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Fundada en 1947
por el Dr. Jesús Enrique Lossada

Ciencias del Agro Ingeniería y Tecnología

Año 11 N° 29
Enero - Abril 2020
Tercera Época
Maracaibo-Venezuela

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Tercera Época

Ciencias del Agro, Ingeniería y Tecnología

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Revista de la Universidad del Zulia

Tercera Época

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El Dr. Jesús Enrique Lossada, luego de trabajar infatigablemente hasta lograr la reapertura de la Universidad del Zulia, el 01 de octubre de 1946, le aportó a esta institución su primera revista científica: la *Revista de la Universidad del Zulia*, fundada por este insigne zuliano, el 31 de mayo de 1947. En su Tercera Época la revista mantiene la orientación que le asignara su fundador: es un órgano científico de difusión de trabajos parciales o definitivos de investigadores y/o equipos de investigación nacionales y extranjeros. La revista posee un carácter multidiscliplinario, por ello su temática se divide en tres grandes ejes: a. ciencias sociales y arte; b. ciencias del agro, ingeniería y tecnología; c. ciencias exactas, naturales y de la salud. Su publicación es cuatrimestral. Cada número, de los tres del año, se corresponde con uno de los tres ejes temáticos. La *Revista de la Universidad del Zulia*, por su naturaleza histórica y patrimonial, está adscrita a la Cátedra libre Historia de la Universidad del Zulia.

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Contenido

Una perspectiva del mundo que se nos avecina

Recién comenzamos a percibir las consecuencias del Covid-19 en nuestro mundo. A partir de esta tragedia volvemos a la certeza de una humanidad que no es capaz de controlar todas las variables del devenir de la historia, donde existen situaciones complejas para las cuales no estamos preparados y, en consecuencia, no tenemos respuestas apropiadas. ¿Qué podemos esperar en un futuro cercano de nosotros mismos, de nuestros gobernantes y de quienes dirigen la economía globalizada, en relación con la impostergable determinación de salvar el planeta de su destrucción? Ciertamente, la familia humana debe atender el desafío urgente de proteger y conservar nuestra casa común (Papa Francisco, 2015).

Entre las trabas que impiden el equilibrio del medio ambiente y, por ende, la preservación de la vida, destaca el actual orden económico, donde el interés por la concentración de la riqueza por parte de unos pocos, hace que se instrumentalice la naturaleza, subordinándola al objetivo de acumular ganancias que terminan en manos de cerca del 1% de la población mundial (Oxfam, 2017). Si bien cabe la duda razonable acerca de la exactitud de los datos disponibles para calcular la distribución o concentración de la riqueza en el mundo, no se puede negar la abismal brecha que separa a una minoría acaudalada de una mayoría empobrecida, realidad que no es exclusiva de nuestra época, sino que tiene amplia trayectoria en la historia de la humanidad.

Con el Covid-19 hemos iniciado una recesión económica similar, en su magnitud, a la del año 2009. Es posible que su alcance sea mayor y genere varios años de recesión. Nos encontramos frente a un complejo panorama cuyo punto de partida es la actual pandemia, pero que trasciende los fueros de esta y abarca el entramado del orden imperante. Los grandes capitales y los principales bloques económicos del mundo globalizado han iniciado sus planes de contención ante esta crisis, apostando a un "equilibrio en el tablero de sus intereses", que minimice en lo posible el desequilibrio creado por ellos mismos.

Independientemente del curso que tome este reacomodo frente a la crisis, las voces críticas de los diversos sectores culturales y científicos del mundo -con sus matices, pero al unísono- pueden alertar sobre la atención inmediata que debe brindarse a los ámbitos más sensibles del contexto actual de la aldea global. La lista de prioridades no es corta, pero podemos destacar dos aspectos que en los próximos años demandarán una respuesta.

Por un lado, el deterioro del medio ambiente al que nos hemos referido continuará amenazando la permanencia de la vida en nuestro planeta, razón por la cual urge insistir en la concreción de un acuerdo viable, que comprometa a los Estados y grandes capitales, a asumir medidas que hagan posible la disminución del calentamiento global.

Por otro lado, una de las consecuencias de la instrumentalización de la naturaleza, se manifiesta en la alteración del promedio de precipitaciones, que a su vez repercute en la producción de alimentos. En este sentido, la prolongación de la crisis económica en conjunción con este factor climático, pueden tener efectos negativos en la producción de alimentos, sobre todo en las regiones del mundo donde la FAO (2019) estima una mayor demanda motivada al crecimiento demográfico, como es el caso de: África subsahariana, India, la región de Oriente Medio y África del Norte. Esta situación, tanto en estas regiones como en otras del mundo, conviene ser abordadas mediante la cooperación intergubernamental, la transferencia tecnológica y el respaldo financiero a los pequeños y medianos productores del campo.

Algunos de los artículos que hoy presentamos en el número 29 de la *Revista de la Universidad del Zulia*, tratan la temática agrícola, y esperamos tocar el ámbito ecológico en nuestra próxima edición. De esta manera, nos involucramos en la discusión de temas de gran importancia para el presente y futuro de la humanidad, con la esperanza de sumar en la tarea de reivindicar la vida.

Dr. Reyber Parra Contreras
Coordinador-Editor de la *Revista de la Universidad del Zulia*

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X-Ray Images Processing to Detect Packaging Defects in Canned Food Industry Using Fuzzy Logic

Marzieh Tafazoli*

ABSTRACT

Taking into account the importance of packaging in the food industry and the need to maintain the health of the materials in the packaging, and with the help of the experiences obtained from previous research with their strengths and weaknesses, we propose a method for the detection of defects in canned packaging, through the use of X-ray radiography, image processing and feature extraction methods, based on fuzzy logic functions for them.

KEY WORDS: radiography, image processing, fuzzy logic, image segmentation, feature extraction

Procesamiento de imágenes de rayos X para detectar defectos en empaques de la industria de alimentos enlatados utilizando la lógica difusa

RESUMEN

Teniendo en cuenta la importancia de los envases en la industria alimentaria y la necesidad de mantener la salud de los materiales en los envases, y con la ayuda de las experiencias obtenidas de investigaciones anteriores con sus fortalezas y debilidades, proponemos un método para la detección de defectos en los envases enlatados, mediante la utilización de radiografía de rayos X, procesamiento de imágenes y métodos de extracción de características, partiendo para ello de funciones de lógica difusa.

PALABRAS CLAVE: radiografía, procesamiento de imágenes, lógica difusa, segmentación de imágenes, extracción de características.

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Introduction

One of the major problems encountered in industrial parts is the defects in welding joints. Failure to timely identify these damages and defects will result in economic and environmental damage. Therefore, accurate and timely diagnosis of welding defects is very important. Industrial radiography is one of the methods of non-destructive tests used to diagnose welding areas (Amza and Cicic, 2015; Namdeo and Vishwakarma, 2013). Non-destructive tests perform the test without any damage to the tested item. Non-destructive testing is an integral part and most important component of any quality assurance program in any industry. The goals of the programs are quality assurance, safety and auditing, reliability and project economics. The qualitative properties of the welds (having defects such as cracking, slag mixing, porosity, incomplete melting, and welded-side sinking) as well as their alloy content can be assessed by non-destructive tests (Pascu, et al., 2014; Namdeo and Vishwakarma, 2013). An industrial radiography test which is one of the methods of non-destructive testing on the principle that X-rays and gamma rays are short wavelength electromagnetic radiation that can penetrate materials. These radiations are absorbed or passed through the material depending on the thickness, density, and atomic number of the material. This absorption phenomenon is used to interpret the information recorded on a photographic film. At this point, there is a need for processing to interpret the imaging information, in order to accurately identify the type of damage to the segment in question, which requires different algorithms or methods for accurate detection. Therefore, in this study, we process X-ray images to detect packaging defects in canned food industry using fuzzy logic.

1. Review of the related literature

Izadbakhsh et al (2017), in their research designing an image processing-based expert system to control the quality of copper wires, concluded that quality control plays a key role in today's industrial environments and whenever necessary take appropriate measures to ensure that products and services manufactured meet quality standards. In this study, they designed an expert system for quality control

automatically. In this input expert system, there are images of the product being manufactured. Image processing techniques have been used for this purpose. First, since the images may be noisy, they are pre-processed and then processed using a fuzzy system. In this fuzzy system, according to the images, certain rules are written to extract the specific properties needed. After the required feature is extracted, the chart is used to classify the product in terms of quality. The proposed approach has been used for copper wires. Rastegari et al. (2017), in their research reviewing the basic concepts of image and image processing, came to the conclusion that with the advancement of the convergence technologies of computer science, electricity and electronics, the application of image processing is becoming increasingly widespread. So digital image processing is a valuable and indispensable area for human life to continue. It has quickly become one of the most widely used sciences in all fields. Image processing has penetrated all sciences and has many applications in a variety of fields. Image processing is the best tool for feature extraction and position analysis and ultimately decision making.

The purpose of image processing is to implement human performance against data and to perform specific processes to extract the features needed to achieve a predetermined goal. The purpose of this article is to introduce the basic concepts for image and digital image processing for further research. Fardin Far (1936), in his study of fuzzy logic based image processing flame detection methods, concluded that image processing based flame detection is now a novel method with significant potential for development. In addition, it can replace conventional photodiode infrared sensors and is more reliable in preventing tunnel accidents or chemical accidents. This article presents a two-step algorithm for detecting flammability to obtain this valuable information. The first step is to identify pixels with color and dynamics similar to real flames. The next step evaluates the instantaneous spreading of the desired pixels using a specific spatial expansion parameter SEP. In parallel, the oscillatory changes in the number of pixels detected over time are transferred to the frequency domain. Frequency spectrum analysis makes it easy to identify the fire by the usual vibration frequency. The proposed identification method uses fuzzy logic classification for each step. Therefore, no static threshold is needed and this makes more choices available to

increase the flexibility of this algorithm. This algorithm is capable of distinguishing between flames and fires with high accuracy. In addition, the expansion of the identified combustion processes is little explained.

2. Statistical population and sample

The number of samples in this study is 100 cans at the end of production line and after packing. In this study, simple random sampling was used. Sampling was done three times during the fall season in the year 2017 in September and October of the factory output. Each item was sampled at three different hours and sent to the laboratory for testing. The following notes are required at the time of sampling:

- Air temperature (in shade)
- Atmospheric conditions of the sampling site
- Location and storage of samples

The specifications of each sample must be clearly specified. This is done by following:

- Storage name
- Sampling location
- Sampler name
- Date and time of sampling

3. Research Method

The present study investigates the processing of X-ray images to detect packaging defects in canned food industry using fuzzy logic. The research method is library and field study and sampling and analysis of samples is from factory output. To conduct this research, the first stage of field survey of the production line and sampling from the storage and the end of the production line (packaging) is performed to explain the performance. After this step, we perform sampling to measure and process X-ray images. The images are specified to eliminate the distortions that occur during the image gathering process, and then image processing, which is an operation that

prioritizes a range of applications. For x-ray images of cracks containing 80 kV voltage generator, 4 mA current, and 3 minutes irradiation time and 400 KODAK AA film irradiation time was used. The images were digitized in TIFF format and stored on the computer. MATLAB R2012b software was used for subsequent processing of these images (Huang and Wu, 2008). A ScanMaker 1000-XL Microtek film scanner is used to convert X-ray film to digital image format, capable of scanning A3 documents with maximum spatial resolution 6400 (dpi) (micron) and it has the highest 4 optical density films and its sensitive element is CCD. For calibration and scanner control, Agfa's standard IT8.7 / 1 calibration film as well as BAM and X-rite calibration step films were used. Radiographic films have to be converted to digital images in order to process them and a scanner is used to achieve this. Since most X-ray films are very dark and high density, so using a conventional scanner cannot produce a good resolution and quality image. After scanning the x-ray film, digital images is acquired, which are stored in JPG format on the computer, so the stored images are now ready for computer processing on them.

Before performing any processing on the radiographic images, first at this stage, a special window around the area suspected of having a defect or the entire welding area is considered (Sargunar and Sukanesh, 2010). Most radiographic images are of poor quality, so in order to improve the quality of the images, special pre-processing of the images is required. In other words, image preprocessing is used to modify the pixel values of digital images to a sufficient extent for subsequent processing (Gonzalez et al., 2004). Techniques used to pre-process images include:

- Histogram Equalization
- Location filtering using the Median Filter
- Gray Levels Slicing Image

4. Research findings

4.1. Proposed Algorithm

In this paper, product failures are diagnosed in two stages, but before the feature extraction, the image is segmented by a neural network. In the first phase, the

geometrical properties of the objects in the segmented image are examined and analyzed. The four properties are extracted from the objects in the binary image. These features are listed below:

- Area: The number of pixels in the image
- Perimeter: The number of pixels on the edge of the image
- Shape: Compression measures the shape and results from dividing the perimeter by area
- Roundness: If an area has a lot of circles it is a circle and if there are oval and other shapes it has a little circle

These criteria are defined using trapezoidal fuzzy sets. If an object has a malfunction, it is geometrically high and has a low shape criterion and has a large environment and its rotation is low. All this is valid when it has a small area. Otherwise it belongs to the background. Therefore, the fuzzy inputs for the cases stated above are expressed as follows (Table 1).

Table 1: First phase fuzzy inputs

Area	Suitable	Notsuitable
Perimeter	Long	Short
Shape	Irregular	Smooth
Roundness	High	Low

And fuzzy outputs include background failures. These are analyzed by the Mamdani fuzzy system. In the second phase the inputs are as follows:

- The average intensity between an object and a rectangular area that surrounds it: DIFFERENCE
- Average intensity for the area of interest and pixels in its neighborhood: TOGETHERNESS

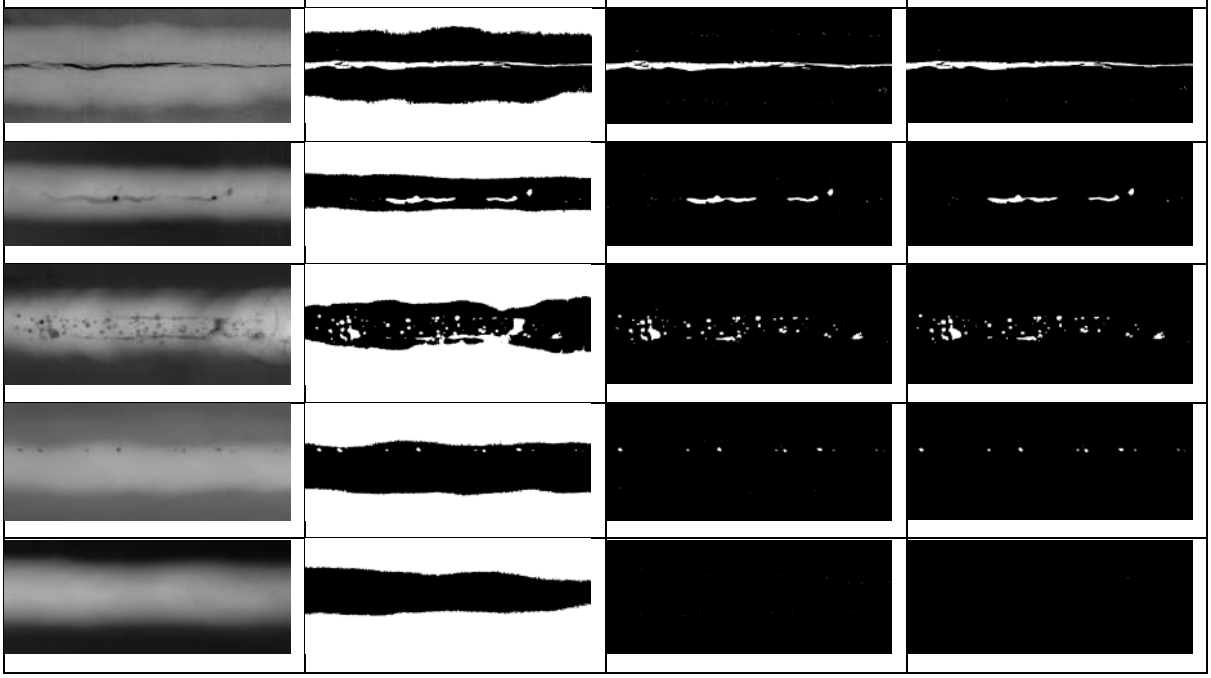
The inputs of these fuzzy sets are expressed as follows (Table 2).

Table 2: Secondary phase fuzzy inputs

Difference	Small	Large
Togetherness	Close	Loose

To detect failures we need to look for objects that have more DIFFERENCE and TOGETHERNESS. Therefore, by considering these fuzzy sets, we identify the failures. The results of the above method are as follows (table 3).

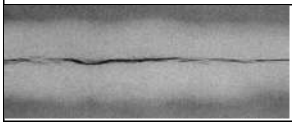
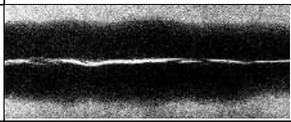
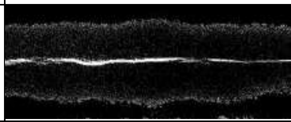
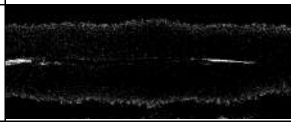
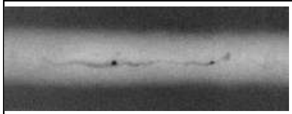
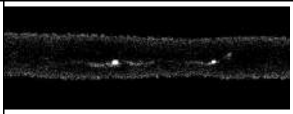
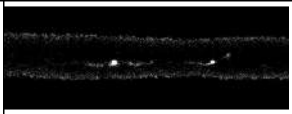
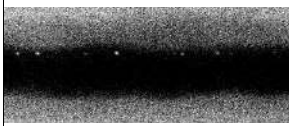
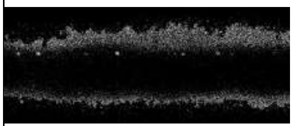
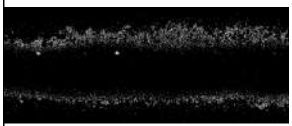
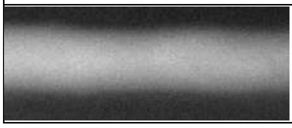
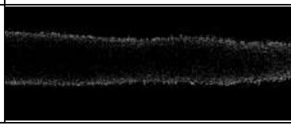
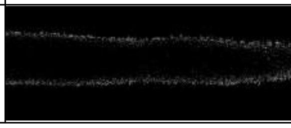
Table 3: Fuzzy outputs of the first and second steps

Main image	Segmentation	Fuzzy first stage	Fuzzy second stage
			

4.2. Results for Gaussian Noise

System performance was evaluated in the presence of Gaussian noise. This noise has an average value of 0.1 and a variance of 0.01. The Gaussian noise results are shown in table 4. The method is not noise resistant and also because the number of objects in the shape increases. In the second phase, the computational speed of the system is very slow, because noise causes interconnected objects to be separated.

Table 4: Fuzzy output of the first and second phase with Gaussian noise

Image of Gaussian noise	Segmentation	Fuzzy first stage	Fuzzy second stage
			
			
			
			
			

MATLAB code

Here, the image is read and resized, and if the image is colored, it would turn black and white otherwise it would not change (Figure 1).

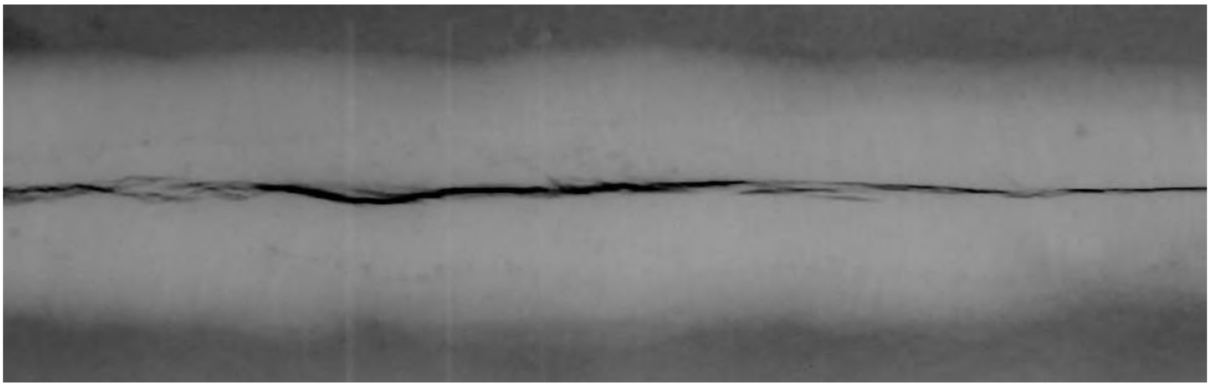


Figure 1: Input image to the system

The image needs to be entered into the neural network for segmentation, for this purpose the image is reshaped to the vector. It should also turn black and white if the image is colored. The post-propagation neural network was used to segment the newff function (Fig. 2). These images instruct the grid to convert each pixel to one or zero of different intensities depending on the corresponding pixel.

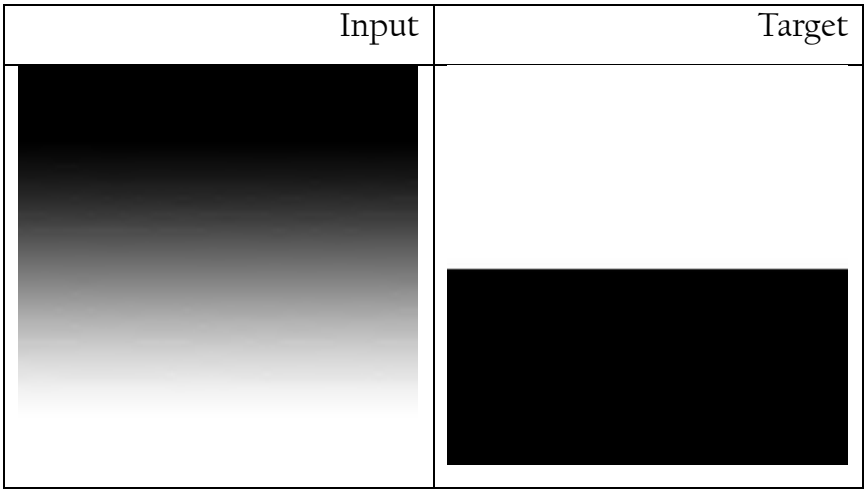


Figure 2: Images for neural network training

Figure 3: Segmentation output stage

This image does not include failures and parts of the background have also been detected. In the later stages, these additional objects can be eliminated (Figure 3).

4.3. Fuzzy system first stage

The fis file is created first. Appropriate inputs and outputs are selected as follows. In each image, the fuzzy sets of inputs and outputs are shown separately.

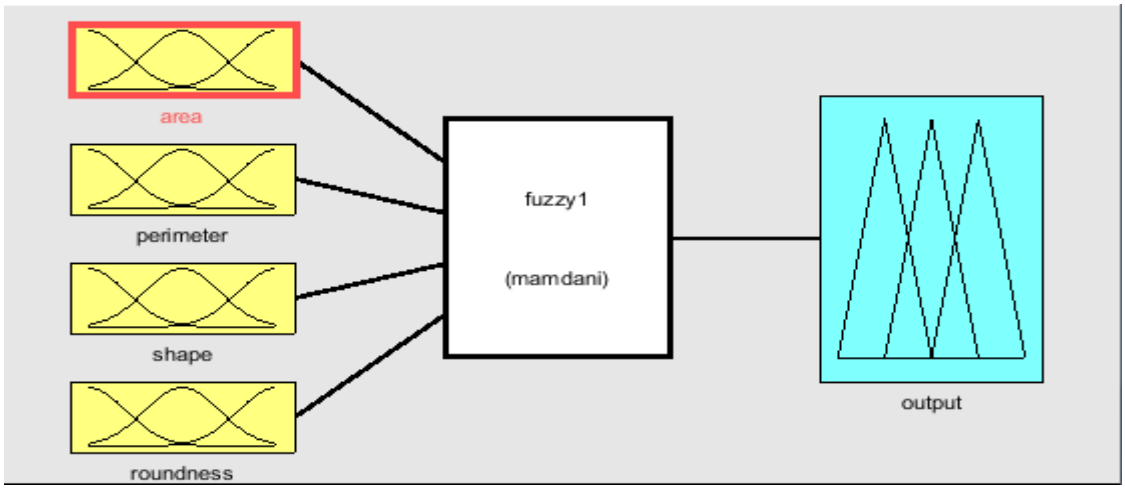


Figure 4: The fis output of the first stage

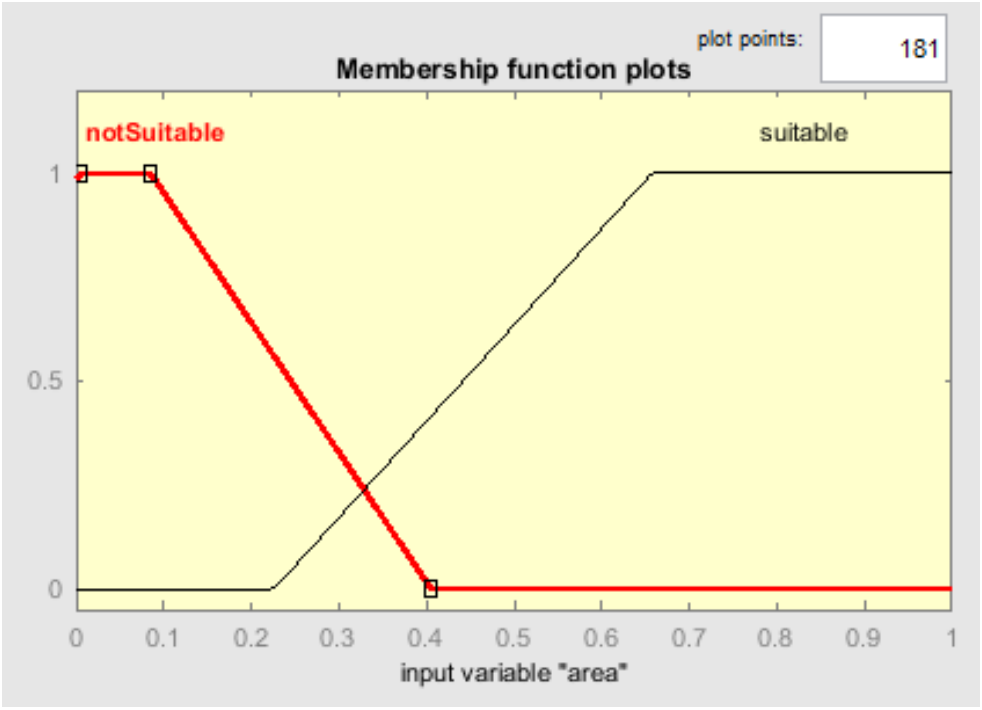


Figure 5: Diagram of area variable membership function.

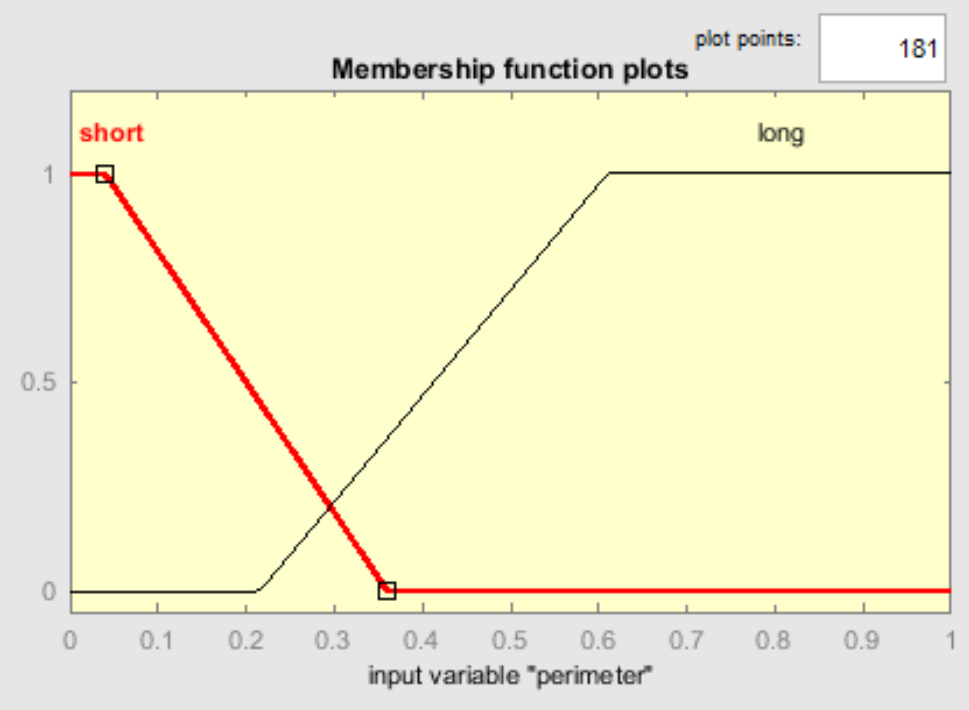


Figure 6: Scheme of variable membership function of perimeter.

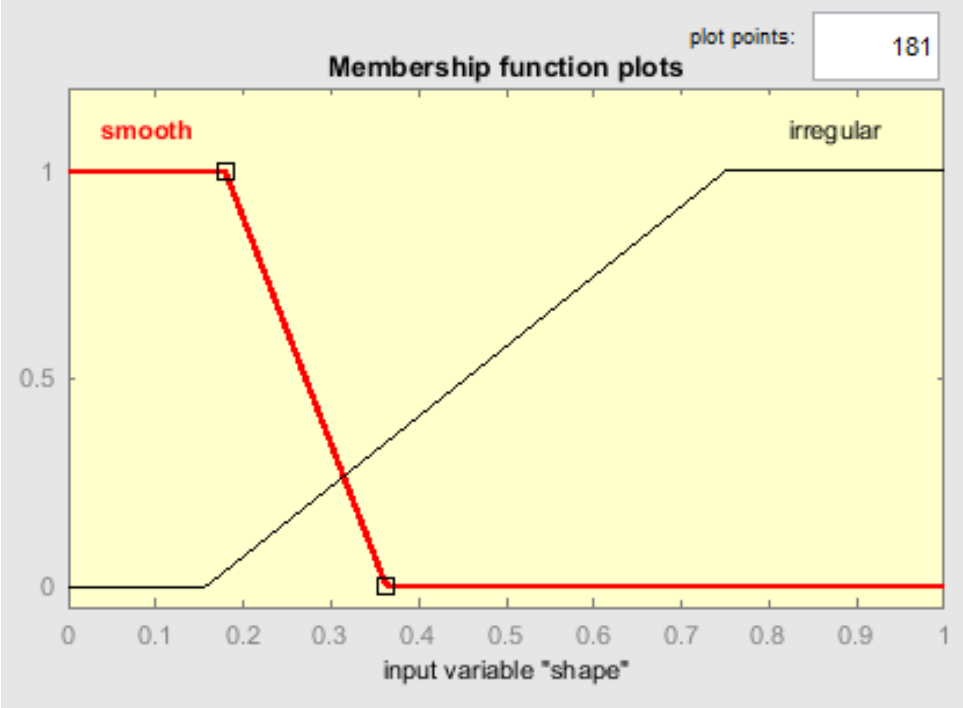


Figure 7: Variable membership function shape.

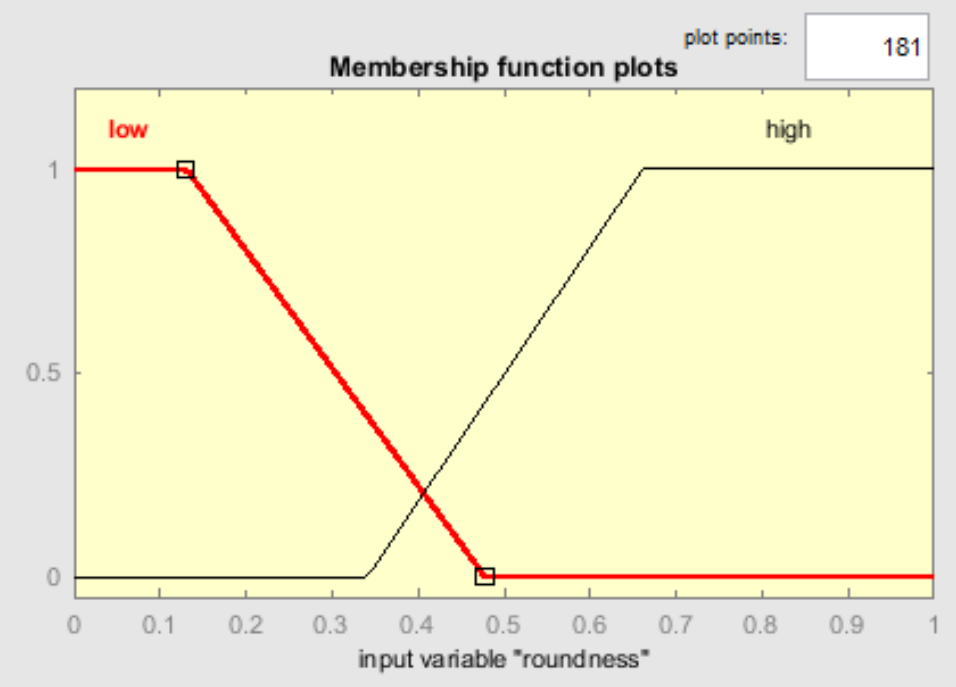


Figure 8: Graph of the variable roundness membership function.

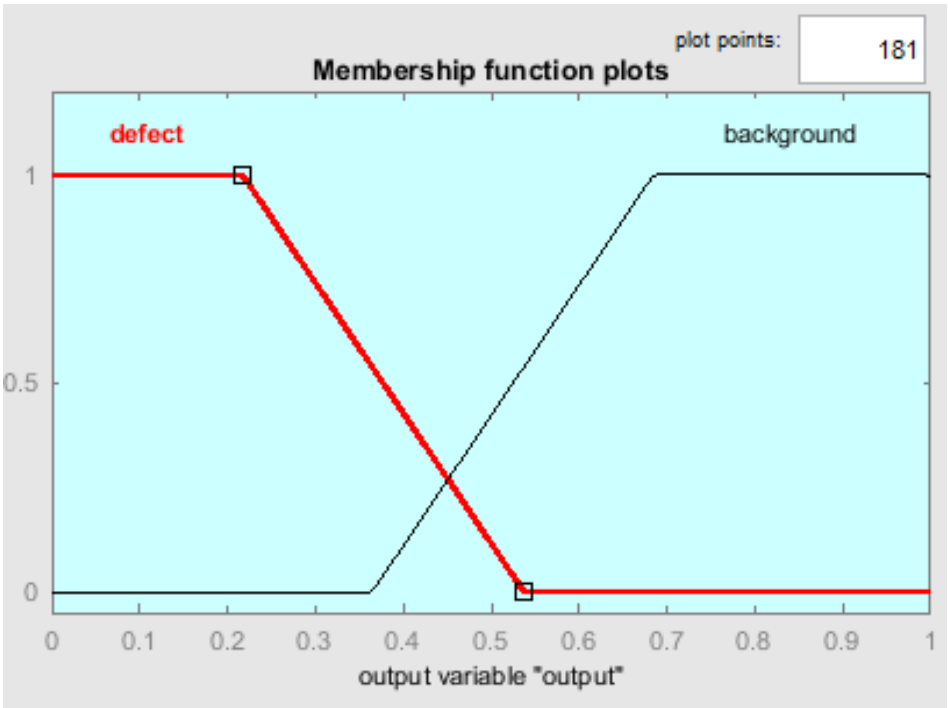


Figure 9: The membership function diagram of the output value.

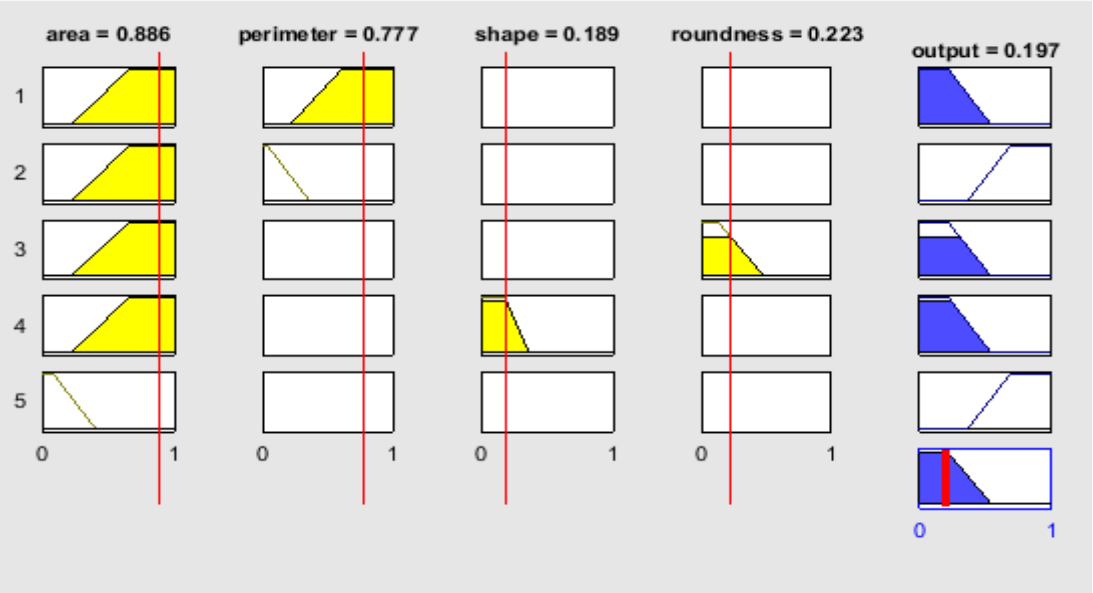


Figure 10: Fuzzy output of the first step of the proposed method for one of the tested samples.

In this section, we first find the interconnected objects in the image with bwconncomp, and then use the regionprops function to obtain the four properties that must be entered into the fuzzy system for each object. At this point, the generated fis file is introduced to the algorithm and placed in ourfis variable. It is then calculated using for loop output based on all the objects in the binary image (Fig. 11).

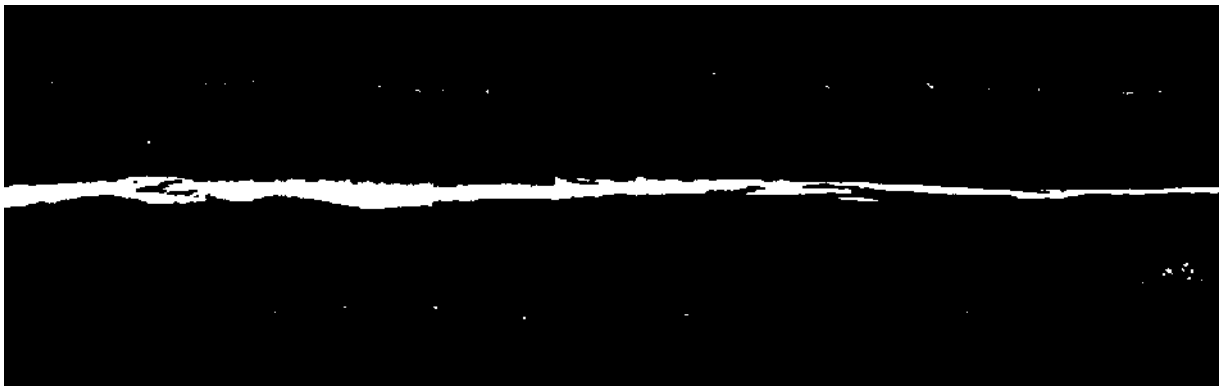


Figure 11: Fuzzy first stage output

4.4. Fuzzy Second Stage

At this point, the fis file is first created based on what the article says. Appropriate inputs and outputs were selected as follows. In each image, the fuzzy sets of inputs and outputs are shown separately.

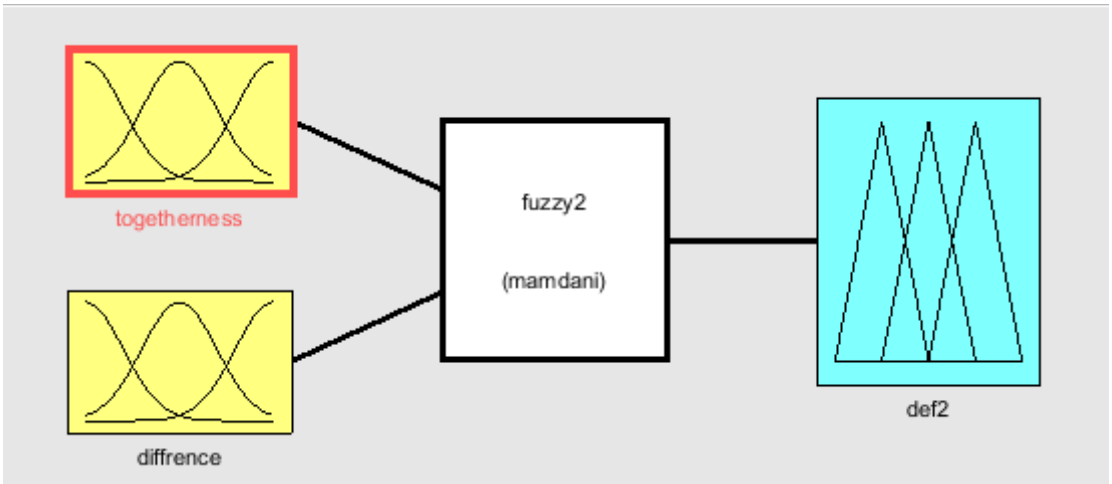


Figure 12: second stage fuzzy output.

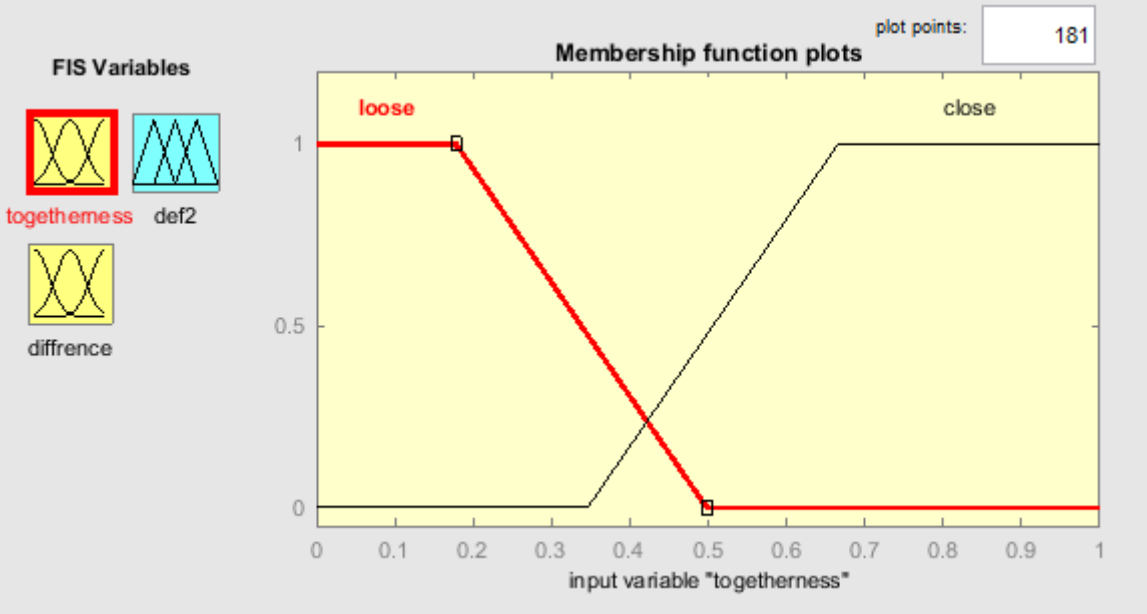


Figure 13: Graph of the correlation variable membership function.

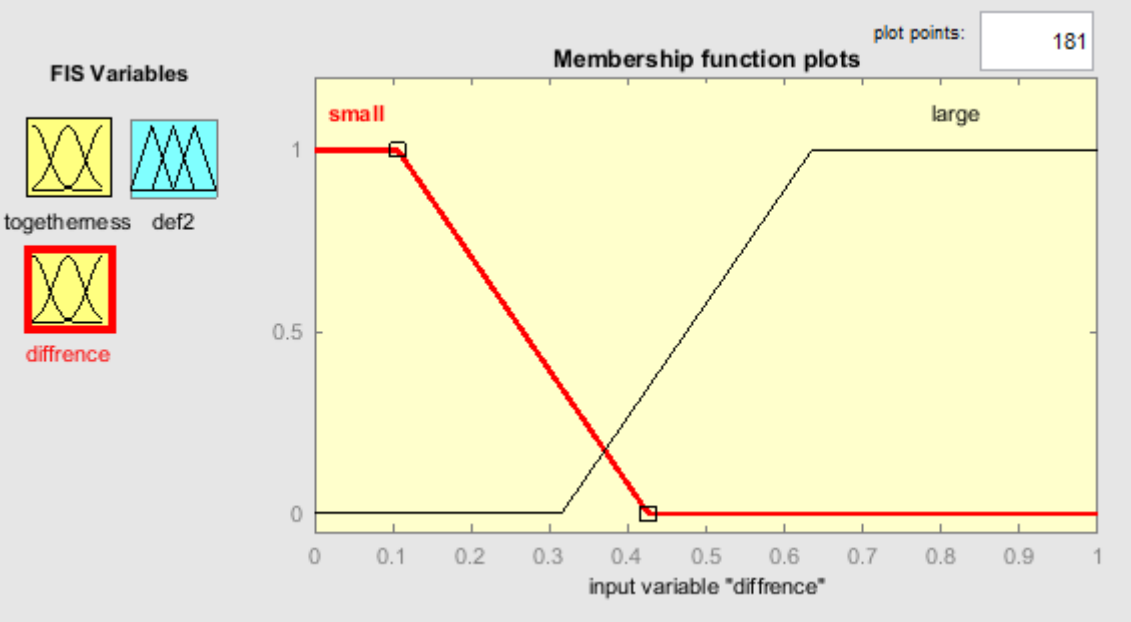


Figure 14: Diagram of the difference membership function.

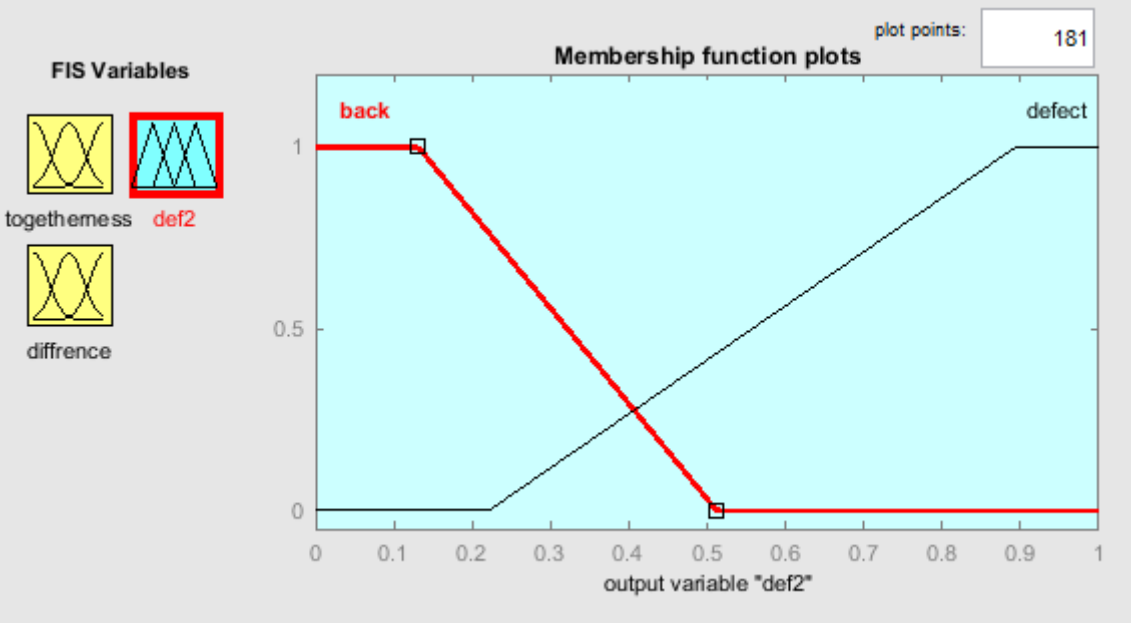


Figure 15: Graph of membership function of output value.

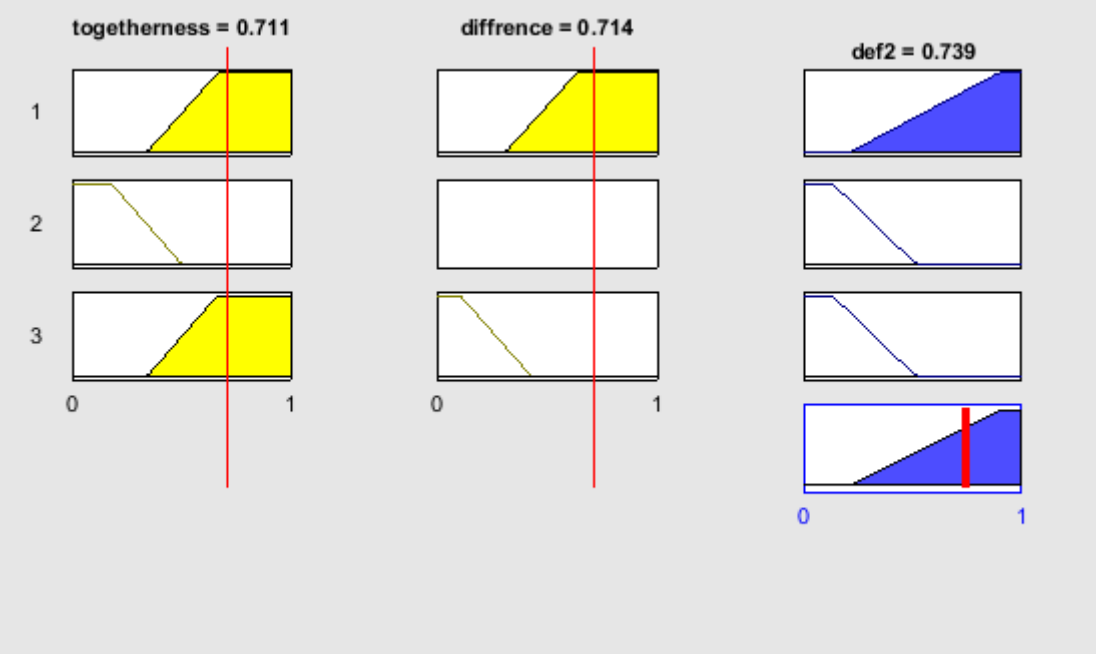


Figure 16: Fuzzy output of the second step of the proposed method for one of the tested samples

The second fis file is introduced to the system and with this output failures can be found. Values of less than 0.4 are considered to be failures. The def2 variable is the final output and represents the failures (Figure 17).

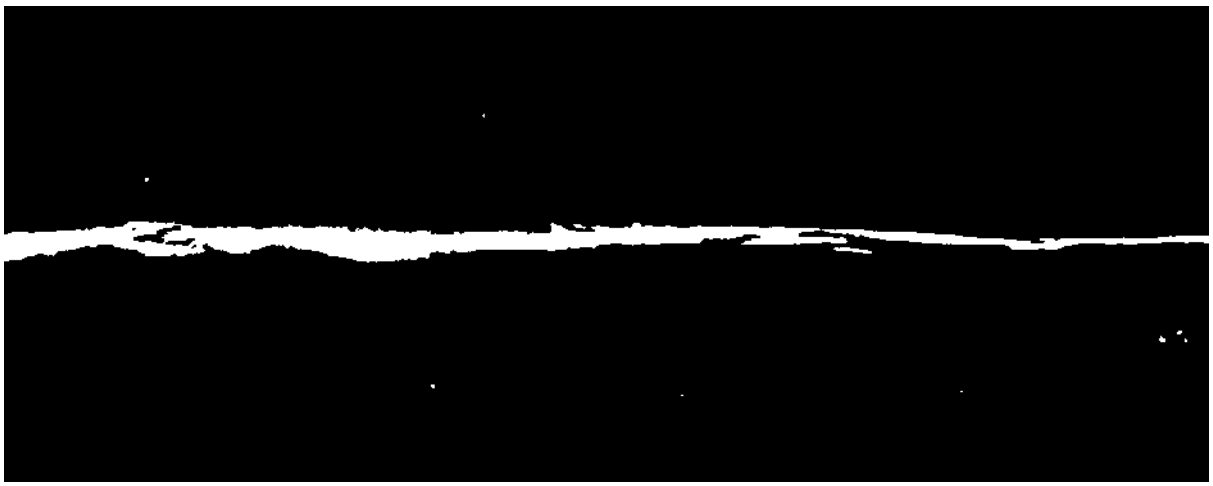


Figure 17: Neural network output

Conclusion

One of the most common tools in diagnosing welding defects is the use of welding radiographs. Due to poor quality of welding radiographic images, some welding defects such as transverse and longitudinal cracks may not be well recognized. This paper was presented to improve the quality of welding radiographic images to detect packaging defects in canned food industry using fuzzy logic. In the proposed method, the input image is first filtered by a 9 * 9 Gaussian filter with a variance of 0.2 and the mixing noise is significantly reduced due to the imaging and scanning of the image.

On the other hand, an approach for using an expert system using image processing and quality control was presented. After pre-processing on images, due to the advantages of fuzzy systems, this system was used in image processing and appropriate feature was extracted. Then, using the extracted feature, each sample was classified into two groups of healthy and damaged. Then, by filtering the image vertically and analyzing the signal by applying a matching threshold, the location of the weld image is determined and the weld image is separated from the rest of the image. In the following, a filter differentiation highlighting algorithm is constructed using a 0.25 image coefficient of amplified detail. The proposed algorithm is implemented in the MATLAB programming environment. Results show that the proposed method is effective in better and easier detection of longitudinal and transverse crack defects.

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Improving the cold flow properties of marine diesel fuel using centrifugation

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ABSTRACT
The possibility of improving the low-temperature properties of marine diesel fuel of the Antipinsky Refinery by dewaxing was studied. Paraffin was isolated from the fuel in a centrifuge in the presence of a depressant additive. The depressant additive is selected from a series of synthesized additives for depressant effectiveness. The influence of the centrifuge rotor speed, the additive content and the initial cooling temperature of the sample on the dewaxing parameters of the fuel was studied. The possibility of isolating the additive from the obtained paraffin concentrates is shown. The dewaxing products obtained under optimal conditions were studied. A paraffin concentrate product containing 40.03% solid paraffins was isolated from fuel. Paraffin was isolated from paraffin concentrate by dewaxing with a selective solvent. The cloud point and freezing point of paraffin were 30 and 29 ° C, respectively. When converted to the original fuel, the amount of released paraffins was 7.3% of the 21% by weight contained in the original fuel. The fuel obtained at optimal parameters for low temperature properties corresponds to grade D of diesel fuel according to EN 590: 2009.

KEY WORDS*:* diesel fuel; low temperature properties; centrifuge; dewaxing; depressant additive.

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Mejora de las propiedades de flujo en frío del combustible diesel marino mediante centrifugación

RESUMEN

Se estudió la posibilidad de mejorar las propiedades de baja temperatura del combustible diesel marino de la Refinería Antipinsky mediante el desparafinado. La parafina se aisló del combustible en una centrífuga en presencia de un aditivo depresor. El aditivo se selecciona de una serie de aditivos sintetizados para la efectividad del depresor. Se estudió la influencia de la velocidad del rotor de la centrífuga, el contenido de aditivos y la temperatura de enfriamiento inicial de la muestra en los parámetros de desparafinado del combustible. Se muestra la posibilidad de aislar el aditivo de los concentrados de parafina obtenidos. Se estudiaron los productos de desparafinado obtenidos en condiciones óptimas. Se aisló del combustible un producto concentrado de parafina que contenía 40,03% de parafinas sólidas. La parafina se aisló del concentrado de parafina desparafinando con un disolvente selectivo. El punto de enturbiamiento y el punto de congelación de la parafina fueron 30 y 29 ° C, respectivamente. Cuando se convirtió al combustible original, la cantidad de parafinas liberadas fue del 7,3% del 21% en peso contenido en el combustible original. El combustible obtenido en los parámetros óptimos para las propiedades de baja temperatura corresponde al grado D del combustible diesel de acuerdo con la norma EN 590: 2009.

PALABRAS CLAVE: combustible diesel; propiedades de baja temperatura; centrífugo; desparafinado; aditivo depresivo.

Introduction

This work deals with the production of diesel fuel with improved cold flow properties by dewaxing of marine diesel fuel without selective solvents. For this, the method of centrifuging the initial diesel fuel in a high-speed centrifuge was used. The method of dewaxing petroleum products using centrifugation has been known for a long time. Its use was limited to dewaxing of oils at Barisol-process plants. In Russia, the last Barisol-process plant was operated until the end of the 70s of the last century (Chernozhukov, 1978). At this plant, a mixture of dichloroethane (80%) and benzene was used as a solvent. The rotor speed of the centrifuges was 6300 rpm. Dichloroethane was also used, among other things, to increase the density difference between the liquid (oil + solvent) and solid (petrolatum with a small solvent content) phases. The performance indicators of such plants are inferior to the current ones that use ketone-aromatic solvents

and vacuum filters. In addition, the centrifuges at a Barisol-process plant are non-tight, which affected the health of the staff. Attempts were made to dewax diesel fuels in centrifuges with a rotor speed of 4000 rpm (Agaev, Yakovlev, Schipanov, 2008). Modern centrifuges are advanced, the speed of rotation of their rotors is increased and they can be manufactured leak-tight. In this regard, the separation of intermediate products for the production of oils and diesel fuels in modern centrifuges becomes relevant. If positive results are obtained, dewaxing of oil products by solvent-free centrifugation will be a significant contribution to the dewaxing technology.

The cloud point (CP) and cold filter plugging point (CFPP) are the most difficult to achieve cold flow properties of diesel fuels (DF). One of the ways to improve the quality of diesel fuel according to these indicators is the method of partial dewaxing of diesel fuel in an electric field, which ensures the removal of high-melting-point n-alkanes C_{19+} from their composition (Agaev, Yakovlev, Zima, 2012; Yakovlev, Agaev, 2012; Agaev, Yakovlev, Stolbov, 2012; Yakovlev, Agaev, 2017). The advantage of this method is the dewaxing of diesel fuel without the use of solvents, which makes it economically advantageous. The method is characterized by positive values of the temperature effect of dewaxing and, therefore, does not require subcooling of raw materials. The disadvantage of the processes of electrical dewaxing of petroleum products is the need to use high-voltage electric fields, which complicates the equipment and makes its operation dangerous.

1. Materials and Methods

The marine diesel fuel of the Antipinsky Refinery (Tyumen) used in the work had the following properties: cloud point - 1ºC, pour point – minus 3ºC, density at 20ºC - $844\ kg/m^3$, viscosity at 20ºC - $6.9 mm^2/s$, refractive index at 35°C - n_D^{35} 1.4640; 10% of diesel fuel boils off at 187ºC, 50% - at 285ºC, 90% - at 366ºC and 96% - at 394ºC, content of hydrocarbons that formed a complex with urea - 21.0%wt. The content of fractions of n-alkanes from their total amount in diesel fuel, % wt.: Σ C_{12-14}=23.31, Σ C_{15-18}=37.11 and Σ C_{19+} =39.58. Marine diesel fuel is enriched with n-alkanes with the number of carbon atoms from 10 to 22, the maximum content falls on medium-melting-point C_{14-16} paraffins. The distribution of n-alkanes in diesel fuel was determined on a Crystal 5000 chromatograph

equipped with an MXT 2887 column 10×0.53×2.65. The column is designed to separate n-alkanes with carbon atoms from C_7 to C_{45}. The content of n-alkanes in the fuel was determined by peaks with automatic integration of their area on a computer using a special program. The volume of sample introduced into the column was 0.06µl. The temperature range was 0 – 300ºC, the rate of temperature rise was 5 – 10ºC/min. The carrier gas was helium. The detector was flame ionization.

To increase the efficiency of centrifuging diesel fuel, the depressant additive DP-5/17 was used, which at a dewaxing temperature ensured a decrease in the structural viscosity of the initial diesel fuel. The amidopolyformaldehyde depressant additive DP-5/17 was a condensation product of polyethylene polyamines (PEPA), stearic acid (SA) and formaldehyde (FA). The molar ratio of the starting reagents SA:PEPA:FA was 1.7:1.0:30.0. The additive was obtained according to the procedure described in (Agaev, Gultyaev, Yakovlev, 2007). The additive DP-5/17 was chosen taking into account its effectiveness from a series of synthesized additives of the same type with different ratios of the starting reagents (Table 1). Efficiency assessment was carried out by a combination of pour points (ASTM D97-05) and cloud points (ASTM D2500-05) of marine diesel fuel when additives were added to its composition in the range from 0.05 to 2.0%wt.

Table 1 – The pour point and cloud point of marine diesel fuel (MDF) with the introduction of depressant additives

Additives	Additives are synthesized at a molar ratio of starting reagents			Content of additives in MDF, %wt.					
	SA	PEPA	FA	0.00	0.05	0.1	0.5	1.0	2.0
				MDF pour point (°C)					
DP-7/16	1.7	1.0	-	-3	-7	-16	-20	-25	-12
DP-12/16	1.7	1.0	10.0	-3	-10	-13	-13	-28	-31
DP-25/16	1.7	1.0	20.0	-3	-12	-21	-24	-24	-28
DP-5/17	1.7	1.0	30.0	-3	-15	-23	-25	-27	-29
				MDF cloud point (°C)					
DP-7/16	1.7	1.0	-	1	1	2	1	37	41
DP-12/16	1.7	1.0	10.0	1	1	3	1	19	36
DP-25/16	1.7	1.0	20.0	1	2	0	13	30	39
DP-5/17	1.7	1.0	30.0	1	0	0	11	27	30

Designations: SA - stearic acid; PEPA – polyethylene polyamines; FA – formaldehyde.

Marine diesel fuel (MDF) dewaxing was carried out on a Thermo Scientific refrigeration centrifuge (Germany). The centrifuge provides temperature control in the

working area in the range from 40 to minus 10°C, and it is equipped with 6 test tubes with a volume of 50 ml each with a total load of 300 ml. The speed of rotation of the centrifuge rotor is adjustable from 1000 to 9500 rpm. The initial DF or its mixture with a depressant additive was preliminarily subjected to heat treatment in a thermostat at 60°C until the raw mixture was completely dissolved. MDF or its mixture with an additive was cooled in a Lauda RP 855 cryostat to a centrifuging temperature of minus 10°C. Next, MDF was transferred to a centrifuge, in the program of which the initial work parameters were preliminarily set: rotation speed of the centrifuge rotor, centrifuging temperature (minus 10°C) and centrifuging time (15 minutes). At the end of centrifuging, the final temperature in the centrifuging tubes is measured. The final temperatures in the tubes due to friction of the centrifuge rotor with the surrounding air are noticeably higher than the initial temperatures in the tubes and the temperature set in the centrifuge. As a result of centrifuging, dewaxed diesel fuel (DDF) and paraffin concentrate (PC) are obtained. The yield of DDF, PC and losses are determined. For DDF, cloud point (ASTM D2500-05), pour point (ASTM D97-05), and refractive index (IRF-454B2M refractometer) at a temperature of 35°C were determined. For paraffin concentrate, the melting temperature and refractive index were determined at a temperature of 35°C. The influence of the centrifuging parameters on the yield and quality indicators of the obtained products was evaluated - the cloud point and the refractive index of DDF. The cloud point t_c of dewaxed diesel fuels, for reasons of simplicity and convenience, was chosen instead of the cold filter plugging point (CFPP) used for summer diesel fuel according to EN 590:2009. CFPP, as a rule, is lower than the cloud point of fuels, which with a margin ensures that DDF meets the requirements of GOST in terms of CFPP.

2. Results

Table 2 presents experimental data on the influence of the rotor speed of the centrifuge and the content of the depressant additive DP-5/17 in diesel fuel on the yield and the main indicator of the quality of diesel fuel - its cloud point. The rotor speed varied from 3000 to 9000 rpm. The content of the additive in the initial fuel ranged from 0.1%wt. up to 1.0%wt.

Table 2 – Effect of marine diesel fuel centrifuging parameters on product yields and DDF cloud point

No. of experiment	Centrifuging parameters		t_f of centrifuging, °C	Yields of centrifuging products, %wt.			t_c of DDF, °C
	ω_r, rpm	Content of DP-5/17 in MDF, % wt.		DDF	PC	Losses	
1	3000	0	-4	No product separation.			
2	4000	0	-4	77.9	20.5	1.7	-1
3	5000	0	-4	68.6	30.3	1.1	-4
4	6000	0	-4	84.5	13.7	1.8	-4
5	7000	0	-2	83.8	14.5	1.7	-8
6	8000	0	-1	80.6	17.2	2.2	-5
7	9000	0	0	86.9	11.8	1.3	-3
8	3000	0.1	-4	69.3	30.3	0.5	-5
9	4000	0.1	-4	70.6	26.6	2.8	-3
10	6000	0.1	-4	82.6	16.4	1.0	-6
11	7000	0.1	-2	85.0	13.5	1.5	-10
12	8000	0.1	-1	79.3	18.2	2.6	-10
13	3000	0.5	-4	74.6	24.3	1.2	-5
14	4000	0.5	-4	75.7	19.4	4.9	-5
15	5000	0.5	-4	71.0	27.7	1.3	-8
16	6000	0.5	-4	82.8	16.6	0.7	-8
17	7000	0.5	-2	80.5	18.0	1.5	-9
18	8000	0.5	-1	78.4	17.7	4.0	-10
19	9000	0.5	0	81.9	16.5	1.5	-5
20	5000	1.0	-4	75.6	21.0	3.4	-9
21	7000	1.0	-2	78.1	20.4	1.5	-10
22	8000	1.0	-1	72.1	23.3	4.6	-10
23	9000	1.0	0	77.2	19.8	3.0	-5

Constant parameters: centrifuging time τ = 15 min; initial temperature of cooling of the DF sample before centrifuging t_{in} = minus 10°C; temperature of a cryostat integrated in a centrifuge t_{cr} = minus 10°C.
Abbreviations: PC – paraffin concentrate; t_f – final centrifuging temperature; ω_r – centrifuge rotor speed, rpm; t_c of DDF – cloud point of DDF.

Centrifuging of marine diesel fuel (MDF) in the absence of a depressant additive (experiments No. 1-7) shows that in the range of rotor speeds from 5000 to 9000 rpm there is a slight decrease in the cloud point of dewaxed diesel fuel (DDF) relative to the cloud point of the initial MDF. By the DDF yield and its cloud point, the best results are observed at a centrifuge rotor speed of 7000 rpm. The yield of DDF reaches 83.8% wt., and its cloud

point is minus 8°C. The temperature difference between the temperature set in the centrifuge and the cloud point of the resulting DDF is minus 2°C. When the speed of rotation of the centrifuge rotor is 8000 - 9000 rpm, the cloud point of DDF increases. At a rotor speed of 3000 rpm, dewaxing of the initial fuel does not occur. A feature of the MDF dewaxing by the centrifuging method is the increase in the final temperature in the centrifuge from minus 10°C (the temperature set in the centrifuge) to 0°C. Moreover, the higher the temperature, the higher the rotation speed of the centrifuge rotor due to its friction with air. The cloud point of DDF at a rotor speed of 7000 - 8000 rpm, which is minus 5 - minus 8°C, is noticeably lower than the temperatures in the centrifuge, which are minus 1 - minus 2°C (see Table 2). Obviously, this is due to the fact that the removal of the crystalline phase from the volume of the tubes into the sediment does not occur in 15 min (time of centrifuging), but much faster. A further increase in temperature in the tubes has little effect on the cloud point of DDF due to the low contact surface of the formed sediment of paraffin and DDF located in the upper part of the tubes.

Dewaxing of MDF when adding to it from 0.1 to 1.0%wt. of depressant additive DP-5/17 at the same rotor speeds from 3000 to 9000 rpm positively affects the performance of the process. The best results are obtained with the lowest content of the additive in MDF - 0.1%wt. and at a rotor speed of 7000 rpm. The yield of DDF reaches 85.0%wt., and its cloud point is minus 10°C. Good results on the yield of DDF and its cloud point are also obtained at a rotor speed of 8000 rpm (see table 2). Note the general patterns of MDF dewaxing in the presence of a depressant additive. An increase in the content of depressant additive in the initial fuel and an increase or decrease in the rotational speed of the centrifuge rotor relative to the optimal 7000-8000 rpm leads to a deterioration in its dewaxing parameters.

Increasing the rotor speed to 9000 rpm worsens dewaxing due to excessive heating of the air in the centrifuging zone, and lowering the centrifuge rotor speed reduces the DDF yield and increases its cloud point. The distribution of n-alkanes in DDF according to chromatography relative to the initial MDF (Figure) under optimal conditions (experiment No.11) shows that the changes in the hydrocarbon composition are insignificant. The maximum content of n-alkane C_{14} in DDF is shifted relative to the maximum content in the initial fuel (C_{15}) by only one carbon atom. There are two peaks in the paraffin concentrate - with a maximum on docosane (C22) and tetradecane (C14),

i.e. the shift in the highest melting n-alkane relative to tetradecane is 8 carbon atoms (see Figure).

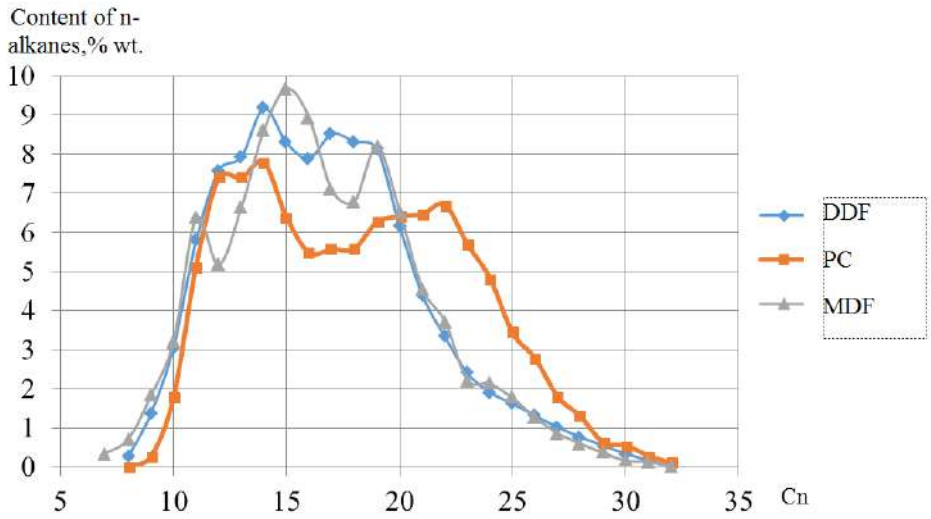

Figure. Distribution of n-alkanes in marine diesel fuel and in dewaxed diesel fuel and paraffin concentrate derived from it

3. Discussion

To assess the influence of the centrifuging parameters on the quality indicators of the obtained paraffin concentrate (PC), additional dewaxing of the initial fuel was carried out under optimal conditions. The following initial parameters of the raw material centrifugation were adopted: the initial cooling temperature of the initial fuel before centrifuging t_{in} - minus 10°C; temperature of a cryostat integrated in a centrifuge t_{cr} - minus 10°C; centrifuging time τ 15 min; rotor speed - 7000 – 8000 rpm, content of the additive in the initial fuel from 0.1%wt. up to 1.0%wt. According to the results of centrifuging, the refractive index of paraffin concentrates does not change significantly - in the range from 1.4628 to 1.4637 (Table 3), i.e. the introduction of the additive in diesel fuel has little effect on the refractive indices of the resulting paraffin. The melting point of paraffin concentrates obtained after centrifugation with increasing additive content in the feedstock increases markedly - from 25 to 35°C. To exclude the possible effect of the depressant additive DP-5/17, whose dropping point is 72°C, on the melting points of paraffin concentrates, the latter were purified from impurities of the polar additive on silica gel. The melting points of paraffin concentrates after purification on silica gel decreased by 9 - 16°C (see Table 3). The slower increase in the melting points of paraffin concentrates before purification on silica gel with an additive content of more than

0.5%wt. in the feedstock is obviously associated with a limited adsorption capacity of paraffin crystals formed in diesel fuel when it is cooled. The obtained results confirm the literature data on the adsorption of depressant additives on solid petroleum hydrocarbons (Savchenkov, Agaev, 1991).

Table 3 – The effect of the centrifuge rotor speed and the content of depressant additive DP-5/17 in the initial fuel on the quality indicators of paraffin concentrate (PC)

Centrifuging parameters		Indicators of paraffin concentrate quality after				Difference in PC melting points before and after purification on silica gel, °C
		centrifugation		centrifugation and purification on silica gel		
ω_r, rpm	C_{DA}, %wt.	t_m, °C	n_D^{35}	t_m, °C	n_D^{35}	
7000	0.1	26	1.4631	17	1.4630	9
	0.5	34	1.4635	18	1.4630	16
	1	35	1.4636	20	1.4632	15
8000	0.1	25	1.4628	16	1.4628	9
	0.5	34	1.4635	20	1.4630	14
	1	35	1.4637	22	1.4632	13

See constant centrifuging parameters in the text
Designations: ω_r – centrifuge rotor speed, rpm; C_{DA} – content of the additive in the feedstock; t_m – PC melting point.

Conclusion

Thus, it is shown that the centrifugation of marine diesel fuel with an initial cloud point of 1°C at a rotor speed of 7000 rpm allows obtaining diesel fuel with a cloud point of minus 8°C and a yield of 83.8%wt. Introduction to the original fuel of 0.1% wt. depressant additive can increase the yield of dewaxed diesel fuel when centrifuging up to 85% wt. and lower its cloud point to minus 10ºC. The summer diesel fuel obtained at optimal parameters in its cold flow properties corresponds to grade D according to EN 590:2009.

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Molecular Dynamic Studies and Experimental Methods for Dispersion of Graphene Sheets with Different Strategies

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Ali Shamel ***

ABSTRACT

Graphene sheets tend to self-associate in microscale aggregates. This occurs in products with less mechanical and electrical action. Recognizing this problem, extensive research has been evidenced in the literature on the development of dispersion technologies, based on both mechanical and chemical approaches. Chemically converted sheets wrapped in surfactants, the ability of surfactants to disperse graphene nanospheres in a medium, was evaluated by different research groups, using both experimental and molecular dynamics (DM) simulation methods; In this article we summarize these methods and techniques. The effect of the influencing factors that count the ions, the pH value and the surfactants in the separation and agglomeration of the gerata sheets is highlighted. Here, we reviewed the recent advances that have been made in the dispersion of graphene sheets in aqueous and organic media by non-covalent adsorption of surfactants and polymers. Graphene structure, properties, and mainly self-assembly are also studied.

KEY WORDS: anionic surfactants, molecular dynamics studies, exfoliation, graphene.

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Estudios de dinámica molecular y métodos experimentales para la dispersión de láminas de grafeno con diferentes estrategias

RESUMEN

Las láminas de grafeno tienden a autoasociarse en agregados a microescala. Esto ocurre en productos con menor acción mecánica y eléctrica. Reconociendo este problema, se ha evidenciado una extensa investigación en la literatura sobre el desarrollo de tecnologías de dispersión, basadas en enfoques tanto mecánicos como químicos. Láminas de grafeno convertidas químicamente envueltas en tensioactivos, la capacidad de los tensioactivos para la dispersión de nanoesferas de grafeno en un medio, fue evaluada por diferentes grupos de investigación, mediante métodos de simulación tanto de experimentación como de dinámica molecular (DM); en este artículo resumimos estos métodos y técnicas. Se destaca el efecto de los factores influyentes que cuentan los iones, el valor del pH y los tensioactivos en la separación y aglomeración de las láminas de gerata. Aquí, se revisaron los avances recientes que se han realizado en la dispersión de láminas de grafeno en medios acuosos y orgánicos por adsorción no covalente de tensioactivos y polímeros. También se estudia la estructura de grafeno, propiedades y principalmente el autoensamblaje.

PALABRAS CLAVE: tensioactivos aniónicos, estudios de dinámica molecular, exfoliación, grafeno.

Introduction

Graphene, a two-dimensional, one-atom-thick hexagonal lattice of carbon atoms has electronic, mechanical, optical, thermal, and chemical properties. graphene has generated huge interest due to its unprecedented physical and chemical properties because of its atom arrangement (Javadian and Khosravian, 2018). A graphene sheet consists of an atomically thin array of sp2-bonded carbon atoms organized in a planar hexagonal arrangement, where each atom is connected evenly to three carbons (120°) in the xy plane, and a weak π bond is present in the z axis. The sp2 set forms the hexagonal (honeycomb) lattice typical of a sheet of graphite. The pz orbital is responsible for van der Waals interactions. The free electrons in the pz orbital move within this cloud and are no longer local to a single carbon atom (Vaisman et. Al, 2006; Bjork, 2010). Owing to graphene's unusual physicochemical properties and

tremendous potential for applications in nanoelectronics, sensors, nanocomposites, batteries, supercapacitors, and hydrogen storage, the development of efficient approaches to producing single-layer. Also the earliest graphene samples were produced using micromechanical cleavage from highly ordered pyrolytic (Du et al., 2008; Morozov et al., 2008).

Graphite has been used by man for thousands of years the details of its layered structure were only revealed by Bernal in 1924 using X-ray crystallography (Bernal, 1924; Boardman et al., 2008). Graphene layers are held together by van der Waals forces in graphite; tend to self-associate into micro-scale aggregates this creates problems both in exfoliating graphene from graphite as well as keeping graphene dispersed in a liquid medium rather than aggregating (Li et al., 2008).

Thermodynamic arguments suggested that graphene could not exist as a freestanding entity. The novel electronic properties of graphene In addition it is the strongest material known to man10 and has been fabricated into large area transparent conductors. graphene sheets has been intensively explored in recent year Du et al., 2008; Bunch et al., 2007).

Micromechanical cleavage from bulk graphite was initially used by Novoselov and coworkers in 2004 to produce graphene flakes, but the yield of this method is extremely low and the process is hard to control (Novoselov et al., 2004). After that several efforts have been reported by several research groups to separate graphene sheets a number of new methods of graphene production have been developed such as annealing SiC substrates12 or growth on metal support and methods based on exfoliation or chemical oxidation of graphite or heat treatment of silicon carbide. Oxidation of graphite to graphene oxide1 (GO) allows for a high-yielding route to exfoliated carbon nanosheets. The GO sheets disperse readily in water due to the presence of hydrophilic oxygen groups on the basal planes and edges (Lomeda et al., 2008).

Two basic methods of top-down, and the bottom-up approaches there are for fabrication of pure single-layer graphene sheets good method for fabrication of single-layer graphene sheets should have two main properties: first, the entire preparation process proceeds under mild conditions, and second no hazardous agents are involved.

Several methods are developed for produce graphene from graphite. , graphene may be produced through exfoliation (through sonication or high shear) of graphite powder . in a solution of stabilizer molecules such as micelle-forming surfactants, polymers, and aromatic hydrocarbons and oxidizing of graphite. A good strategy for producing high quality single-layer graphene sheets is using anionic and cationic surfactants. Main challenges for integration of this unique nano-material include: (1) uniform dispersion; (2) preferential alignment in liquid and melt phases; and (3) mass-production of high-purity material at low costs (Vaisman et al., 2006).

1. Graphen Dispersion methods

1.1. Liquid Exfoliation of Graphite

Liquid exfoliated graphene can be used for a range of applications: graphene dispersions as optical limiters, films of graphene flakes as transparent conductors or sensors, and exfoliated graphene as a mechanical reinforcement for polymer-based composites (Coleman, 2012).

Graphite is exfoliated either in organic solvents with the suitable surface energies or in aqueous solution of surfactants (Ciesielski and Samorì, 2014; Bourlinos et al., 2006). Different factors including ions, pH value and surfactants on graphene sheets separation and agglomeration are very important. Different research groups studied the effect of these parameters.

1.1.1.Surfactant

It is still challenging to synchronize prime goals of high quality, good yield, large sheet size, stable long term storage and low cost eco-friendly processing. We present a simple and inexpensive green route for large scale production of exfoliated graphene. self-assembly of surfactant molecules on the graphene surface is of great importance for better preparation and application of graphene: In the dispersion and preparation of graphene, surfactant adsorption on the graphene surfaces can assist the exfoliation and dispersion of graphene nanoparticles in aqueous media. Meanwhile, the adsorption can be used to isolate the graphene sheets with controlled thickness in the density gradient ultracentrifugation (DGU) method (Blanch et al., 2010). In next scheme (Fig.

1) some usual surfactant for dispersion and preparation of graphene sheets are presented.

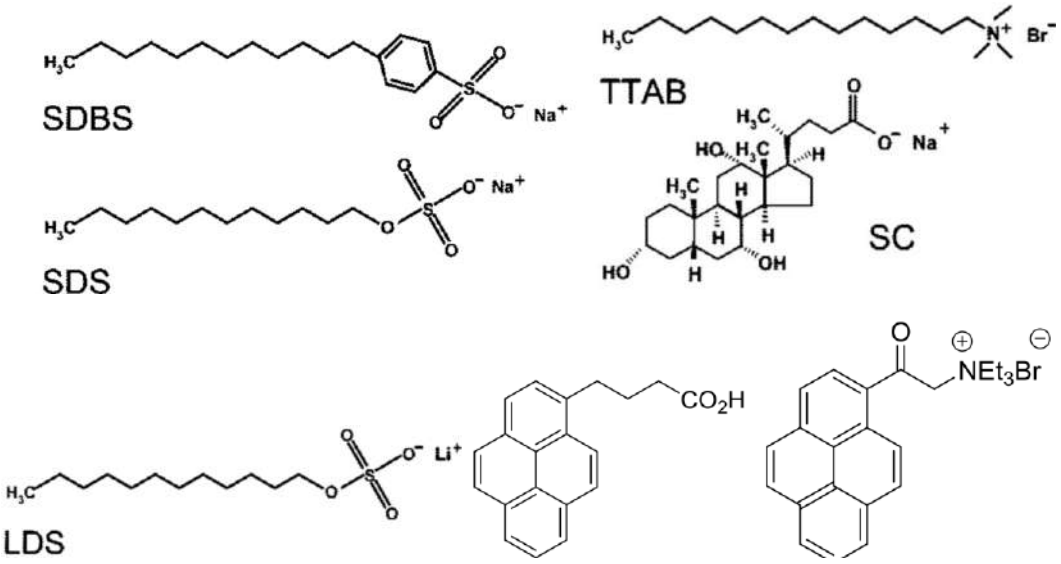

Fig.1 some usual surfactant for dispersion and preparation of graphene sheets

Javadian, and Khosravian in 2018 studied Self-Assembly Morphology of Fatty Acid on Graphene Synthesized by Surfactant Assisted LPE by A Joint MD, SAPT(DFT) and Experimental Study. They investigated different factors. such as surface density, environment pH, substrate size and number of layer. The results show that the decrease in pH transmutes the nature of the classical electrostatic interaction between the surfactants from repulsion to attraction leading to a decline in the stability of the colloidal systems. The morphology of self-assembly on the graphene surface and the factors tailoring the morphology were surveyed in light of classical molecular dynamic (MD) and symmetry-adapted perturbation theory (SAPT) have applied Docosahexaenoic acid (DHA) fatty acid to disperse graphite (Javadian and Khosravian, 2018).

Two important features which characterize surfactants, namely adsorption at interface and self-accumulation into supramolecular structures, are advantageously used in processing stable colloidal dispersions. The adsorption of surfactants onto inorganic and organic surfaces usually depends on the chemical characteristics of particles, surfactant molecules and solvent (Vaisman et al., 2006). Surfactant self-assembly structures on carbon surfaces have been extensively studied by several

research groups (Wu and Yang, 2012; Xu et al., 2010).

Haar and Coworkers developed A Supramolecular Strategy to Leverage the Liquid-Phase Exfoliation of Graphene in the Presence of Surfactants. They also investigated the Role of the Length of Fatty Acids. Here, a fundamental understanding on a straightforward supramolecular approach for producing homogenous dispersions of unfunctionalized and non-oxidized graphene nanosheets in four different solvents is attained, namely N -methyl-2-pyrrolidinone, N, N -dimethylformamide, ortho -dichlorobenzene, and 1,2,4-trichlorobenzene (Haar et al., 2016).

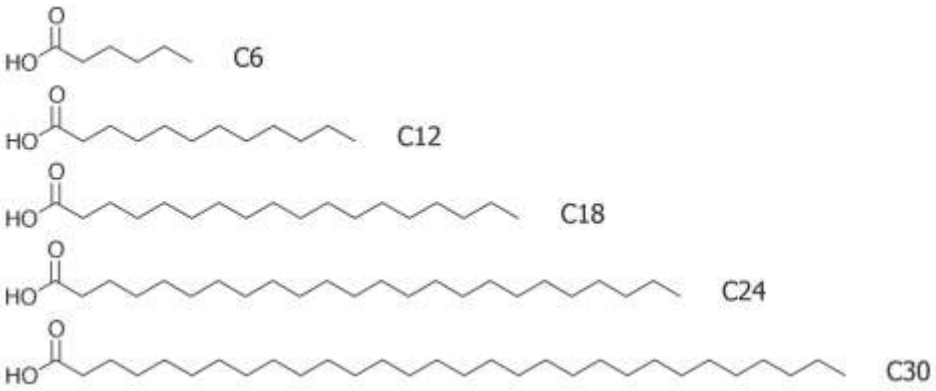

Fig.2 Chemical structures of investigated carboxylic acid derivatives by Haar and coworkers.

The addition of the C24 and C30 molecules reduces significantly the amounts of thick graphitic flakes (Fig.2)

Narayan and coworkers studied Perylene tetracarboxylate surfactant assisted liquid phase exfoliation of graphite into graphene nanosheets with facile re-dispersibility in aqueous/organic polar solvents. non-covalent surface chemistry between graphene and perylene tetracarboxylate (PTCA) aromatic semiconducting surfactant was studied by this research group. Significantly, pure aromatic semiconducting nature of surfactant without dielectric moiety ensures tight electrical contact among graphene sheets in thin films. The approach exploiting the simple molecular design of aromatic charged surfactants for graphene exfoliation holds a great prospect for solution processed graphene based nanomaterials and devices (Nayaran et al., 2017.

The strategy of this research is showed in Figure. Graphite flakes are first non-covalently functionalized with PTCA in water via p-p stacking interactions. Subsequent low power sonication releases exfoliated graphene sheets stabilized by electrostatic repulsion given by adsorbed PTCA molecules.

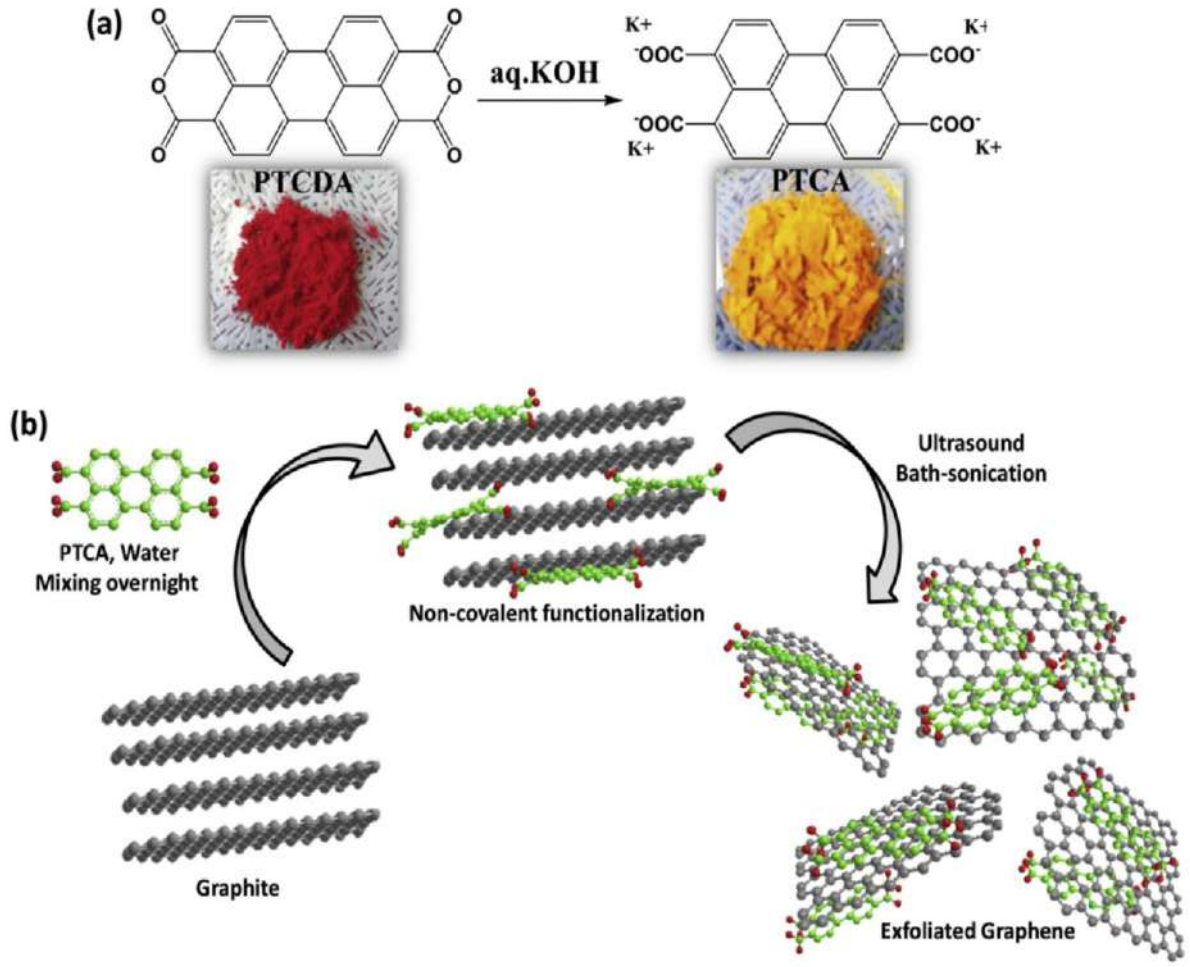

Fig.3 The diffirent step of NAYARAn and coworkers. (a) Synthesis of PTCA surfactant from PTCDA precursor. (b) Schematic process for PTCA assisted liquid phase exfoliation of graphite.

Nayaran and coworkers (2017) proposed the following schem (Fig. 4) for mechanism of electronic interaction between graphene and PTCA Surfactant in the non-covalent structure.

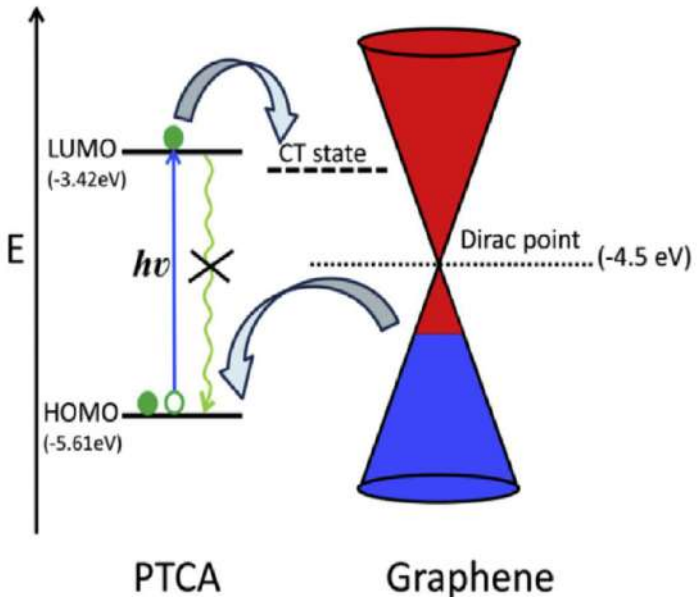

Fig.4 mechanism of electronic interaction between graphene and PTCA in the non-covalent **Structure**

Ahmadin and coworkers in 2019 used Computational Methods for Graphite delamination using Anionic Surfactants to produced pgraphene. They compared the capability of two different anionic surfactant sodium 4- actyloxybenzoate and Sodium Laurate. Gaussian calculation was applied in order to perform molecular dynamics analysis, first, (the minimum) force that each atom imposes to other atoms was calculated. The optimal structure showed that the presence of benzene, ether and carboxylic groups lead to facilitate the entry of surfactants into the plates and is a factor for starting the separation of grapheme sheets. The longer the surfactant sequence is the desire and ability to separate the plates by surfactant increase. The presence of an aromatic group in surfactant causes π-π interaction among the surfactants and graphene sheets, and makes the placement of the plates in parallel with the plate of the benzene ring and also creates distance in flat graphene sheets (fig. 5) (Ahmadin et al., 2019).

This research group also determined the HOMO and LUMO arbital of the System of Interaction of Surfactant and graphene sheets. In figure 6, the Laurate surfactant and graphene system is showed.

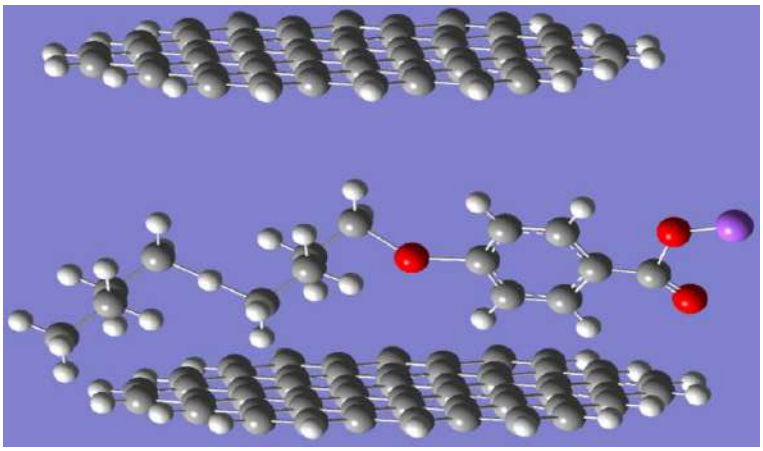

Fig.5 Gaussian view schem of dynamic modeling of surfactant and graphen sheet interaction by Ahmadin and coworkers.

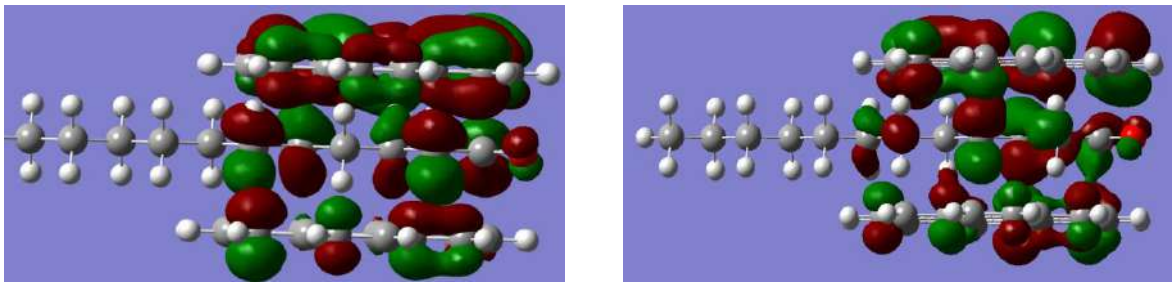

Fig.6 Double layer graphite HOMO (Left) an LUMO (right) orbital in the presence of sodium laurate surfactant

In Figure 7, the electrostatic interaction of graphite plates and sodium laurates surfactant is presented. In red areas, negative charge accumulation is more than white and blue areas and on the other hand, the negative charge accumulation of graphene sheet and anionic surfactant causes electrostatic repulsion and, consequently, increases the gap between graphite layers (Ahmadin et al., 2019).

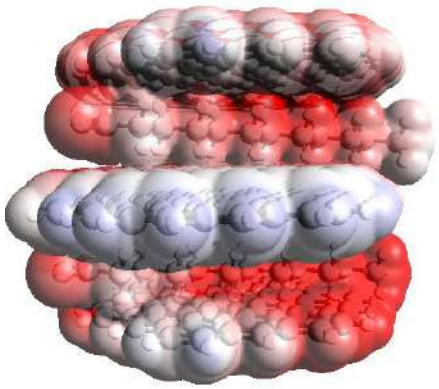

Fig.7 Electrostatic interaction of graphite plates and parallel sodium laurate surfactant

Heard and coworkers in 2019 studied the Rational Design of Aqueous Graphene Dispersants. This study presents preliminary experimental data suggesting that sodium 4-(pyrene-1-yl)butane-1-sulfonate (PBSA), 5, an analogue of sodium pyrene-1-sulfonate (PSA), 1, enhances the stability of aqueous reduced graphene oxide (RGO) graphene dispersions (Heard et al., 2019). The strategy of Heard and coworkers is showed in Fig.8.

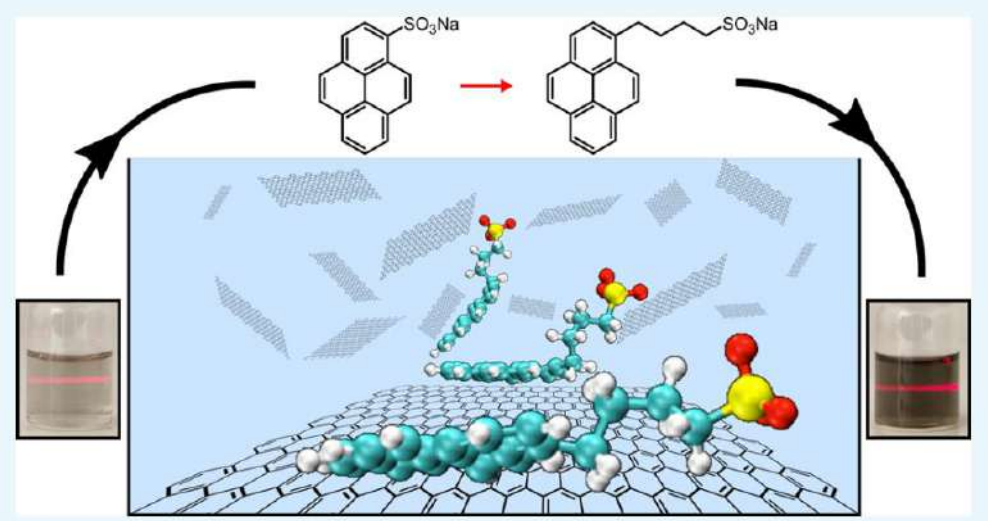

Fig.8 The strategy of Heard and coworkers

Zhang et al. (2018) investigated the direct exfoliation of graphite in graphene aqueous solution using a new surfactant derived from motor oil. This study presents a new classification of dispersion factors for graphene, which helps the process of exfoliating in water with high-concentration and stabilization of graphene plates against the reaccumulation.

Monajjemi (2017) in a research investigated the liquid phase exfoliating (LPE) of graphite for graphene. In this study, by ab initio study, they showed that sulfone groups in surfactants are most effective for any dispersion in the LPE process.

Haar and coworkers in 206 developed Liquid-Phase Exfoliation of Graphite into Single- and Few-Layer Graphene with α-Functionalized Alkanes. Report the exfoliation of graphite in N-methyl-2-pyrrolidinone, in the presence of heneicosane linear alkanes terminated with different head groups. These molecules act as stabilizing agents during exfoliation. The efficiency of the exfoliation in terms of the

concentration of exfoliated single- and few-layer graphene flakes depends on the functional head group determining the strength of the molecular dimerization through dipole-dipole interactions. A thermodynamic analysis is carried out to interpret the impact of the termination group of the alkyl chain on the exfoliation yield (Haar et al., 2016).

Sun and Yang in 2014, used Molecular simulation by classical molecular dynamics has been performed to study the adsorption self-assembly of sodium dodecylbenzene sulfonate (SDBS) on nanosized graphene sheets. They found Under higher surfactant concentration, multilayered micelles can be formed on the graphene surfaces. Also by using MD calculation they probed unique supramolecular morphology with SDBS adsorption on multilayer graphene nanosheets. also simulated the potential of mean force (PMF) between two nanoscale graphene sheets covered by SDBS surfactants in order to understand the interaction mechanism in the SDBS-based graphene dispersion and stabilization (Sun et al., 2014).

Side and front views of representative simulation snapshots of their calculation for the self-assembly of SDBS surfactants absorbed on graphene sheets are showed in fig. 8.

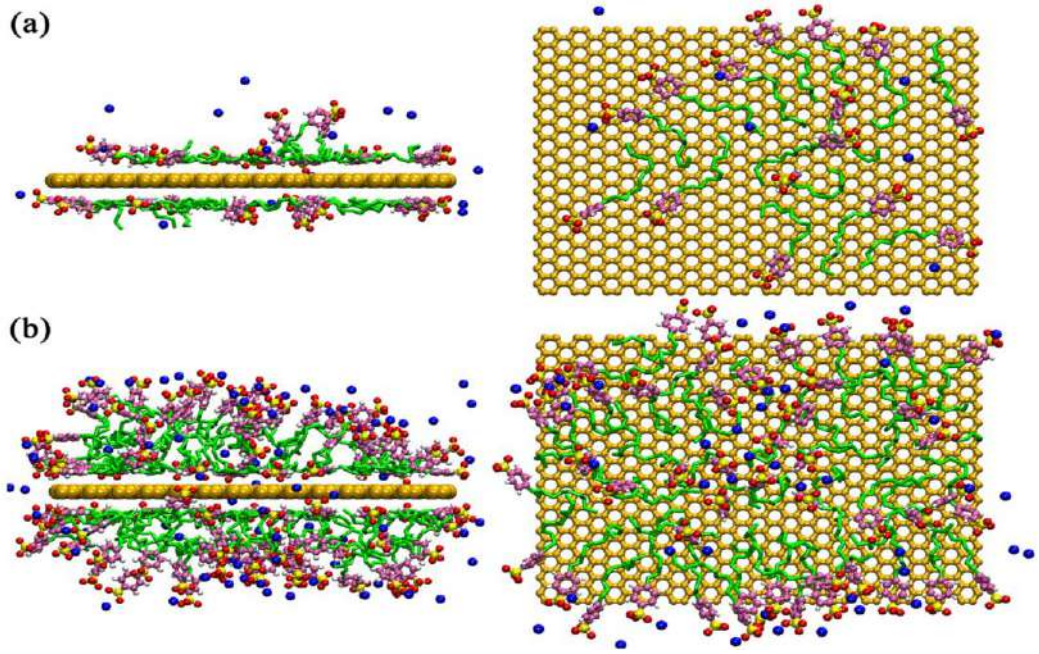

Fig.8. Side and front views of representative simulation snapshots for the self-assembly of SDBS surfactants absorbed on graphene sheets: (a) at low surface coverage; (b) at high surface coverage. Color code: green for CHn groups; purple for carbon atoms in benzene rings; yellow for sulfur atoms; red for oxygen atoms; blue for sodium counterions; orange for carbon atoms in graphene.

Lomeda et al. reported diazonium functionalization of surfactant-wrapped chemically converted graphene sheets (Lomeda et al., 2008).

1.1.2. Graphite Oxidizing

Graphene layers are held together by van der Waals forces in graphite; The most common approach to of producing graphene from graphite involves oxidizing the graphite to produce graphite oxide, which may then be exfoliated to yield dispersions of graphene oxide. While the graphitic nature of the resulting nanosheets is highly compromised by oxidation, leading to loss of conductivity, reduction by chemical,2b,5 thermal,6 or electrochemical7 treatment results in partial recovery of the graphitic character (Stankovich et al. 2006, 2007). Graphene oxide (GO) may subsequently be chemically or thermally treated to remove the covalent functional groups and produce reduced graphene oxide (rGO).

Sabziparvar and coworkers investigated that Ca^{2+} cation effect on graphene oxide sheets. They found Ca2+ cation is more detrimental in case of GO agglomeration in the cementitious environment, compared to the monovalents Dispersion of GO in water mainly occurs via its oxygen functional groups including hydroxyl and epoxide functional groups. They found in mild alkali media, an increment in pH from 7 to about 10.9 causes more ionization and electrostatic repulsion, which leads to better dispersion. However, at high alkali media with pH larger than 10.9 GO dispersion undergoes reduction when pH increases, because GO loses the most of its functional groups and then will agglomerates (Sabziparvar et al., 2019).

Lomeda and coworkers developed a new methos as Diazonium Functionalization of Surfactant-Wrapped Chemically Converted Graphene Sheets. It was obtained from reduction of graphene oxide with hydrazine were functionalized by treatment with aryl diazonium salts. *Their resuls showed* The resulting functionalized nanosheets disperse readily in polar aprotic solvents, allowing alternative avenues for simple incorporation into different polymer matrices (Lomeda, 2008).

The functionalize Graphen with high amounts of varying aryl addends, allowing these nanosheets to be solubilized in organic solvents. This strutegy may prove to be useful in the area of composites, especially in the use of these 2-D structures as

reinforcing agents where intimate interfacial bonding between the host and the structural modifier is critical *(Fig. 9)*

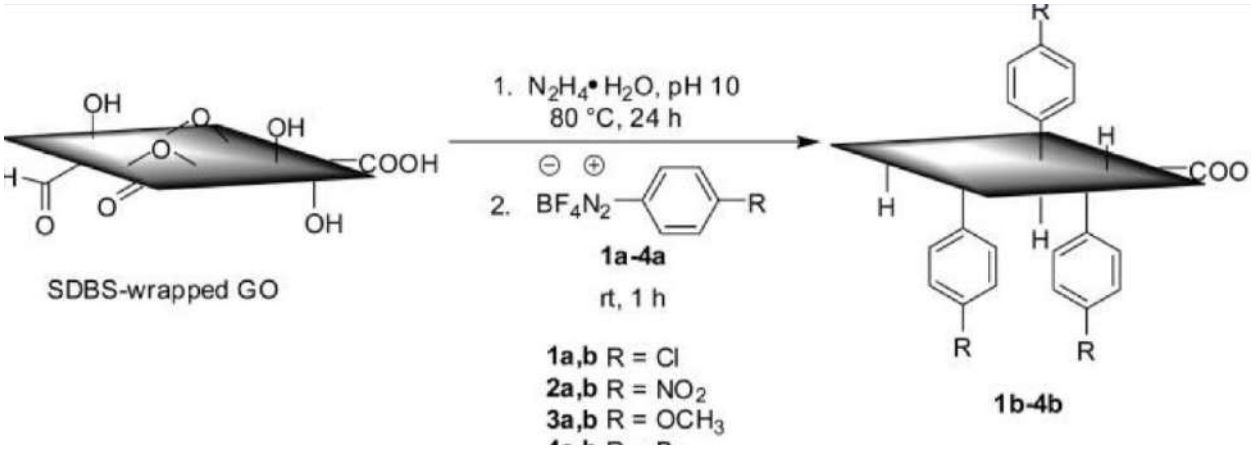

Fig.9. SChem of methods of Lomeda and coworkers by Starting with SDBS-Wrapped GO, Reduction, and Functionalization of Intermediate SDBS-Wrapped hemically converted graphen (CCG) with Diazonium Salts

Stankovich et al. chemically modified the graphite oxide using phenyl isocyanate in N,N′-dimethylformamide (DMF). The grafting of long alkyl chain or six-armed poly- (ethylene glycol) on the graphite oxide surface through amideformation with the carboxyl groups was reported (Stankovich et al., 2006, 2007).

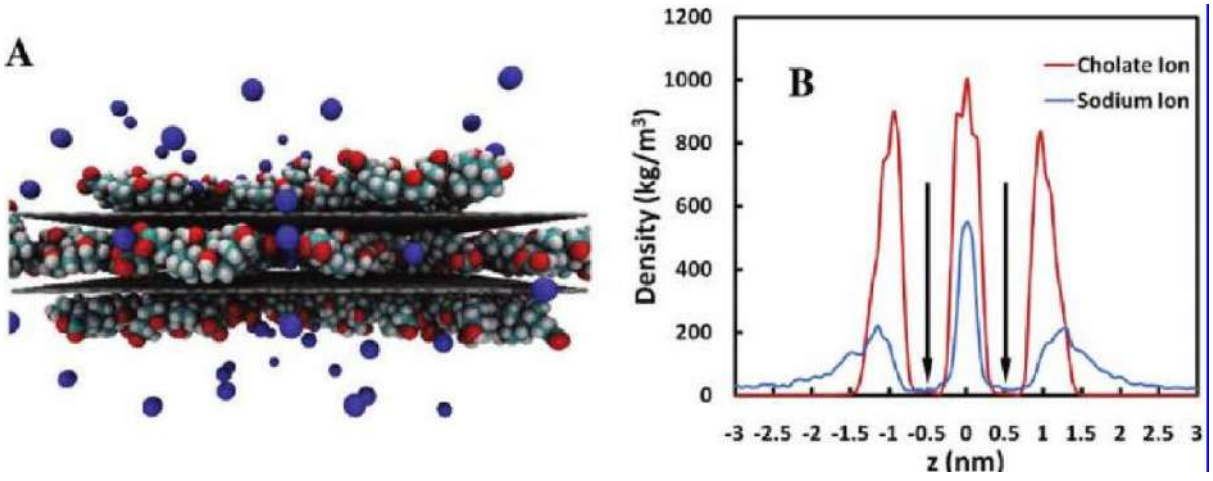

Figure 10. (A) Postequilibrium simulation snapshot of the metastable bilayer grapheneSC assembly at an intersheet separation of d = 1.05 nm, showing a single layer of cholate ions and a sodium counterion wall confined between the two graphene sheets. Water molecules are not shown for clarity. The color code is the same as in Figure 1. (B) The simulated density profiles of the cholate ions and the sodium counterions along the z-axis, showing a single layer of cholate ions and a sodium counterion wall (both peaked at z = 0 nm) being confined between the two graphene sheets. (Lin et al, 2011).

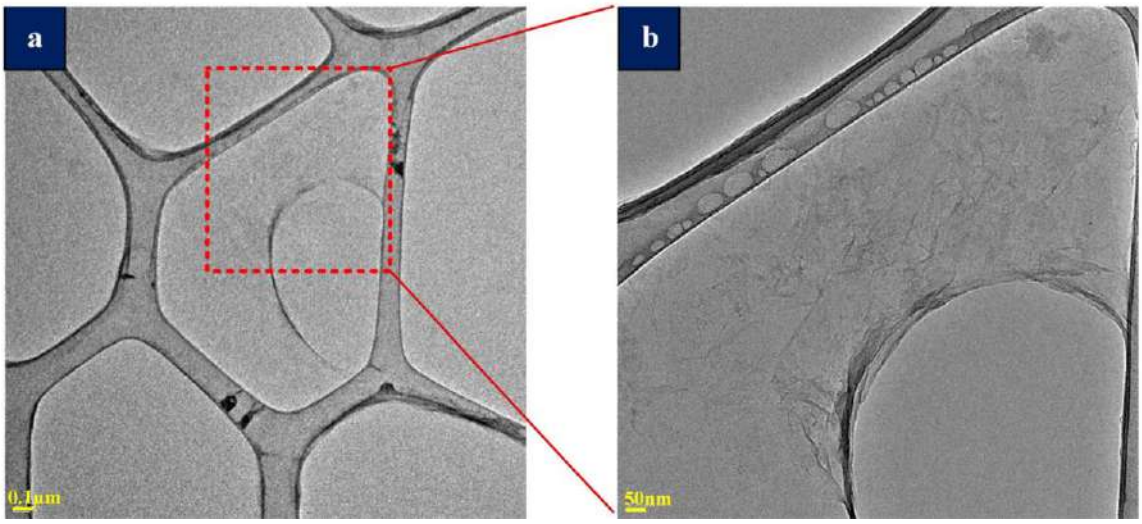

Fig.11 TEM image of as-received GO nanosheets, (a) low magnification and (b) high magnification.

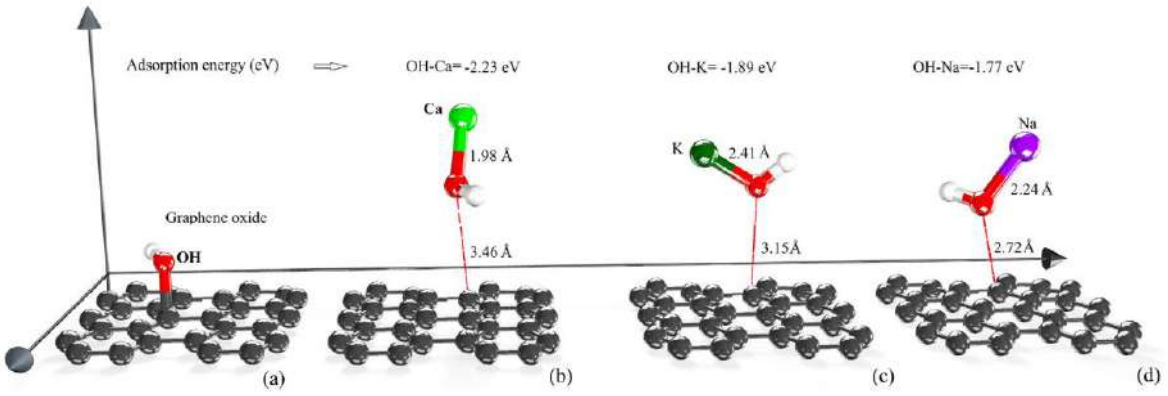

Fig. 12. Hydroxyl group location (a) before adsorption and after adsorption of (b) calcium, (c) potassium, and (d) sodium.

OH group detachment and physical interaction between graphene and calcium hydroxide could be found. Fig.12(a) shows the electron density difference before the adsorption of calcium on the GO, which represents a covalent bond between the hydroxyl and GO surface and no electron exchanging between calcium and GO. However, after the adsorption (Fig. 12(b) and (c)), calcium ion disrupts CAO covalent bond by transferring the charge to OH and making an electrostatic interaction. Through this mechanism, the hydroxyl group is being located at a relative location respect to GO surface in which a vdW physical interaction creates and eventually diminish polarity of GO surface (Lin et al., 2011).

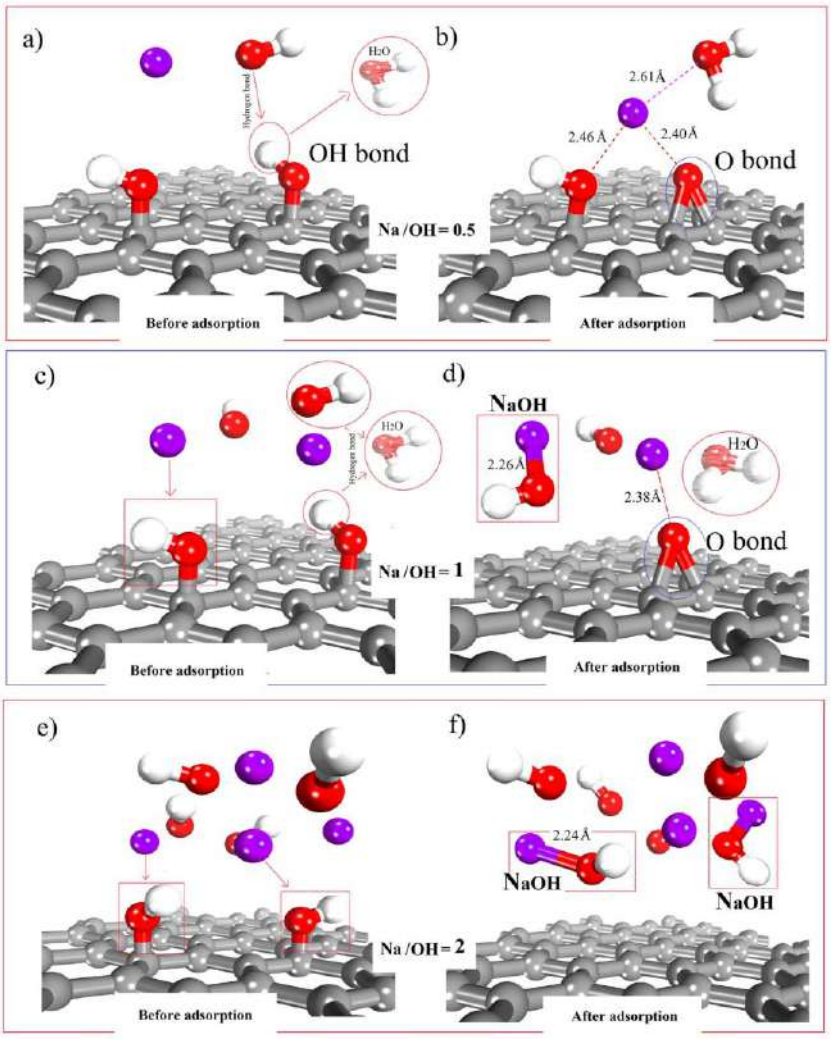

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Fig.13. Interaction of GO with NaOH at different ratios of sodium to the hydroxyl group of GO; (a), (b) Na/OH = 0.5, (c), (d) Na/OH = 1, and (e), (f) Na/OH = 2.

1.1.3. Self-Assembly Approach for Exfoliation of Graphite

But Zhang research geoup a new tempelate base strategy as Based on a Confined Self-Assembly Approach for production single seet graphen. The three-step procedure of this strategy is showed in Figure 5. A special structure-directing surfactant containing a pyrrole moiety is used to construct lamellar mesostructured silica. Since polypyrrole is an ideal carbon precursor to form raphite, this surfactant can serve simultaneously both as the structure-directing agent and as the carbon source. During the formation of the lamellar silica framework, the pyrrole moieties could be densely packed in a controlled fashion within confined 2D spaces between silica layers, providing the prerequisite for quantitative production of isolated graphene sheets after

carbonization. After the in situ polymerization of the organized pyrrole moieties using FeCl3 as oxidant, the resulting polypyrrole nanosheets were individually transformed into single-layer graphene sheets in N2 atmosphere (Fig. 14), for which the residual iron salts from the polymerization process were directly employed as catalyst for the conversion (Zhang et al., 2018).

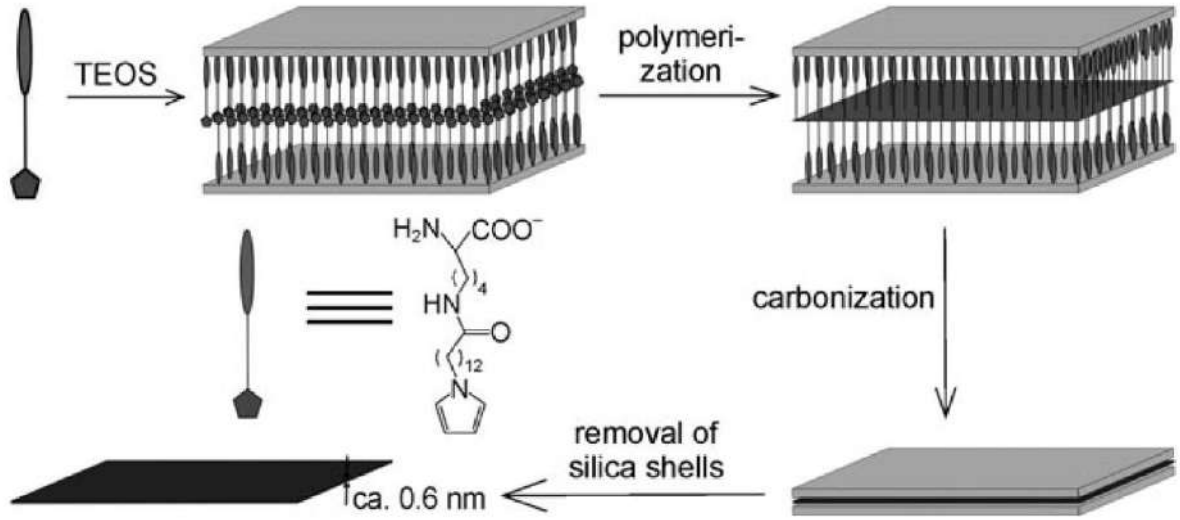

Fig14 Schem of Zhang'S strategy for fabrication of pure single-layergraphene with a thickness about.0.6 nm. TEOS=tetraethoxysilane

Lin and coworkers, graphene-based electronic and optical devices requires synthesis methods to either control the number of layers to enrich AB-stacked bilayer or trilayer graphene or control the extent of functionalization of monolayer graphene. Over the past decade research efforts devoted to graphene fabrication (Lin et al., 2011).

Poorsargol and coworkers (2014) developed an method of Dispersion of Graphene using Surfactant Mixtures. They investigated Experimental and Molecular Dynamics Simulation for The capability of sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB), cationic-rich and anionic-rich mixtures for dispersion of graphene nanosheets in an aqueous medium. In MD simulation The ζ-potential about surfactant mixture-graphene assemblies was estimated using Poisson's theory. The ζ-potential about surfactant mixture-graphene assemblies was estimated using the results of MD simulation and Poisson's theory the design and selection of appropriate surfactants, the optimization of the process and the

improvement of graphene dispersion in aqueous solutions of surfactants. Interactions between two surfactant mixture-graphene assemblies were evaluated through calculating the potential of mean force (PMF), and it was found that increasing surfactant surface coverage would lead to an enhanced repulsive barrier of PMF Using surfactant mixtures for dispersing graphene nanosheets is promising. Moreover, MD simulations were used to examine surfactant mixture assemblies' structure on graphene and explain the experimental results, which showed that the random adsorption model first changes to the monolayer model and then the hemispherical model with an increased surfactant concentration. novel method based on the controlled electrochemical exfoliation of graphite in aqueous ammonium sulfate electrolyte to produce graphene in large quantities and with outstanding quality.

Common challenges, including controlling the surface morphology, reducing the turbostratic layering, and enhancing the dispersion stability (Lin et al., 2011). The latter, solution-phase method offers several significant advantages since it: (i) utilizes inexpensive and readily available graphite flakes, (ii) does not require transferring the graphene from the growth substrate, (iii) employs existing technologies (e.g., sonication and centrifugation) for scaled-up large volume processing, and (iv) allows solution-phase chemical functionalization of graphene.

1.1.4. Electrochemical exfoliation

Electrochemical exfoliation has recently emerged as a promising strategy for producing graphene on an industrial scale with high efficiency, at low cost, and in an environmentally friendly manner (Bunch et al., 2007; Yang et al., 2015; Liu et al., 2008). Either cathodic or anodic potentials are able to drive guest ions into graphitic layers which promotes the structural deformation of a graphite working electrode. Organic Radical-Assisted Electrochemical (Yang et al., 2015; Xia et al., 2013). Morphology ographen obtained by electrochemical methods were investigated by researchers for tha capability of its for electrical and mechanical purpose (Eredia et al., 2017).

A facile approach to disperse graphene in aqueous solution is described (Li et al., 2008). Graphene can be prepared via top-down approach from graphite through physical exfoliation ("peel-off")1 and chemical exfoliation. The latter method generally

produces a large-scale amount up to grams. However, chemical exfoliation gives graphite oxide which contains lots of hydrophilic oxygencontaining groups such as carboxyl, hydroxyl, and epoxide (Zu and Han, 2009).

1.2.7. Polymeric and copolymeric hydrogels

Zu And Han in 2009 produced Graphene Sheets Formation of Supramolecular Hydrogel and Stabilized by Pluronic Copolymers: Proposed strategy of the formation hydrogel by Copolymers for Production graphene sheets is showed in next figure. utilizing the dual roles of Pluronic copolymer in dispersing graphene in aqueous solution and forming supramolecular hydrogel with R-CDs through the penetration of PEO chains into the cyclodextrin cavities, (fig. 15). They developed a facile and effective method to hybridize the well-dispersed graphene into a supramolecular hydrogel (Zu and Han, 2009).

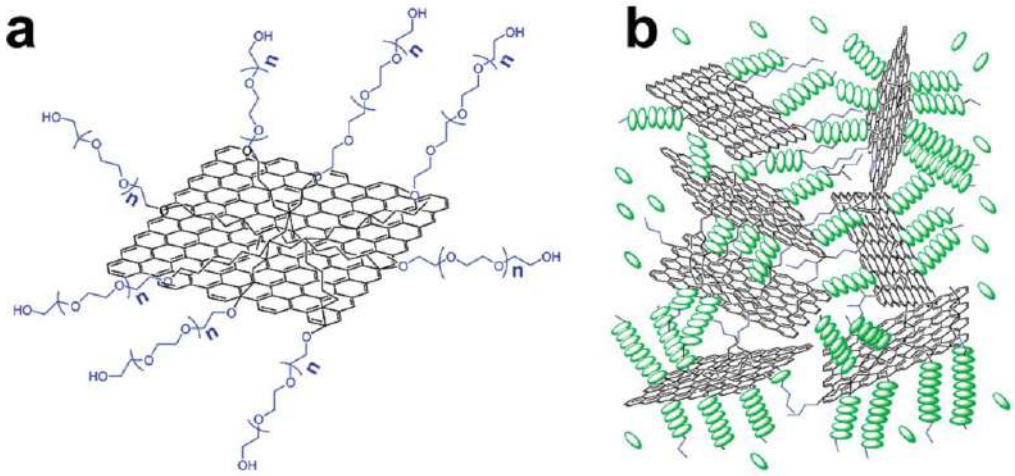

Fig.15. Proposed structure of the copolymer coated graphene (a) and supramolecular well-dispersed graphene sheet containing hybridhydrogel (b).

1.1.5. Ionic Liquid

Novel ionic liquids (ILs) were designed and synthesized to contain aromatic groups for Direct exfoliation of graphene (Porsargol, 2014) Ionic liquids (ILs) are organic molten salts with melting point temperatures below 100 ◦C, which have been

used extensively as solvents. ILs are non-volatile, thermally stable, nonflammable, recyclable, and capable of dissolving a range of solutes. Furthermore, their properties such as miscibility and viscosity can be tuned via chemical changes to the cation or anion (Zheng et al., 2011; Ravula et al., 2015). Additionally, ILs are attractive because of their status as green solvents due to their low vapor pressures and ease of recycling, in contrast to common organic solvents.

ILs can disperse graphene directly (Wang et al., 2010). The mechanisms behind IL–graphene interactions are just beginning to be understood (Porsargol, 2014).

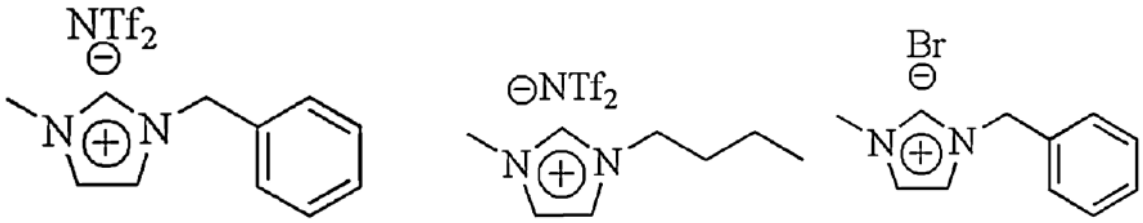

Fig.16. Usual ionic liquids for dispersion of graphene.

Bari and coworkers, used ionic liquids with aromatic groups for direct exfoliation of graphene. Novel ionic liquids (ILs) were designed and synthesized to contain aromatic groups on the imidazolium cation that non-covalently interact with graphene surfaces. In Figure 17 the schematic strategy of this research group is showed.

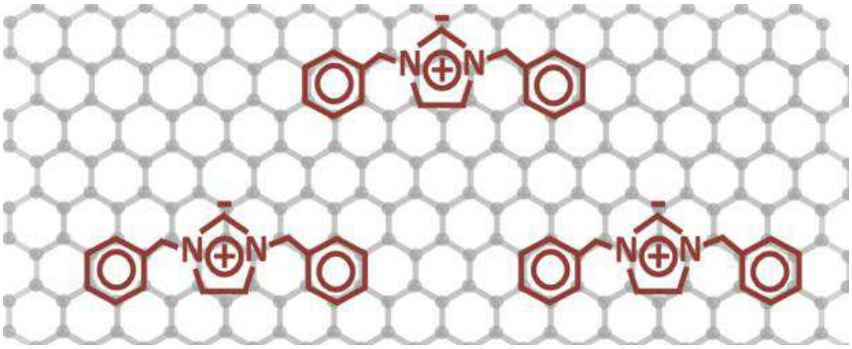

Fig.17. schematic of the strategy of Bari and coworkers

They used Density functional theory (DFT-D3) calculations used for predictive modeling of IL design for optimal graphene dispersions. Interaction of Graphene and IL computed at the PBE-RI/TZVPP level is showed in next figure. In their results IL-4

with two phenyl groups was the most effective one in stabilizing the graphene dispersion with a high yield of 5.8 mg mL-1. the dispersion of graphene in ILs at high concentrations without covalent functionalization or additive stabilizer was the result of their investigation. These preliminary computational calculations suggest that the addition of π-stacking capable substituents will increase the adsorption of the ionic liquids on the graphene surface with a possible favorable effect on the exfoliation and stabilization processes(Fig. 18) (Bari et al., 2014).

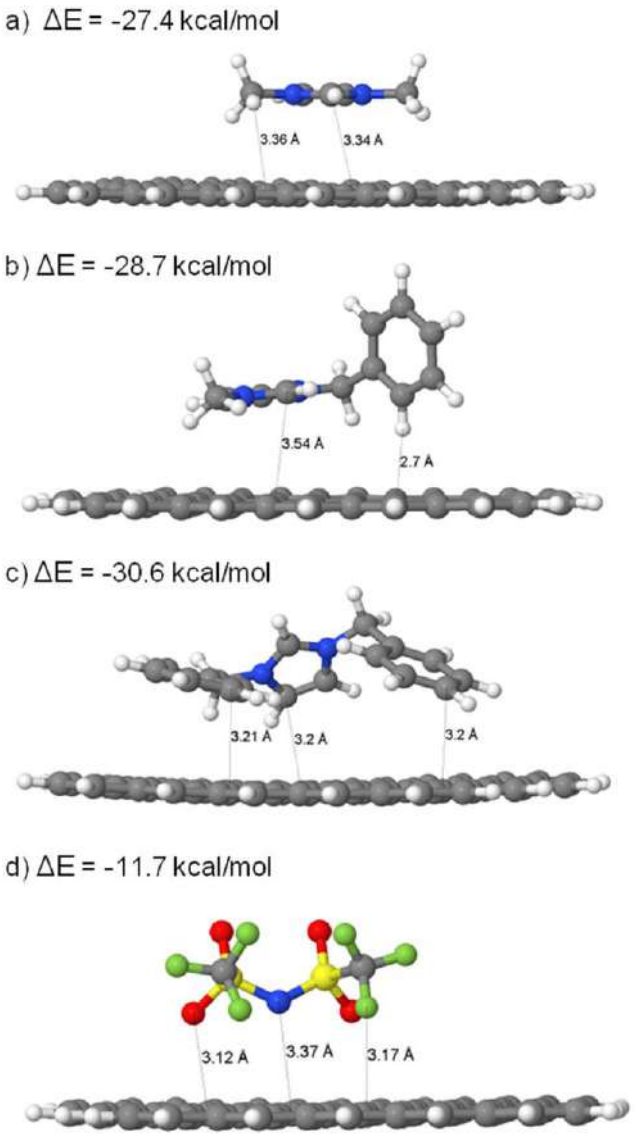

Fig. 18. Graphene and IL interaction computed at the PBE-RI/TZVPP level: (a) [C1C1im]+ cation and graphene, (b) IL-1 [BnzC1im]+ cation and graphene, (c) IL-4 [(Bnz)2im]+ and graphene, and (d) [NTf2]- anion and graphene. The two additional aromatic rings on IL-4 provide an increased interaction with graphene relative tostructure (a). Shorter distances between the cation and graphene can be observed and also a slight curvature of the carbon sheet as an effect of stronger – interactions (Liu et al., 2008).

1.1.6. Other Delamination strategy

High pressure homogenizer combines surfactant were used by Peukert's research group for graphene prodiction from graphite. principle of graphite delamination by high pressure homogenizer (HPH). The suspension is pumped through a nozzle and released into an expansion chamber. A counter pressure can be applied to the suspension by closing the valve after the expansion chamber. HPH devices are commonly used in food industry, cell disintegration 24, emulsification 25, 26 or dispersion of active pharmaceutical ingredients.27,28 Recently, HPH devices were employed for graphene production by exfoliation of thermally reduced graphite oxide (Nacken et al., 2015).

The Resulted graphene dispersions were used for manufacturing graphene films by printing techniques or for preparation of graphene nanocomposites with superior mechanical and electrical properties (Appel et al., 2012).

Chiesielski and SAmori in 2014 developed a simple method for this purpose as Graphene via sonication assisted liquid-phase exfoliation (Ciesielski and Samori, 2014).

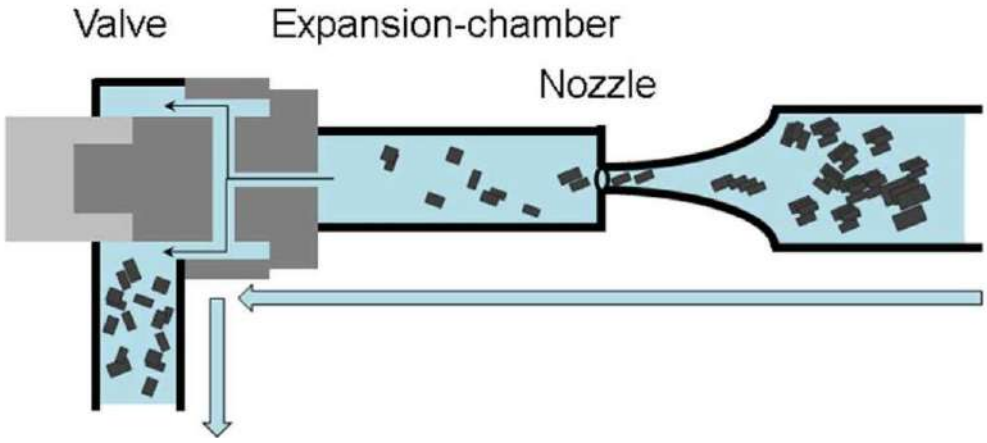

Fig. principle of graphite delamination by HPH.

1.2. Thermodynamic and electrostatic equation of Graphene sheets

1.2.1-Total Graphene Dispersion Stability

To utilize the kinetic model described above to calculate the time-dependent number concentration of various graphene layer

$$N_{total}(t) = \sum_{i=1}^{M} N_i(t)$$

1.2.2. Interactions between two parallel graphene sheets

To assess the optimum and appropriate interactions between two parallel graphene sheets that coated with surfactant, the PMF was evaluated through the numerical integration (the trapezoidal method) of the interaction forces needed to separate two parallel graphene sheets fixed at different intersheet separations d (along the z-axis of the simulation box) from d1 = 0.7 nm to d2 = 2.0 nm. The PMF between two graphene sheet covered by pure SDS and CTAB surfactants was also calculated for comparison. The PMF is found through integrating constraint force ($F_C(r)$) as follows:

$$PMF(r) = \int_{d1}^{d_2} F_C(r)dr$$

To calculate the average total forces exerted on both graphene sheets (F_{tot}):

$$F_C(d) = \frac{1}{2}\left\langle \vec{d}_v.(\vec{F}^1_{tot}(\vec{d}_1) - \vec{F}^2_{tot}(\vec{d}_2)) \right\rangle$$

$$\vec{d}_v = \frac{(\vec{d}_1 - \vec{d}_2)}{\left|\vec{d}_1 - \vec{d}_2\right|}$$

where d_v, d_1 and d_2 are the unit vector and the position of center of mass of graphene sheets 1 and 2, respectively. To find the PMF, a series of initial configurations were constructed by positioning two parallel graphene sheets coated with surfactants at different intersheet separations.

In 2008, Bergin et al. combined experiment and thermodynamic modeling to show that the enthalpy of mixing of nanotubes per volume of solvent is given by. surface energy of graphite is similar to that of carbon nanotubes, it might be possible to exfoliate graphite to give graphene in certain solvents:
enthalpy of mixing of graphite: per volume of solvent is given by

$$\Delta H_{mix}/V \approx 4(\sqrt{E_{S,NT}} - \sqrt{E_{S,Sol}})^2 \phi/D$$

Here where φ is the dispersed nanotube volume fraction, D is the dispersed

graphite diameter, and $E_{S,NT}$ and $E_{S,Sol}$ are the graphite and solvent surface energies, respectively. This suggested successful solvents to be those with surface energy close to that of the graphite. he maximum dispersible concentration of graphite in solvents is given by

$$\phi \approx K' \exp\left[\frac{\overline{V}}{RT} \frac{\partial(\Delta H_{Mix}/V)}{\partial\phi} \right]$$

here K_0 is a constant and vh is the molar volume of rods. Applying to nanotubes by mixing two above equation:

$$\phi \approx K' \exp\left[-\frac{\pi DL}{4E_{S,NT}kT}(E_{S,NT} - E_{S,Sol})^2 \right]$$

here L is the mean nanotube length. This expression represents a Gaussian function when φ is plotted versus the solvent surface energy.

1.2.3. Electrostatic Potential of Surfactant graphene system

The electrostatic potential about assemblies of surfactant graphene mixture, Ψ(z), along the z-axis simulation box, correlated with local charge density, ρ(z), through the Poisson equation

$$\frac{d^2\Psi(z)}{dz^2} = -\frac{\rho(z)}{\varepsilon\varepsilon_0}$$

Here ε = 78.5 is the relative dielectric permittivity of water at room temperature. To calculate Ψ(z), we first divided the simulation box into a number of thin slices and obtained the mass density of surfactant ions $\varepsilon_0 = 8.85 \times 10^{-12}$ C/m.V is the vacuum dielectric permittivity

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Increased efficiency of a fuel cell using h-BN electrodes and Teflon polymer electrolyte [-C2F4-]n

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M. Monajjemi **
H. Aghaei *

ABSTRACT

Graphene and h-BN have been theoretically simulated for hydrogen storage and oxygen diffusion in a single fuel cell unit. Obviously, the efficiency of the PEM hydrogen fuel cells was significantly related to the amount of H2 concentration, the water activities in catalyst substrates and the polymer of the electrolyte membranes, the temperature and the dependence of such variables in the direction of the fuel and air currents between the anode path and the cathode. The single PEM parameter has been estimated and the results show greater fuel cell efficiency using graphene sheets and h-BN. Maximum efficiency is observed with the stoichiometry of the 5H2, 5O2 and 3 C2F4 molecules during adsorption.

KEY WORDS: fuel cell, h-BN, electrodes, teflon, [-C2F4-] n polymer, electrolyte

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Aumento de la eficiencia de una pila de combustible mediante electrodos h-BN y electrolito de polímero de teflón $[-C_2F_4-]_n$

RESUMEN

El grafeno y el h-BN se han simulado teóricamente para el almacenamiento de hidrógeno y la difusión de oxígeno en una sola unidad de pila de combustible. Obviamente, la eficiencia de las celdas de combustible de hidrógeno PEM se relacionó considerablemente con la cantidad de concentración de H2, las actividades del agua en sustratos catalizadores y el polímero de las membranas de electrolitos, la temperatura y la dependencia de tales variables en la dirección de las corrientes de combustible y aire entre la vía del ánodo y el cátodo. Se ha estimado el parámetro de un solo PEM y los resultados muestran una mayor eficiencia de la pila de combustible utilizando láminas de grafeno y h-BN. La máxima eficiencia se observa con la estequiometría de las moléculas de 5H2, 5O2 y 3 C2F4 durante la adsorción.

PALABRAS CLAVE: pila de combustible, h-BN, electrodos, teflón, [-C2F4-] n polímero, electrolito.

Introduction

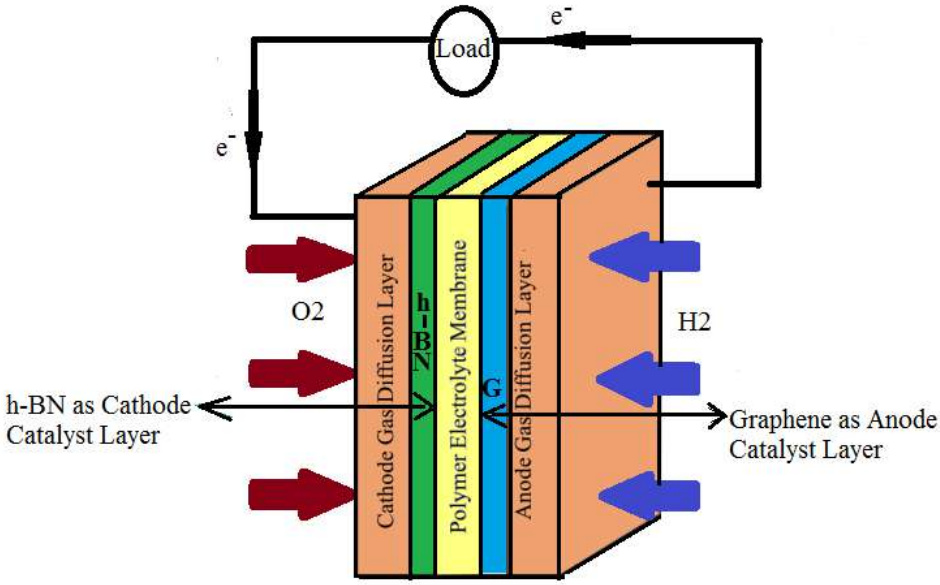
Currently, fuels same as petrol, gasoline, oil, gas and coal, supply the 90% environmental energies. The demands have been raising since the 1975s and this rise is expected for continuing due to the fast and advanced world technologies. In order to consider both efficiency and ecology, hydrogen/ oxygen fuel cells are being important key element. H_2/O_2 fuel cells are clean efficient production of energy sources in the 21st century (Ciureanu, 2004). In H_2/O_2 fuel cells, two half- cell reactions accomplish simultaneously including, loss of electrons (an oxidation reaction) and gain of electrons (a reduction reaction) in anode and anode electrodes respectively (De Bruijn and Dam, 2008). These processes make up the formation of water from hydrogen and oxygen gases through the total redox reaction of this fuel cell (Cruz-Manzo et al., 2013).

The electrolyte in the fuel cell consists of a solid acid supported within the membrane which is saturated with H_2O for any further ions transporting. Anode reaction:

$H_2 \rightarrow 2H^+ + 2e^-$ and Cathode reaction: $1/2\ O_2 + 2e^- + 2H^+ \rightarrow H_2O$ **(1)** with an overall reaction: $H_2 + 1/2\ O_2 \rightarrow H_2O$ **(2)**. In viewpoint of mechanism, at the anode, H_2 first come into contact with a nickel catalyst and break apart, bonding to the nickel surface forming weak H-Ni bonds consequently the oxidation reaction can be proceed. Each H_2 releases its electron, which moves around the external circuit to the cathode which is electrical current. Then the H^+ bonds with H_2O on the membrane surface for forming H_3O^+ that moves through the membrane to the cathode electrode, leaving the nickel catalyst for the next H_2. At the cathode, O_2 come into contact with nickel catalyst on the electrode surface and break apart bonding to the nickel sheet forming weak O-Ni bonds, enabling the reduction reaction to proceed. O_2 then leaves the nickel catalyst site, combining with two electrons that move in external circuit and two protons which have moved through the membrane for forming H_2O. Increasing the H_2 storage is a major section for the transition more and more hydrogen molecules in a fuel cell (Larminie and Dicks, 2003).

1. PEM fuel cells

Obviously fuel cells as an electrochemical instrument are able to convert chemical energies straightly into direct electrical currents (DC) through a sufficient electrolyte. Therefore, it is usually far yields than combustion engines. A fuel cell needs a stable reservoir of fuels and oxidants for to keeping the electrochemical reactions, same as hydrogen and oxygen (Kazmi et al., 2009). Although Hydrogen can be used in a mixture with other gasses such as N2O, N2, NO2, C2H6, the major fuel cell is electrolysis reversed consist of hydrogen and oxygen for producing electricity with high efficiency. It is notable that electrolyte has major roles which are different types this work is focused on graphene and h-BN electrodes with polymer membrane electrolyte (PEM) in low temperature. In the PEM fuels cell, the electrolytes are thin polymeric membrane including proton permeability. At low temperature around 90◦C the presence of the catalyst such as typically nickel is needed for hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR) on anode and cathode electrodes respectively (Scheme.1).

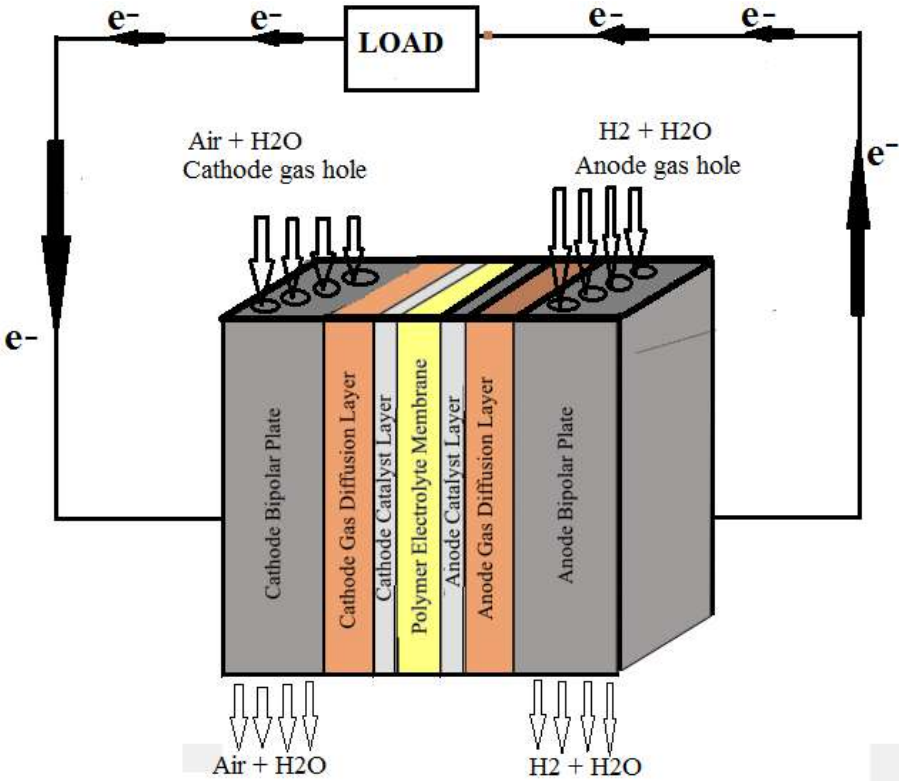


Scheme 1: A schematic components of fuel cells

Cathode and anode gases diffusion layers, generally made of carbon porous including graphene layer for cathode and h-BN for anode adjacent to catalyst, respectively which are distributed on each side of the polymer membrane. Currently, PEM fuel cell technologies have been combined to the R&D approaches in the automotive sections such as Chrysler, Toyota, Suzuki, Ford, General Motors, Volvo, Hyundai, Nissan and BMW and also as power back-up sources (Kazmi et al., 2009). The electrochemical reactions accomplish at the catalyst electrodes on both sides polymer material including oxidation and reduction (equations 1&2). Hydrogen flows into the PEM fuel cell and diffuses through the gases diffusion layers to the catalyst layers, where catalyst particles facilitate fuel oxidation and protons trap onto water molecules to form H_3O^+ that move via the membrane from the anode towards cathode. In addition two electrons from above equations (1&2) reach to the cathode electrode over the bipolar plates and over an external circuit. It is notable that this mechanism is known as electro-osmotic drag. On the cathode electrode, oxygen gases diffuse to the catalyst layer and chemically combined with protons and electrons to form water (ORR). Obviously, the electrodes must be selected of porous materials that facilitate water moving to outside and the excess oxygen gases might

be help for pushing water out of the cell (scheme 2 & 3). Efficiency, permanence and cost reduction effort are the most important items for PEM fuel cells that cover construction and assembly methods (Litster and McLean, 2004). There are several major items for increasing the life cycle and PEM fuel cells efficiency which are thermal management, water management, new catalysts, and novel material of membranes and also quality of electrodes. Operating conditions and operating strategies play an important role in a fuel cell lifecycle. Bad distribution of fuel cell reactants can appear in the presence of high cell currents, liquid water, fuel impurities, and different flows of fuel due to the sudden changes in the power demand and conditions between cell inlet and outlet.

In other hand, fuel starvation can cause severe degradation during of gross fuel starvation that cell voltages can become negative (as the anode) and the carbon is consumed given the lack of fuel, consequently anodic current will be provided by carbon corrosion to form carbon dioxide (Schmittinger and Vahidi, 2008).

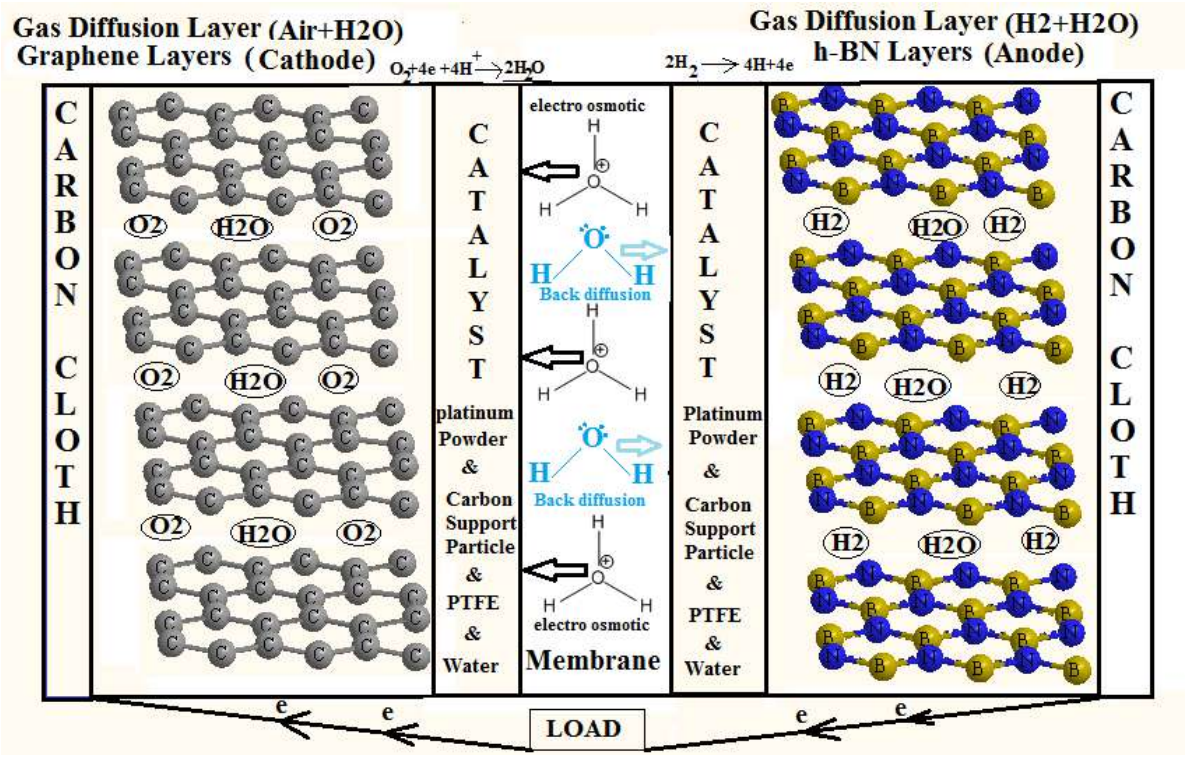


Scheme 2: one unit of PEM fuel cell structure

In addition, oxygen starvation can result in generation of hydrogen in the cathode or oxygen in the anode similarly during oxygen starvation the reaction at the cathode will

produce hydrogen. For avoiding these problems the suitable monitoring controlling sensors and indicators are needed (Borup, 2007). Several studies have shown that thermal management is important, higher temperature might be producing the radicals consequently the electrochemical surface area (ECSA) decrease the life time. There are various cooling methods for PEM fuel cells which one important has been investigated by Fly among Liquid- cooled air-cooled and evaporative-cooled fuel cells. Water management is essential and most important issues in PEM fuel cell technologies which dependent to adequate membrane hydration and avoidance of water flooding in the catalyst layers. It is important to keep the membrane and the catalyst layer humidified for high proton conductivity. In the presence of H2O, the protons produce H3O+ on the boundaries of the catalyst layer and the membrane which prevent of the proper activity of the protons from the anode catalyst layer to the cathode catalyst layer in aqueous phase. Therefore, tuning humidification of the membranes is also a basic way of cell performance while accumulation of too much water also impacts performance and lifetime (Zawodzinski et al., 1993).

Excess water blockages can instantly lead to reactant starvation and water flooding is an important limiting factor of PEM fuel cell efficiency and life time. Flooding appears in both cathode and anode electrodes with three mechanisms as; (a) Water generated in the cathode side of the membrane by the electrochemical reaction (ORR), (b) electro-osmotic drag and (c) over-humidified reactant gases. Anode flooding is much longer than the cathode flooding (Mollaamin et al., 2019). Although flooding in the cathode is much common compared to anode, flooding on the anode side of the membrane can also have serious consequences on the operation, performance and degradation and due to low fuel flow rates, removing H2O from anode is much more difficult compared to cathode.



Scheme 3: Schematic model of all layers including h-BN and graphene layers and their activities in a whole unit of the fuel cell

Pasaogullari has reported, anode flooding is most probable for happening at low current, low reactant flow rates and low temperatures due to the lower electro-osmotic forces (Pasaogullari and Wang, 2005). In other words proton flux is large in the anode electrode; therefore a strong electro-osmotic force pulls the H2O from anode to cathode (due to the low water content). In contrast to the inlet of the anode side, at the exit current density is lower and H_2 concentration has decreased, so, the partial pressure of water is high and closer to total anode pressure (Futerko and Hsing, 2000). Several researchers (Wang et al., 2001) have assessment various tactics and technics for water managing (Dutta et al., 2000). He et al. associated partial pressure straightly to the flooding level and considered it to be a suitable indicator for efficiency. They planned a tool for monitoring the flooding measure in PEM fuel cell with inters digitized flow field. Diperno and coworkers (Bosco and Fronk, 2000) record a USA patent for a simple way which monitors the pressure drop across the flow field to detect flooding in PEM fuel cells. Problem of

membrane dehydration is related to drying out in anode which causes a protonic resistance and consequently collapse in cell voltage. Therefore in dried situation radicals will produce and increased, to enhanced membrane degradation (Le et al., 2006). Anode dehydration is might be serious both at the inlet of the cell and at the outlet trajectory. In addition due to dehydrating conditions, the membrane leads to lower diffusion. One of the main reasons for dehydration is the strong electro-osmotic forces in the condition of high current densities where water replenishment by reactant humidification or back-diffusion is not quick enough to cope with the lack of water (Ciureanu, 2004).

2. Theoretical Background

The enthalpy of hydrogen combustion reaction or hydrogen heating amount for one mole of hydrogen can be calculated via $\Delta H = \Delta H_f^0(H2O) - \Delta H_f^0(H2) - \frac{1}{2}\Delta H_f^0\ (O2) = -286.31\ Kj/mol$. Hydrogen heating amounts are used as a measure of energies input for the fuel cells and this is the maximum value of thermal energy which can be extracted from hydrogen. In addition Gibbs free energy is given by the following equation: $\Delta G = \Delta H - T\Delta S$. which the difference between entropies of products and reactants can be calculated as $\Delta S = \Delta S_f^0(H2O) - \Delta S_f^0(H2) - \frac{1}{2}\Delta S_f^0(O2)$. The maximum electrical work is:$W_{max} = -n(emf)F = -\Delta G$ where F is Faraday's constant and "emf" is the ideal electro motor force or potential of the cell. Therefore the theoretical hydrogen/oxygen fuel cell potential or maximum voltage of fuel cells is: $emf = E = \frac{-\Delta G}{nF} = \frac{237.342\ J\ mol^{-1}}{2*98486.5\ Coulmb} = 1.231\ Volt$. The thermal efficiency is defined based on amount of useful energy released when a fuel is reacted with an oxidant (ΔG), relative to the change in stored chemical energy (ΔH) therefore The maximum theoretical yields in a fuel cell is $\eta = \frac{\Delta G}{\Delta H} = \frac{237.342}{-286.31} = \%82.9$ [5]. Based on Nernst equation a function of temperature and pressure can be applied for any fuel cells as; $emf = E_{(T,P)} = -\left(\frac{\Delta H}{nF} - \frac{T\Delta s}{nF}\right) + \frac{RT}{nF} Ln\left[\frac{P_{H_2} P_{O_2}^{0.5}}{P_{H2O}}\right]$, (1) based on this equation, in an open circuit with reactant gases the actual cell potential is decreased (usually less than 1V) and it is called open circuit voltage (OCV) . This decreasing of actual cell

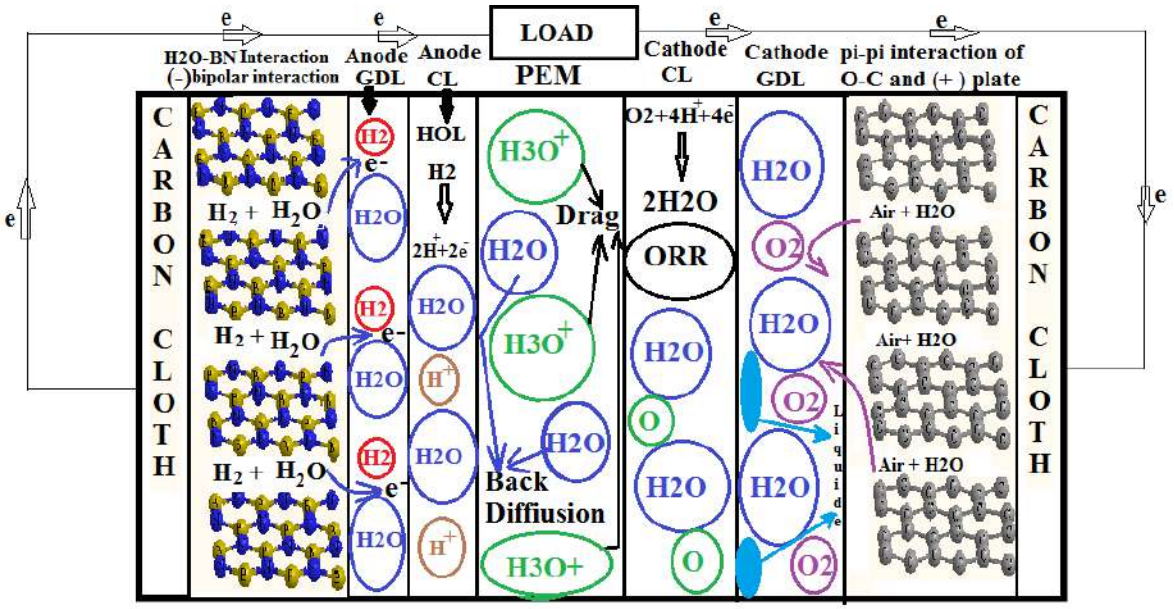
potential is due to irreversible losses and hydrogen crossover losses which often called polarization, over potential, or over voltage including activation polarization, ohmic polarization and concentration polarization. Activation polarization is associated with sluggish electrode kinetics which happens at both anode and cathode which can be expressed with Tafel equation: $\Delta V_{act} = \frac{RT}{\alpha F} ln \frac{i}{i_0}$ (2) where α is the electron transfer coefficient of the reaction at the electrodes and i0 is the exchange current density.

The ohmic polarization appears due to resistance against the flow of protons in the electrolyte and also resistance to the flow of electrons through the electrode materials as the equation $\Delta V_{ohm} = i\Omega$ where i is the current flowing through the cell and Ω is the total cell resistances consist of electronic, ionic and contact resistance. Concentration polarization is due to loss of potential because of inability of the surrounding material for maintaining the initial concentration of the bulk fluid, thus, a concentration gradient is formed. $\Delta V_{conc} = \frac{RT}{nF} \ln \left[\frac{i_L}{i_L - i}\right]$, That i_L is the limiting current. The actual cell voltage can be written as: $V_{cell} = E(T,P) - (\Delta V_{act} + \Delta V_{conc})_a - (\Delta V_{act} + \Delta V_{conc})_c - \Delta V_{ohm}$ (3) by replacing the above equations in this equation the fuel cell polarization curve is: $V_{cell} = E(T,P) - \frac{RT}{\alpha_c F} ln \frac{i}{i_{0,c}} - \frac{RT}{\alpha_a F} ln \frac{i}{i_{0,a}} - \frac{RT}{nF} \ln \left[\frac{i_{L,a}}{i_{L,a} - i}\right] - \frac{RT}{nF} \ln \left[\frac{i_{L,C}}{i_{L,C} - i}\right] - i\Omega.$ (4) Due to the activation energy barriers the polarization terms voltage collapse very fast and in the ohmic term polarization voltage falls slower due to the membrane and electrode ohmic resistance.

2.1. Modelling and simulation

The details mechanism of the PEM fuel cells are very complex due to the different and tightly phenomenon which occur within a cell-fluid-dynamic, migration, electro chemical reaction, diffusions, water transports inside polymer membrane involving both electro-osmotic drag and back diffusion, proton transports via proton-conductivities of the polymer membranes, electron conduction via electrically conductivities of the cell components, heat transfer involving both conduction via solids components of the cells

and convection of reactant gases and cooling medium, water transports both evaporation and liquids via porous catalyst layer, gas diffusion layer , and phase Changes (scheme 4).



Scheme 4.

Processing and operating of a PEM fuel including h-BN and cell Modelling is needed for describing the basically phenomenon to evaluate the cells steady-state and dynamic behavior. However, the complex mechanism inside the fuel cell causes challenging in some models involving reactants, cooling, and humidification and conditioning systems. Models are able to predict fuel cell efficiency under different operating situations and optimization and designing of control systems (Rowe and Li, 2001). In past decades, several of PEM fuel cell models are defined to the purpose of gas channel, gas diffusion layers, catalyst layers and polymer membrane of electrolyte (Siegel, 2008). Models can also be categorized based on their dimension, single, double or triple which can be considered either isothermal or non-isothermal (Yao et al., 2004). Single cell model explain the electrochemical and transporting processes in the fuel cell component including pressure drop, flow distribution, and temperature profile in the gas channel (Pukrushpan et al., 2004). This simulation, quantitatively explain interaction between physical and electrochemical phenomenon which can also be divided into two sections,

first an empirical simulation for prediction how the fuel cell voltages change with the current densities with polarization curves and second principle simulation is built- up from ordinary differential equations or solving partial differential equations (PDEs) including distributed parameter, Stefan-Maxwell convection and diffusion account for species conservation. Based on Darcy's law, the principle of mass conservation is applied to simulate reactant concentration (Gurau, 1998).

Recently, in advance simulation, two-dimensional and three dimensional simulations have been developed. The two-dimensional simulation can be separated into two classes, first one explain the plane perpendicular to the flow channels and second describes the direction along the flow channel (Karimi, 2011) An extended simulation of 3-dimensional, 2-phase, non-isothermal unit cell systems were investigated by Tao for performing parameters sensitivities examination. Generally, simulated systems are lumped data of parameters for evaluating fuel cell efficiency under various operating situations for any controlling as a function of time through solving differential equations (ODEs) (Tao et al., 2006). Pukrushpan investigated a system including fuel cell stack, hydrogen supply, air supply, cooling and the humidification systems with a constant temperature due to the dynamics variables (Pukrushpan et al., 2004).

3. Computational details

Calculations were accomplished via GAMESS-US package (Schmidt et al., 2004). DFT methods such as m062x, m06-L, and m06 for the non-bonded interaction of fuel cell layers including G/h-BN// h-BN / G have been used. The m062x, m06-L and m06-HF are new DFT functional with a good correspondence in non-bonded calculations which are useful for estimating the energies of distance between layers in the fuel cells simulation (Zhao and Truhlar, 2008). The double ζ-basis set with polarization orbitals (DZP) were applied for calculated for inputs and outputs parameters for the simulation fuel cells. Graphene is known to relax in 2-D honeycomb structures and the h-BN also will be assumed to have a similar structure. A monolayer of graphene containing 76 atoms with zigzag edges was optimized and allowed to relax to its minimum energies structures. The

edges were saturated with the hydrogen atoms for neutralizing the valance of terminal carbon, reducing the edge effect after relaxation. The C-C-C angle was calculated to be around 120.0 and the C-C and C-H bound lengths are about 1.422 and 1.086, respectively which are corresponds to reported paper (Zhao and Truhlar, 2008). Generalized gradient approximation (GGA) is adopted. In our model, the electrodes have been doped by various percentages of boron atoms which are likely to be adjusted by the surrounding host C atoms. Therefore, when the graphene sheet is doped with one boron atom, the boron atom also undergoes the sp^2 hybridization (Perdew and Burke, 1996). Using the computational procedure as stated above, the electronic properties, especially the band structure can be calculated. Via doping boron atoms in graphene, Fermi levels shifts significantly below the Dirac point resulting in a p-type doping. This would break the symmetry of graphene into two graphene sub-lattices due to presence of the B atoms which would eventually lead towards a change of the behavior of graphene from semimetal to conductor which significantly is useful for fuel cells. The charge transfer and electrostatic potential-derived charge were also calculated using the Merz-Kollman-Singh (Besler et al., 1990; Chirlian and Francl, 1987). We have also extracted the charge density profiles from first-principles calculation through an averaging process described.

Conclusion

For the model of these fuel cells, the adsorption energies of various number of H_2, O_2 over the surfaces of graphene and h-BN sheets have been calculated both in the anode and cathode plates (Figs.1 & 2).

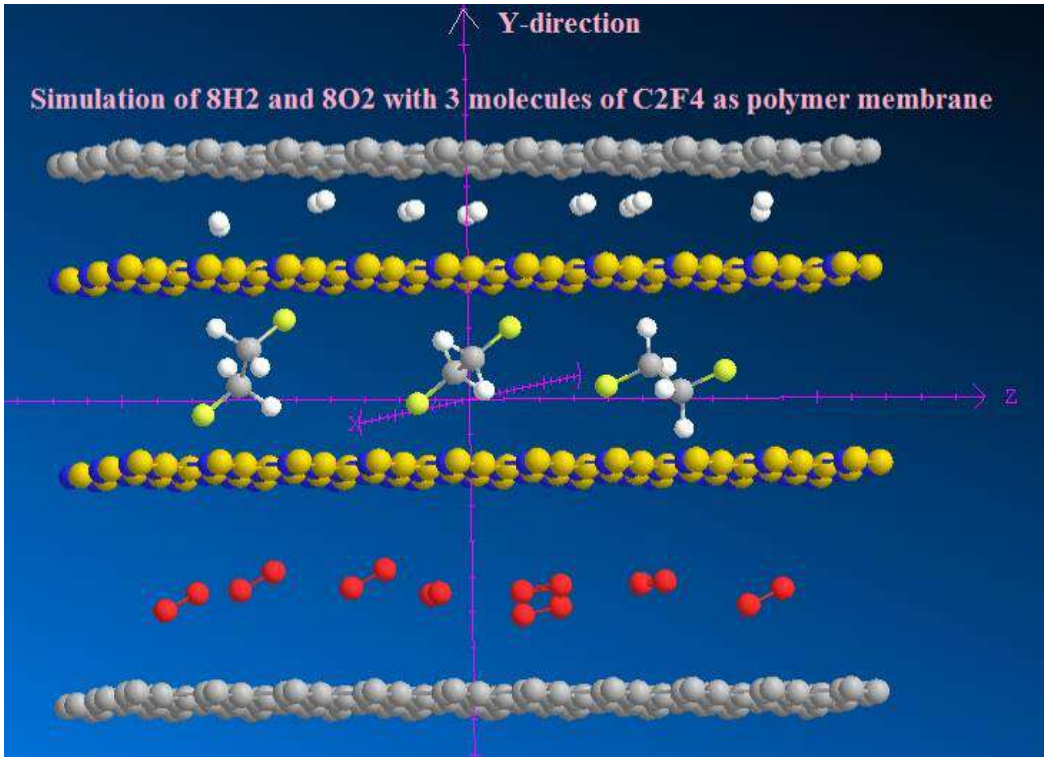


Fig. 1: Adsorption of $8H_2$, $8O_2$ and 3 C_2F_4 as polymer membrane for a unit cell.

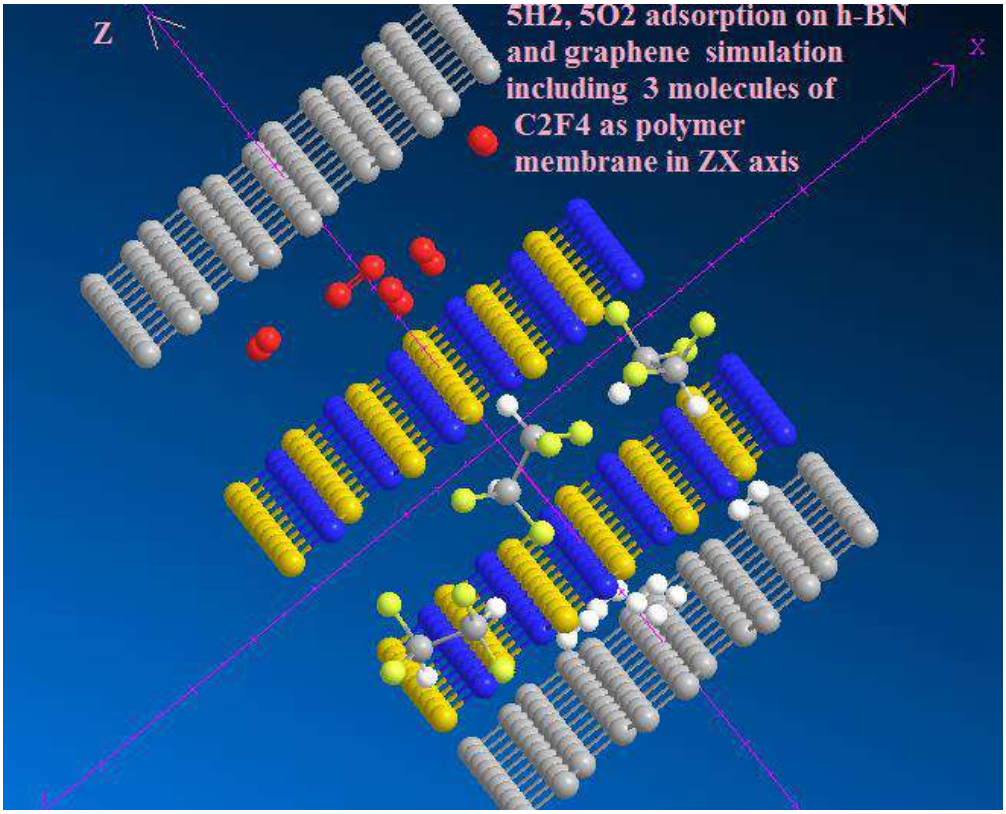


Fig. 2: Adsorption of $5H_2$, $5O_2$ and 3 C_2F_4

Initially, we assume that the adsorption is Langmuir uniformly both on graphene and h-BN sheet. The adsorption energies can be calculated as follows: $E_{adsorb}^{H2} = \frac{1}{n}\left(E_{total} - E_{h-BN} - nE_{H_2}\right) + E_{BSSE}$ Where BSSE is basis set error position. We obtain the stable situation after the modified system is fully relaxed. The activation energy barrier for O2 diffusion from h-BN to graphene found to be as low as 0.05 eV. The barriers for the rest of the considered path are also quite low. The adsorption energies is are listed in table 1. The best simulation was found for 5; 5; 3 mole ratio of H_2, O_2 and C_2F_4 (Table 1).

Table 1: The adsorption of H2 and N2 on surface of graphene

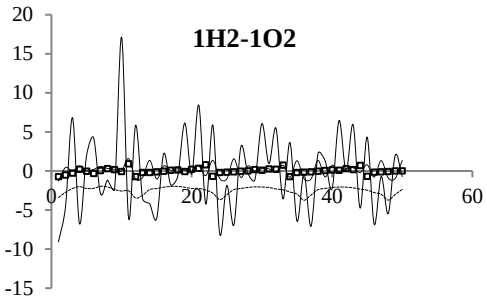
No. H_2	E_{adsorb}^{H2} eV/H_2	E_{adsorb}^{O2} eV/O_2
$1H_2$	-0.65	-0.36
$2H_2$	-0.58	-0.38
$3H_2$	-0.54	-0.44
$4H_2$	-0.61	-0.39
$5H_2$	-0.69	-0.48
$6H_2$	-0.57	-0.41
$7H_2$	-0.55	-0.43
$8H_2$	-0.51	-0.46
$9H_2$	-0.54	-0.42
$10H_2$	-0.56	-0.39

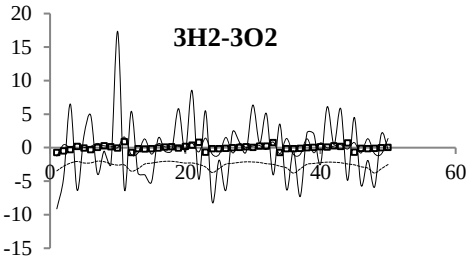
For any further adsorption model, the validation of the Langmuir-Freundlich multilayer isotherm model is done by using breakthrough experiments with binary mixtures of H_2/O_2, O_2/N_2 and H_2/H_2O (steam) and, a few component mixture composed by H_2/ $O_2/H_2O/N_2$. Breakthrough simulations are performed for different pressures, flow rates and different number molecules of adsorbent and also different sheets including graphite and h-BN. The results are then compared with experimental data from the

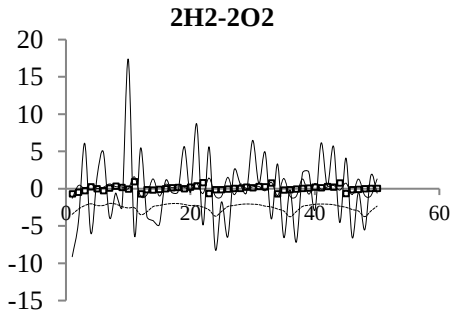
literature. The Multisite Langmuir multilayer isotherm model and simulations with a four component mixtures of H_2/ O_2/H_2O/N_2 and are listed in table 2.

Table 2. Langmuir multilayer isotherm model of H_2/ O_2/H_2O/N_2

Gas	K_1 $Mol.Kg^{-1}.K^{-1}$	K_2 $Mol.Kg^{-1}.$ $K^{-1}T^{-1}$	K_3 atm^{-1}	k K
Graphene				
H_2	16.9	$-2*10^2$	$0.6*10^4$	1200
N_2	1.7	$-0.8*10^2$	$5*10^6$	320
O_2	30.1	$-9.0*10^2$	$2.1*10^4$	-650
H_2O	27.5	$-7.0*10^2$	$9*10^5$	1002
h-BN				
H_2	1.3	$-1.5*10^2$	$25.1*10^4$	450
N_2	4.8	$-0.65*10^2$	$5.6*10^4$	1530
O_2	11.8	$-3.1*10^2$	$199*10^4$	730
H_2O	10.3	$-1.8*10^2$	$1.6*10^4$	209


1H2-1O2
20
15
10
5
0
-5
-10
-15
0
20
40
60


3H2-3O2
20
15
10
5
0
-5
-10
-15
0
20
40
60


2H2-2O2
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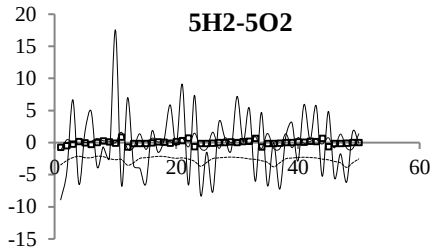
5H2-5O2
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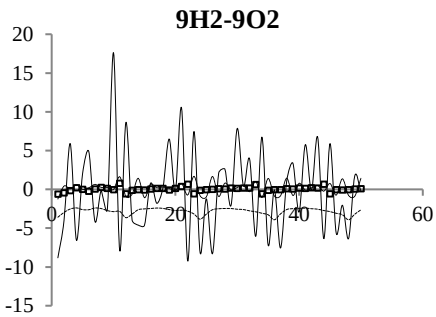
9H2-9O2
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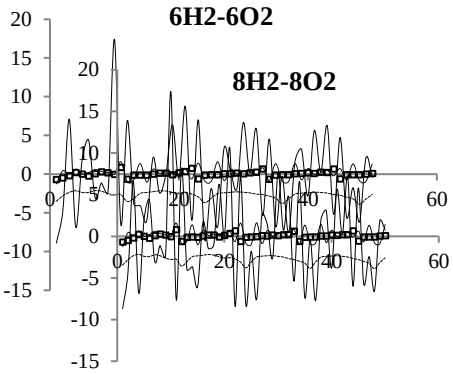
6H2-6O2
8H2-8O2
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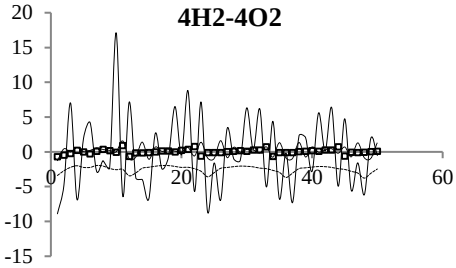
4H2-4O2
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-5
-10
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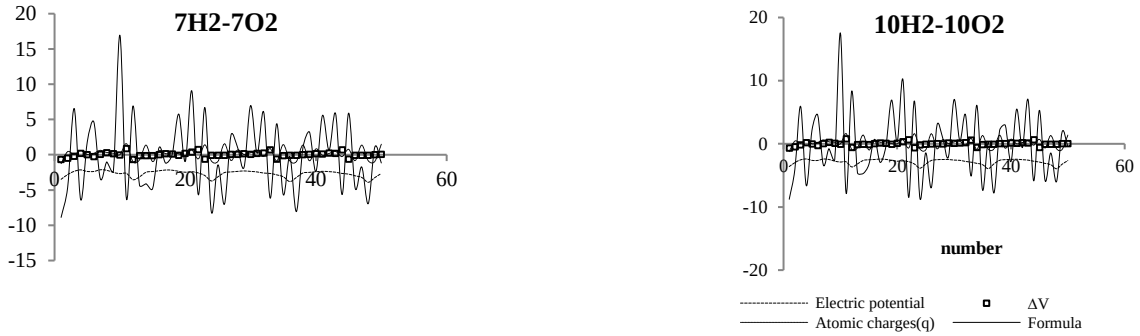

Fig.3 Electrical potential and Difference voltages of 10 situations of H2 and O2 adsorption versus distance

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Investigation about electrostatic three-wall carbon nanotubes (MWCNT), including doping with BN: a model for the nano capacitor

Nabieh Farhami*
Majid Monajjemi**

ABSTRACT

Three-walled boron & nitride nanotubes are used for a theoretical study of a cylindrical molecular capacitor, including an inner cylinder with a positive charge distribution and an outer cylinder with a negative charge distribution. Due to the semiconductor characteristic and dielectric functionality of SWBNTs, DWBNTs and TW (B&C) NTs can be used as a capacitor. Although the SWBNTs @ SWCNTs behave like Nano cylindrical capacitors, we have shown in this study that a dopant of BN in the inner cylinder reduces the energy gap and yields a better capacitance. The dopant of BN in the outer cylinder results in an inverse charge distribution (outer is positive and inner is negative). Therefore under these circumstances, the term capacitor would be meaningless, thought, the gap and the interaction energy decreases compared to the non-dopant form of those capacitors. Density functional theory (DFT) calculations have performed for the structure and stability of three wall carbon Nano tubes (TW (BN&C) NTs). In this work, it was calculated the geometrical structure, and stability to predict NMR and thermodynamics parameters. A mixing of SWBNNTs @ DWCNTs has been modeled and calculated for the suitable structures to storage the H_2 molecules for increasing the dielectric. We have found these kinds of Nano-structures are useful for maximum storages of charges compare to other cylindrical capacitor.

KEYWORDS: three wall carbon nanotubes (TWCNTs), BN doping, Nano capacitor, cylindrical molecular capacitor.

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Investigación acerca de la electrostática de tres nanotubos de carbono de pared (MWCNT), incluido el dopaje con BN: un modelo para el condensador nano

RESUMEN

Los nanotubos de boro y nitruro de tres paredes se utilizan para un estudio teórico de un condensador molecular cilíndrico, que incluye un cilindro interno con una distribución de carga positiva y un cilindro externo con una distribución de carga negativa. Debido a la característica semiconductora y la funcionalidad dieléctrica de los SWBNT, los DWBNT y los TW (B&C) NT se pueden usar como condensadores. Aunque los SWBNTs & SWCNTs se comportan como condensadores cilíndricos nano, hemos demostrado en este estudio que un dopante de BN en el cilindro interno reduce la brecha de energía y produce una mejor capacitancia. El dopante de BN en el cilindro externo da como resultado una distribución de carga inversa (el exterior es positivo y el interior es negativo). Por lo tanto, en estas circunstancias, el término condensador no tendría sentido, aunque el espacio y la energía de interacción disminuyan en comparación con la forma no dopante de esos condensadores. Los cálculos de la teoría funcional de la densidad (DFT) se han realizado para la estructura y la estabilidad de los tubos nano de carbono de tres paredes (NT (BN&C) NT). En este trabajo, se calculó la estructura geométrica y la estabilidad para predecir los parámetros de RMN y termodinámica. Se ha modelado y calculado una mezcla de SWBNNTs @ DWCNTs para las estructuras adecuadas a objeto de almacenar las moléculas de H2 para aumentar el dieléctrico. Hemos encontrado que este tipo de nanoestructuras son útiles para el almacenamiento máximo de cargas en comparación con otros condensadores cilíndricos.

PALABRAS CLAVE: nanotubos de carbono de tres paredes (TWCNT), dopaje BN, condensador nano, condensador molecular cilíndrico.

Introduction

Although much study has been done for nanotube carbon phenomenon, there are a few studies for MWCNTs such as TWCNTs (Bourgeois et al., 2000). The carbon nanotube (CNT) is a representative Nano-material. CNT is a cylindrically shaped carbon material with a Nano-metric-level diameter. Its structure, which is in

the form of a hexagonal mesh, resembles a graphite sheet and it carries a carbon atom located on the vertex of each mesh. The sheet has rolled and its two edges have connected seamlessly (Iijima Sumio, 1991).

Although it is a commonplace material using in pencil leads, its unique structure causes it to present characteristics that had not found with any other materials. CNT can be classified into single-wall CNT, double-wall CNT and multi-wall CNT according to the number of layers of the rolled graphite (Iijima Sumio, 1991). The type attracting most attention is the single-wall CNT, which has a diameter deserving the name of "nanotube" of 0.4 to 2 nanometers. The length is usually in the order of microns, but single-wall CNT with a length in the order of centimeters has recently released (Frackowiak, Béguin, 2002). CNT can be classified into single-wall CNT, double-wall CNT and multi-wall CNT according to the number of layers of the rolled graphite. The type attracting most attention is the single-wall CNT, which has a diameter deserving the name of "nanotube" of 0.4 to 2 nanometers (Bourgeois et al., 2000).

The length is usually in the order of microns, but single-wall CNT with a length about centimeters have recently released. The extremities of the CNT have usually closed with lids of the graphite sheet. The lids consist of hexagonal crystalline structures (six-membered ring structures) and a total of six pentagonal structures (five-membered ring structures) placed here and there in the hexagonal structure (Monajjemi et al., 2011). The first report by Iijima was on the multiwall form, coaxial carbon cylinders with a few tens of nanometers in outer diameter. Two years later, up to now, single walled nanotubes were reported in various works (Iijima Sumio, 1991). SWCNTs have considered as the leading candidate for Nano-device applications because of their one-dimensional electronic bond structure, molecular size, and biocompatibility, controllable property of conducting electrical current and reversible response to biological reagents hence SWCNTs make possible bonding to polymers and biological systems such as DNA and carbohydrates. Boron nitride

nanotube (BNNTs) has attracted many interests due to their large gap semi conducting character. Boron nitride (BN) is a structural existing in cubic (diamond-like), hexagonal (graphite-like), turbo static, and amorphous forms .these compounds have been produced by a variety of methods, such as arc melting, high temperature chemical reaction, carbon nanotube templates, and laser ablating. The most attention has been focused on the development of new methods for the production of nanotube and inorganic fullerene of other materials (Lee et al., 2009).

In addition, theoretical calculations have been described the possible existence of small BN clusters. Theoretical studies have been performed for BN doped in CNTs which it has been found that a structure built from squares and hexagons is more stable than those built from pentagons and hexagons. This is because in the second case less stable B-B and N-N bonds are formed (Derakhshandeh, 2015). The most stable TWCNTs structure is built from CNTs doping with BN. In this work, we focused on TWCNTs and TWC (BN) NTs Nano-con. Our aim was to obtain the global minimum energy structure (Fig.1). For this structure, we use the hybrid B3LYP exchange-correlation functional within density functional theory. Primary, structure optimization calculated and then Nuclear Magnetic Resonance (NMR) parameters by density Functional Theory (DFT) method calculated on the optimized structure. In material sciences Boron nitride, which appears in a manifold of crystalline modifications, has been an extremely practical material with hexagonal and cubic boron nitride as most outstanding materials (for doping). The BN cluster is a polar molecule and BN doped in nanotubes have an inert chemical structure. We can see that there is a negative charge at nitrogen atom and a positive charge at boron atom, so we can use an electrophilic or nucleophilic reagent as a solution for BN clusters (Farhami et al., 2017).

BN nanotubes are very suitable for composite materials because these structures have a higher temperature resistance to oxidation than the carbon nanotubes. All the BN nanotubes are semiconductors. The BN doped in nanotubes

have the band gaps which can be greater than 2 eV for most tubes also we know that the smallest carbon nanotubes are semiconductor and these structures obtain the properties of graphite when the diameter of these structures increases but BN nanotubes are semiconductors without attention to the diameter. On the basis of the similarities in characteristics between carbon and BN-based (BN=boron nitride) substances, BN-based nanotubes can be stable and therefore their electronic structure can be studied. The comparison between BN nanotubes and carbon nanotubes shows that BN nanotubes have more interesting characteristics for doping in carbon nanotubes. Recently the mixing of boron nitride (BNNTs) and (CNTs) in a nanoscale particles have been investigated and these structures are made up of conical shells without any seamless. Most of the studies about these compounds have been done so far with carbon structures. Considering the above mentioned, (BN-C) NTs nanotubes are very important and interesting for new research, especially for H2 storage and can open a huge spectrum in the field of theoretical and experimental research. In the Fig.1 structure of TWCNTs is shown and this particular nanometer configuration has been proposed in this research (Madani et al., 2017).

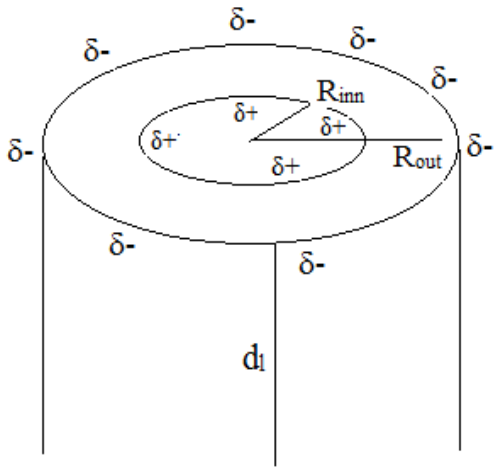
1. Theoretical background

Our system is similar to narrow seamless graphitic carbon nanotube cylinders, showing an unusual combination of a nanometer-size diameter and millimeter-size length. This topology, combined with the absence of defects on a macroscopic scale, gives rise to uncommon electronic properties of individual single-wall nanotubes which can be metallic, semiconducting or insulating, depending on their diameter and chirality.

Consider a cylindrical capacitor of length "d_l", inner radius "R_{inn}", outer radius "R_{out}", and charge Q = $d_l.q_\lambda$ which q_λ is the charge per unit length (magnitude) on each cylinder (Schemel). Assume "d_l" ›› "R_{out}" and Neglect fringing and electric field between cylinders: use Gauss' law $E[2\pi r d_l] = \frac{d_l.q_\lambda}{\varepsilon_0} \Rightarrow E(r) = \frac{q_\lambda}{2\pi\varepsilon_0 r}$ **(1)** and

electric potential between cylinders: use V_{out} =0 $\Rightarrow V(r) = -\int_{R_{inn}}^{r} E(r)dr = \frac{-q_\lambda}{2\pi\varepsilon_0}\int_o^r \frac{dr}{r} = \frac{-q_\lambda}{2\pi\varepsilon_0} ln\frac{r}{R_{inn}}$ (2)

And $V = V_+ - V_- = V_{(inn)} - V_{(out)} = \frac{Q}{2\pi\varepsilon_0 L} ln\frac{R_{out}}{R_{inn}}$ **(3)** and capacitance for cylindrical geometry is: $\bar{C}_g \equiv \frac{Q}{V} = \frac{2\pi\varepsilon_0 d_l}{ln\frac{R_{out}}{R_{inn}}}$ **(4).** Where$\Delta V_{(inn-out)}$, is a positive quantity because $2kln\left(\frac{R_{out}}{R_{inn}}\right)$ is a positive quantity. This is due to the fact that the outer layer is at a higher potential than the inner layer. In our system the calculation of the Nano-cylindrical capacitors can be obtained from the electrical potential $\emptyset(r,Z)$ in the space between two coaxial cylinders of radii R_{inn} and R_{out} finite length d_l in the z direction $(0 \le z \le d_l)$. We have assumed that the geometrical capacitance in our system is a function of d_l ,R_{inn} R_{out} or$C_g = F(d_l, R_{inn}, R_{out})$.



Scheme 1: A schematic of a cylindrical Nano-capacitor

The capacitance in our model can be calculated via $C_g = \frac{2\pi R_{inn}\varepsilon_0}{V}\int_0^{d_l}(\frac{\partial\emptyset}{\partial r})_{r=R_{inn}}dz$ **(5)** in a finite nanometer-scale cylindrical capacitor (based on the classical electrodynamics). However, on very small scales the quantum corrections will appear. It is known that typical inhomogeneous electric fields used in the polarizability measurements for metallic clusters are in the order of 10^5V cm^{-1}

and field gradients are approximately 10^5 V cm^{-2}. These fields induce a dipole moment and slightly deformed clusters. Therefore, to strictly preserve the shape of a nanometer-scale capacitor, weaker and homogeneous fields should be applied in electronic devices. To calculate the capacitance in eq.4 and eq.5 for $(\bar{C}_g\ , C_g)$, the potential difference applied between two cylindrical plates V=$V_{(inn)} - V_{(out)}$ has been calculated by the total different of atomic point charges versus the bond distances. The original total DOS (TDOS) of this system has been calculated based on, $TDOS(E) = \sum_i \delta(E - \varepsilon_i)$ **(6).** Where the eigenvalue "ε" is set of single-particle Hamilton and "δ" is the Dirac delta function which can be yielded after replacing Gaussian. There is another Gaussian function as: $G(X) = \frac{1}{c\sqrt{2\pi}} e^{\frac{-x^2}{2c^2}}$ Which the FWHM ($c = \frac{FWHM}{2\sqrt{2ln2}}$) stands for "full width at half maximum", an adjustable parameter in multi-wave function program where the larger FWHM results in a smoother looking TDOS graph, making the analysis to be performed easier. The normalized Lorentzian function is defined as $L(X) = \frac{FWHM}{2\pi} \frac{1}{x^2 + 0.25FWHM^2}$ Pseudo-Voigt function is weighted as linear combination of Gaussian function and Lorentzian function $P(x) = w_{gauss}\, G(x) + (1 - w_{gauss})\, L(x)$. The curve map of broadened partial DOS (PDOS) and overlap DOS (OPDOS) are valuable for visualizing orbital composition analysis PDOS function of fragment which *A* is defined as $PDOS_A(E) = \sum_i \Xi_{i,A}\, F(E - \varepsilon_i)$ **(7)** where $\Xi_{i,A}$ is the composition of fragment "A" in orbital *i*. The OPDOS between fragment "A" and "B" is defined as$OPDOS_{A,B}(E) = \sum_i X^i_{A,B}\, F(E - \varepsilon_i)$ **(8)** where $X^i_{A,B}$ A, B is the composition of total cross term between fragment A and B in orbital. Both original and broadened TDOS/PDOS/OPDOS are shown in this study. It is important to note that the height is only meaningful for lines (original data) and not for curves and left-axis and right-axis correspond to TDOS/PDOS and OPDOS respectively (Lu, Chen, 2012).

2. Computational details

Calculations were performed using GAMESS-US packages as well as some other parallel ab-initio and molecular mechanics programs. In this study, we have mainly focused on getting the optimized structures for each tube from DFT methods including the m05 and m06 groups. The m062x, m06-L, and m06-HF are a novel Meta hybrid DFT functional with a good correspondence in non-bonded calculations and are useful for calculating the energies of the distance between two coaxial cylinders of radii R_{inn} and R_{out} in the cylindrical capacitor. ONIOM methods including 3 levels of 1-high calculation (H), 2-medium calculation (M), and 3-low calculation (L) have been performed in our study. The ab-initio and DFT methods are used for the model system of the ONIOM layers and the semi empirical methods of Pm6 (including pseudo=lanl2) and Pm3MM are used for the medium and low layers, respectively. The semi empirical methods have been used in order to treat the non-bonded interactions between two parts of SW-BN-NTs and SWCNTs cylinders. M06 and m06-L (DFT) functional are based on an iterative solution of the Kohn-Sham equation from density functional theory in a plane-wave set with the projector-augmented wave pseudo-potentials.

The Perdew-Burke-Ernzerhof (PBE) exchange-correlation (XC) functional of the generalized gradient approximation (GGA) has also been used. The optimizations of the lattice constants and the atomic coordinates are made by the minimization of the total energy. It is interesting to note that the tubular morphology of SW-BN-NTs is fundamentally different from the usual tubular forms of carbon and boron nitride (BN) nanotubes. In the outer shell, the more electronegative atoms (N atoms) are pushed radially outward and the more electropositive atoms (Ga atoms) are displaced inward. In the inner shell, the opposite phenomenon occurs and the Ga atoms move outward while the N atoms move inward. This result for BN nanotubes is expected since the overlap between the B and N, PZ orbitals is weaker. According to the Mulliken population analysis, a considerable amount of electron charge is

transferred from Ga to N, resulting in an ionic bonding nature. N loses some *s* electrons and gains more *p* electrons, whereas Ga loses more *p* than *s* electrons. The average B-N bond length in the optimized structure of SW-BN-NTs in our calculation is between 1.9-1.945 A°, which is shorter than the bond length of 1.95A ° in the crystal structure of Wurtzite. A fixed SW-BN-NTs geometry with BN bond lengths of 1.45 Å is chosen with no further geometry optimization.

The outer ring, initially placed at the center of the inner tube, is rigidly axially been shifted and rotated around the fixed inner shell. At each inter-tube configuration, a single-point calculation is carried out and the total energy is recorded. The resulting sliding-rotation energy surfaces are used to fix our model in a better position. We employed density functional theory with the van der Waals density functional to model the exchange-correlation energies of SW-BN-NTs. The double ζ-basis set with polarization orbitals (DZP) were used for tubes. For non-covalent interactions, the B3LYP method is unable to describe the van der Waals interactions, e.g., the capacitor systems by medium-range interactions such as the interactions of two cylinders. The B3LYP and most other functional are rather insufficient to illustrate the exchange and correlation energy for distant non-bonded medium-range systems. Moreover, some recent studies have shown that inaccuracy for the medium-range exchange energies leads to large systematic errors in the prediction of molecular properties. Therefore, we further calculated the interaction energy between two coaxial cylinders of radii R_{inn} and R_{out} for each tubes in our structures (The number of nanotubes was varied to examine size-dependent electrical properties) using other ab-initio method. The interaction energy "ΔE_S" between two cylinders of the capacitor has been calculated via an Mp6 method based on the eq.6. $\Delta E_S(eV) = E_{total} - \left(E_{SW-GaN-NT(inn)} + E_{SWCNT(out)}\right)$ **(9)** (Table 1).

The charge transfer and the electrostatic potential-derived charges were also calculated using the Mullikan charge distribution the representative atomic charges for molecules should be computed as average values over several molecular

conformations. A detailed overview of the effects of the basis set and the Hamiltonian on the charge distribution can be found in previous studies. We have also extracted the charge density profiles from the first principle calculations through an averaging process. DFT (density functional theory) is one of the computational methods which can be used in different systems and it is more useful for some calculations than other methods. It is clear that basis sets are vast various. The Gaussian 98 program was run to obtain the best prediction of this particular structure. Also all Ab-Initio and DFT (density functional theory) calculations were done with the Gaussian 98 program. Frequency analyses were carried out to show that the optimized structures are true minima or transition states on the potential energy surfaces of a specific structure without imaginary frequencies. In this work, geometry optimizations in the gas phase for TWCNTs were performed at density functional theory (DFT) level with B3LYP and Ab-Initio with HF methods in different basis sets at the temperature of 298.15K.

The parameters were calculated for TWCNTs in the gas phase in different methods and basis sets include thermodynamic and NMR parameters. The chemical shielding shows the phenomenon which is dependent on the secondary magnetic field which is built by the induced movements of the electrons which encompass the nuclei. The chemical shielding is built by a three-by-three matrix which is biodegraded into a single scalar term, three antisymmetric pseudo vector components, and five components which correspond to a symmetric tensor. It can be observed the single scalar and the five symmetric tensor elements in the normal NMR spectra of the solids. The chemical shielding tensor includes the chemical shift isotropy (CSI) and chemical shift anisotropy (CSA) and the anisotropy ($\Delta\sigma$) of the tensor, the shielding tensor asymmetry parameter (η) and chemical shift (δ) are calculated. The thermodynamic parameters that were calculated in this research are Gibbs free energy, enthalpy, internal energy (It is clear that the sum of zero point energy (ZPE) and thermal energy is internal energy.) and entropy then these reports

were compared with each other in order to obtain the best results. These results were reported in tables.

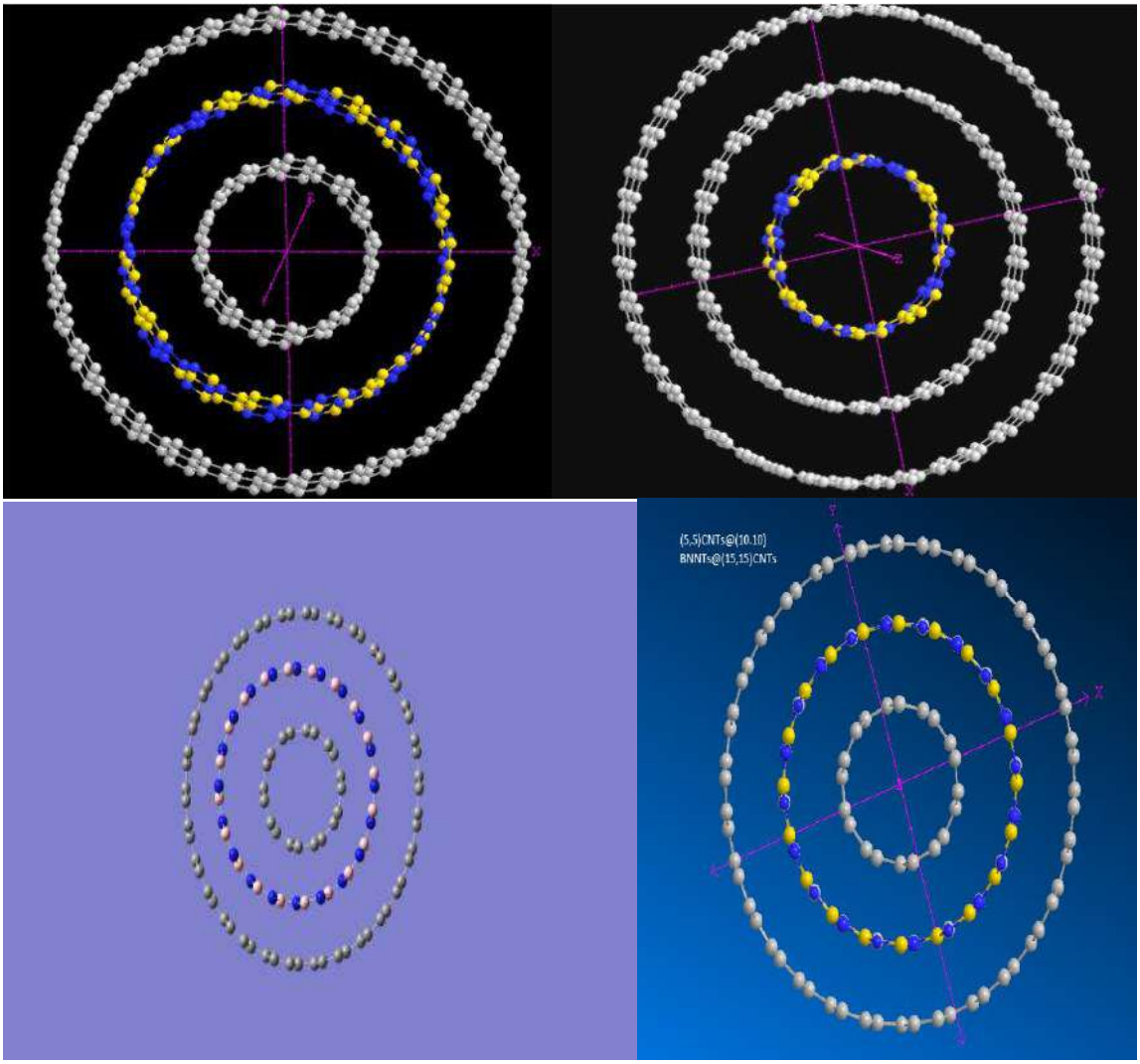


Fig.1: Optimized of Various TW(C&BN)NTs

3. Results and Discussion

The 3D BN tubes in various diameter and chirality are designed for finding a stable form inside the SWCNTs. The stability depends on the distance between inner

radius "R_{inn}", and outer radius "R_{out} in one hand and the chirality on other hand Table 1.

Energies and HOMO LUMO for several capacitors are listed in Table 1.

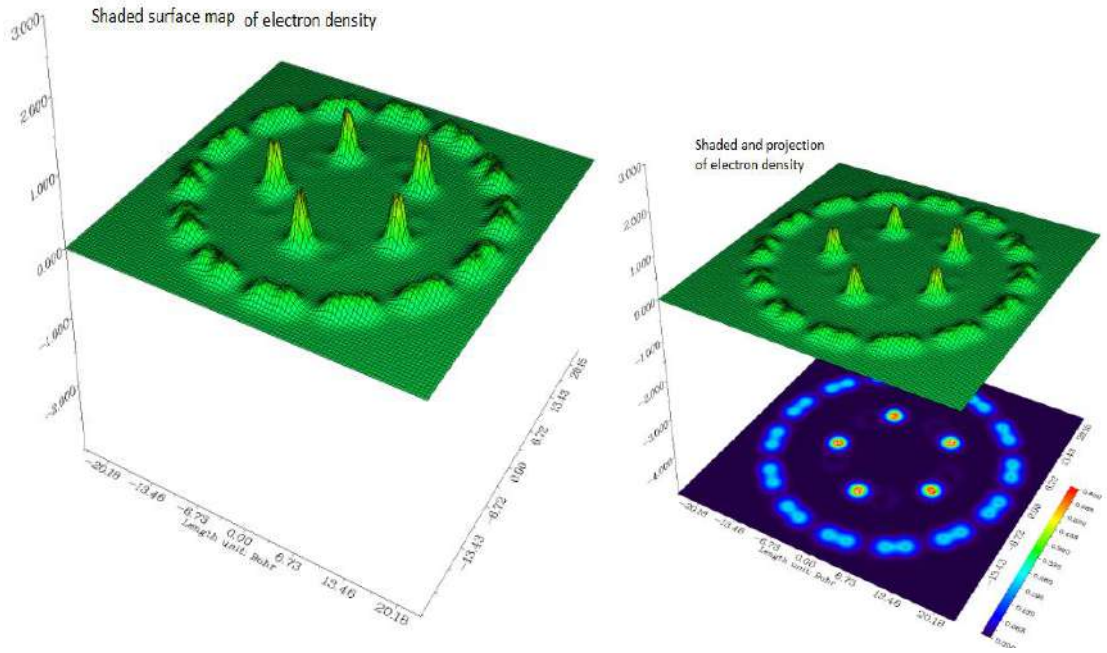


Fig. 2: Shaded surface map of cylindrical capacitor

Table 1. The band structure, Fermi level energy, stability and relative energy of the C (m, m) NTs @ C (n, n)NTs structures, including 7 molecule of BN dopant in outer cylinder. And 3 molecule of BN dopant in inner cylinder.

CNTs@CNTs	Fermi energy	HOMO	LUMO	Gap energies	Relative energies	Stability energy	R(in)-R(out)
(4,4)@(9,9)	-814.2	-0.310109	-0.215009	249.68	-	-5.53 eV	3.58
(5,5)@(10,10)	-901.7	-0.34345	-0.228012	303.15	+0.057903	-0.69 eV	4.53
(3,3)@(7,7)	-913.5	-0.34795	-0.240903	281.06	-1.9068974	-4.39 eV	3.58
(4,4)@(11,11)	-905.6	-0.34494	-0.227262	308.98	0.0000000	+0.25 eV	6.37
(5,5)@(12,12)	-850.9	-0.324091	-0.227069	254.72	+0.522609	+10.00 eV	6.39

The differences in the band structure and Fermi level energy of different tubes have been calculated. Furthermore, we have presented the number of states in unit energy interval through density of states (DOS) (Table 1 and Figs.2 & 3). Since the energy levels are contiguous and our system is isolated (the energy levels are discrete), DOS was plotted as a curved map and we have considered those graphs as a tool for analyzing the nature of electronic structure in our systems. The original total DOS (TDOS) of our system was calculated based on eq.6 and are shown in We have calculated the amount of charge on constituent B and N atoms in our systems by performing the Mulliken atomic charges.

The SWBNNT in the form of inner cylindrical are semiconductors due to the existence of an energy gap in the range of (250-310) KJ/mol (Table1) which are between the valence bands and the conductor bands. The (n,n) and (m,n) single-walled boron nitrogen nanotubes (SWBNNTs) that have similar diameter . The partial density of states (PDOS) of different contributions of B and N are plotted in Fig2-5 with the total DOS for comparison. The data for interaction energy shows that the (3, 3) @ (7, 7) DWBNNTs have a stable form comparing to other systems which yields a suitable charge transfer for the Nano capacitor.

The calculated values of charge transfer for (3, 3BNNTs @ (7, 7) CNNTs, (3,3)BNNTs @ (7, 7)CNNTs and (3, 3)BNNTs @ (7, 7)CNNTs from inner to outer tubes is found to be 1.02, 0.47 and 1.22 electrons respectively, which is an acceptable value (Table2) and it is negligible for the (5, 5) @ (12, 12) structures due to their unstable forms. This analysis clearly indicates that a significant amount of charge is transferred from inner tubes which are closed to outer tubes. However the values of -q may scatter owing to the ambiguities in placing boundary between Zn and O in the structure.

Table 2. Δ(stability energy) and charge distribution based on the geometry of BN(m, m)NTs @ C(n, n)NTs structures

BNNTs @CNNTs	$Ln(R_{OUT}/R_{inn})$	Σ Q(+)	Σ Q(-)	Δ(stability energy)
(3,3)@(7,7)	0.80	+1.07	- 1.01	-4.19 eV
(4,4)@(9,9)	0.79	0.09	-0.08	-0.99 eV
(4,4)@(11,11)	0.99	0.11	-0.08	+0.35 eV
(5,5)@(10,10)	0.61	0. 04	-0. 04	-0.60 eV
(5,5)@(12,12)	0.80	0.06	-0.05	+11.00 eV

Table3: Several DFT methods including two levels of of DFT/Semi empirical

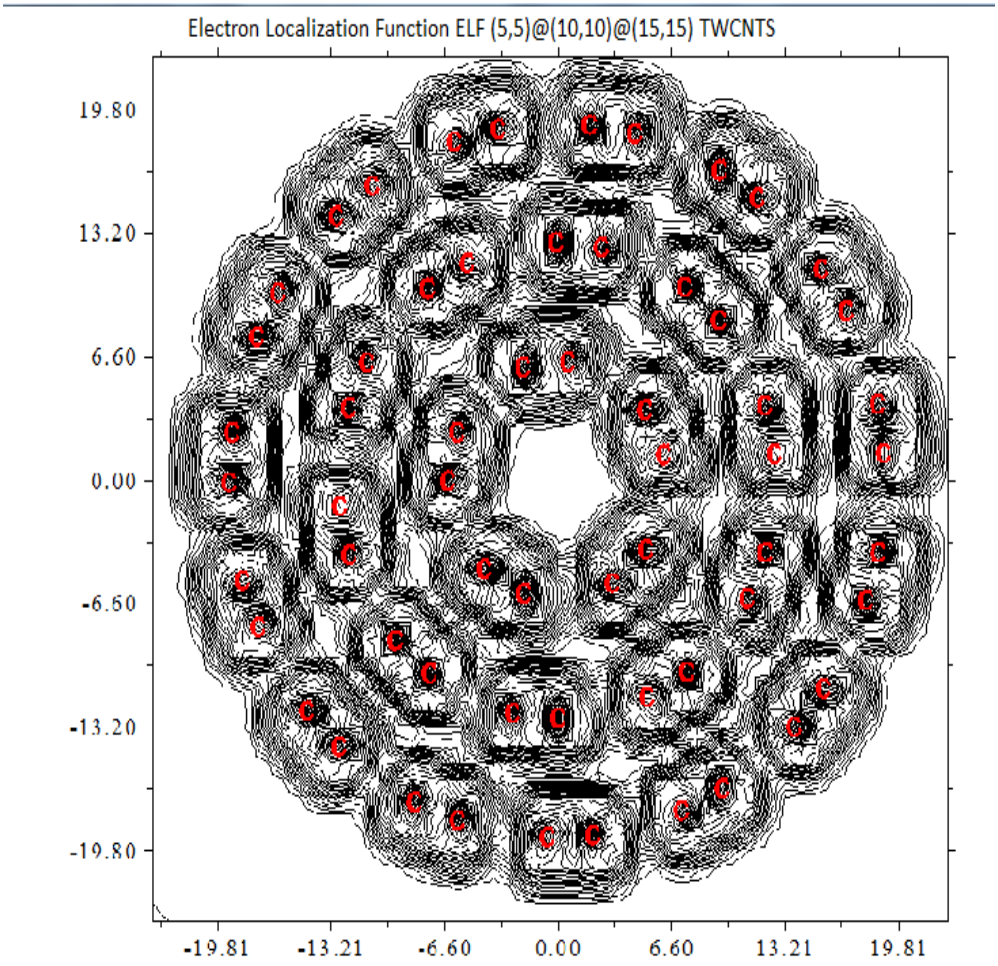
Methode	Σ Q(out)	Σ Q(inn)	Fermi energy	Partial charges	HOMO	LUMO	Gap
M06HF/PM6	-0.42	+0.42	-814.3	**±0.47**	-0.31011	-0.21500	249.6
M06/PM6	-0.44	+0.44	-814.1	**±0.46**	-0.310109	-0.21500	249.5
M052x/PM6	-0.47	+0.47	-814.4	**±0.45**	-0.31011	-0.21500	249.7
M062x/PM6	-0.43	+0.43	-817.0	**±0.62**	-0.31119	-0.211091	-262.6
M05/PM3MM	+0.03	-0.03	-890.6	**±0.54**	-0.339219	-0.07527	692.7

Table4. The dielectric constant and capacitance C(g) for inner and outer BN dopant

SWBNTs@SWCNTs	$Ln(R_{OUT}/R_{inn})$	Σ Q(out)(+)	Σ Q(inn)(-)	Σ V(2)-V(1)	C(G)	k
(3,3)@(7,7)* (inner)	0.82	1.22	-1.22	2.3	9.29	1.37
(3,3)@(7,7)	0.82	1.02	-1.02	1.88	8.58	1.26
(3,3)@(7,7)* (outer)	0.82	-0.47	+0.47	1.44	5.78	0.85

The results are listed in tables 1-4, and the figures are explained in Figs 2-4. The geometry optimization for TWCNTs has been done with HF and B3LYP methods at different basis sets such as 4-31G, 6-31G, 6-31G* and 6-311G*. Then thermodynamic properties were calculated for this structure in gas phase at 298.15K in the same methods and basis sets. A comparison of Gibbs free energy (G), Enthalpy (H), Entropy (S) and Internal energy (E) in different methods and basis sets are shown in table 4. As shown in table 4, the maximum values for Gibbs free-energy (G) , Enthalpy (H) and Internal energy (E) were calculated when 6-311G* basis set had been applied at B3LYP method.

HOMO and LUMO and Gap energy of TWCNTs (atoms between, 500-540) are listed in Table 1.



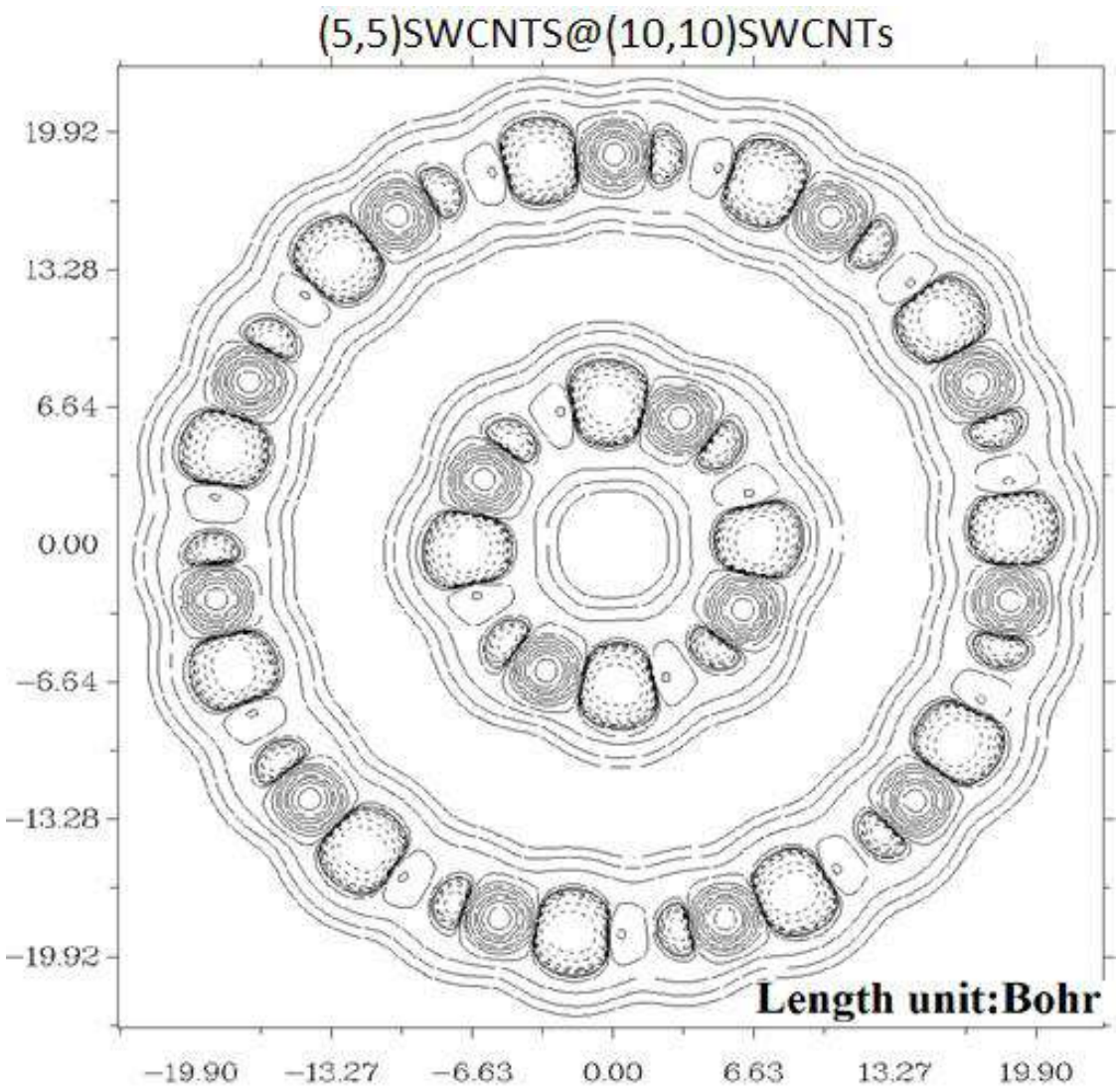


Fig3. ELF of (5,5)@(10,10)@(15,15) TWCNTS

Out Put and plot of density electron from Atoms 1-540 are shown. Localized Orbital Locator (LOL)@Electron Localization Function ELF of (5,5)@(10,10)@(15,15) TWCNTS are shown in Figs2-5. Relief map and Shaded Surface map with projection for electron density of (5,5)@(10,10)@(15,15) TWCNTs in Fig3&4. According to the results that are shown in table2, the largest values have been obtained in B3LYP method.

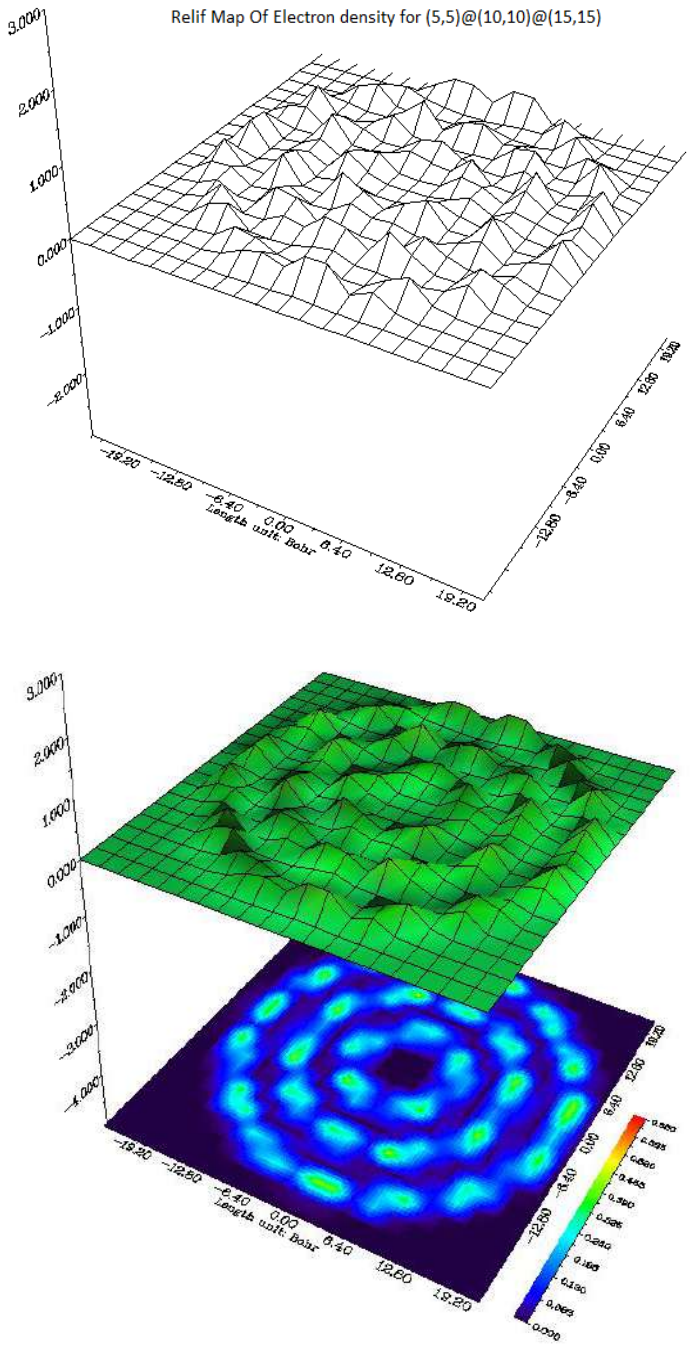


Fig. 4. Relief map and Shaded Surface map with projection for electron density of (5,5)@(10,10)@(15,15) TWCNTs

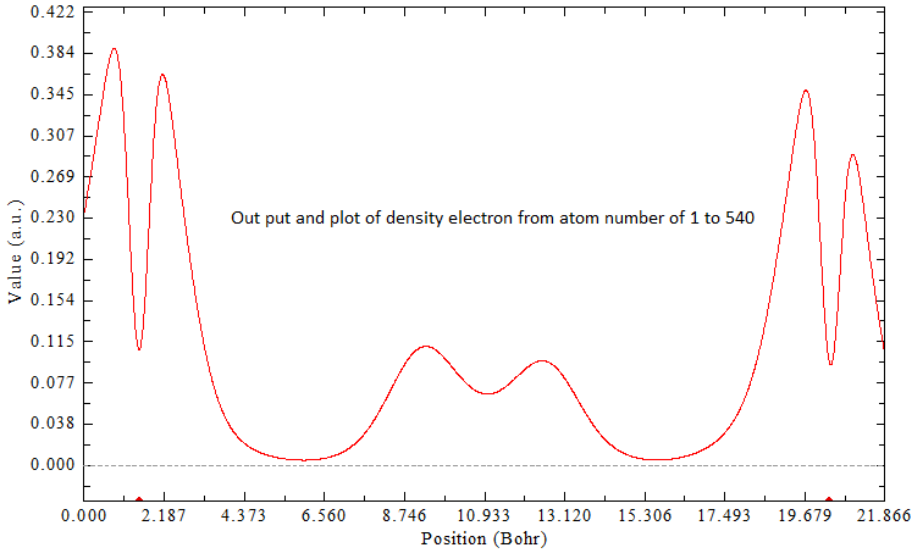


Fig 5. Out Put and plot of density electron from Atoms 1-540

Conclusion

The stability of TWCNTs and SWBNNTs @ DWCNTs were investigated. It is found that the amount of Gibbs free energy (G) , Enthalpy (H) and internal Energy (E) obtained in DFT levels in the gas phase are the largest amount and also optimization of TWCNTs and SWBNNTs @ DWCNTs at the HF levels which means DFT calculation are more accurate and suitable for these Nano structures.

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Drug delivery via α-Cyclodextrin: A Statistical-Nucleus Independent Chemical Shifts (S-NICS) study

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ABSRTACT

This study aims to investigate a novel method by using nucleus independent chemical shifts or S-NICS method of cyclo-dextrin. Monajjemi et.al (2008 a, 2015) has exhibited this novel method which so called "S-NICS" a few years ago. This program is arranged to calculate the aromaticities in some non-benzene rings. As the asymmetry (η) and skew (κ) parameters are fluctuated in a short and are alternative in lengthy distances, the S-NICS is a certain criterion for estimating the aromaticity. By generation of pseudo-random numbers in a Monte Carlo calculation which distributed in different function, the maximum abundant of skew and asymmetry parameters have been calculated for (η^*), (κ^*), and lastly the modified isotropy (σ^*_{iso}) has been calculated for α-Cyclodextrin as an electromagnetic criterion. The results revealed that positive S-NICS and NICS values for α-Cyclodextrin indicate anti-aromaticity. It was observed from the values of (η^*), (κ^*) based on our calculations for α-Cyclodextrin is negatives which are depending on the distances to the center of those rings. At last, by this work it has been presented a schematic diagram of S-NICS for post-ab-initio calculations.

KEYWORDS: Independent chemical shifts, S-NICS, Aromaticity, Monte Carlo, α-Cyclodextrin.

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Suministro de fármacos a través de la α-ciclodextrina: un estudio de cambios químicos independientes del núcleo estadístico (S-NICS)

Este estudio tiene como objetivo investigar un método novedoso mediante el uso de desplazamientos químicos independientes del núcleo, o el método S-NICS de ciclodextrina. Monajjemi et.al (2008 a, 2015) han exhibido este método novedoso que se llamó "S-NICS". Este programa está diseñado para calcular las aromaticidades en algunos anillos sin benceno. Como los parámetros de asimetría (η) y sesgo (κ) fluctúan de forma breve y son alternativas en distancias largas, el S-NICS es un criterio determinado para estimar la aromaticidad. Mediante la generación de números pseudoaleatorios en un cálculo de Monte Carlo que se distribuyó en diferentes funciones, se calculó el máximo abundante de parámetros de asimetría y asimetría para (η ∗), (κ ∗), y finalmente la isotropía modificada (σ_iso ^ *) se ha calculado para la α-ciclodextrina como criterio electromagnético. Los resultados revelaron que los valores positivos de S-NICS y NICS para la α-ciclodextrina indican anti-aromaticidad. Se observó que a partir de los valores de (η ∗), (κ ∗) basados en nuestros cálculos para α-ciclodextrina son negativos, que dependen de las distancias al centro de esos anillos. Finalmente, en este trabajo se ha presentado un diagrama esquemático de S-NICS para cálculos post-ab-initio.

PALABRAS CLAVE: Desplazamientos químicos independientes, S-NICS, Aromaticidad, Monte Carlo, α-Ciclodextrina.

Introduction

The chemical shifts for molecular rings happen from the nucleolus of the magnetic fields with the steadiness of those external magnetic fields (B_0). Generally, B_0 is a uniform field in the z-axis. The frequency, ν_i, of an each nucleus inside of molecules are related to their gyromagnetic ratios, ν_i, as specified by $\nu_i = (\gamma_i/2\pi)B_0(1 - \sigma_i)$ (Mason, 1993).

The NICS (nucleus independent chemical shifts) method is a statistical computing approach that calculates the absolute magnetic shielding in the center of the ring. Negative S-NICS (Statistical-Nucleus Independent Chemical Shifts) values

indicate aromaticity and in contrast the positive values are anti-aromaticity (Schleyer et al., 1996 and 1997).

For comparing the data together, another method which so-called "harmonic oscillator model" is used for estimating the aromaticity (HOMA) (Kruszewski and Krygowski, 1972), which are: (1) magnetic parameters of aromaticity (2) reactivity of aromatic compounds (3) geometrical considerations (4) the energetic approach to aromaticity (Stepien et al., 2004; Katritzky et al., 1989).

Through using of the energetic criterion for organizing of the aromatic molecules (Feixas et al., 2008), it is obvious that more stability of the structure might be appeared due to the cyclic electron delocalization (Fias et al., 2008; Hehre et al., 1970). Monajjemi and Boggs (2013) have demonstrated the low aromaticity for the borazine's ring of $B_{18}N_{18}$ and $B_{15}N_{15}$ (Monajjemi et al., 2010; Monajjemi and Khaleghian; 2011; Monajjemi 2012 and 2013).

Usually, aromatic ring has a downfield shift from the olefin area; hence, up-field shifts appear in the PNMR spectrums (Frueh,2002) which might be described as potential of a structure for sustaining a precipitated ring current. These molecules are known as dia-tropic and anti-aromatic and are called Para-tropic (Jiao and Schleyer, 1995).

In recent decades, aromaticity in terms of NICS in a long distances as the, NICS (0), at the center of ring through the aromatic ring current shielding (ARCS) method was estimated in several studies (Martin and Nance, 2002). In addition, S-NICS calculations, particularly in shortest ranges, have been investigated for relaxing of CSA (chemical shift anisotropies), dipole-dipole (Luginbhl and Wuthrich, 2002). It was shown that the asymmetry or (η) and skew (κ) parameters are fluctuated around the center of each ring.

This work is based on random movement of a probe in the shielding and de-shielding space of aromatic and anti-aromatic molecules for understanding the anisotropic spin–spin interactions and spin-relaxation in short ranges (Beenakker et al., 1973).

In other investigations, the components of Herzfeld and Haeberlen (Herzfeld and Berger, 1980), and CSA tensor has been calculated for $B_nN_nH_x$ rings (n=12, 15, 18) and $B_3N_3H_n$ (n = 0, 2, 4, 6, 8,) (Monajjemi and Mohammadian, 2015). NICS values exhabite a little currents with no aromaticity for borazine because of the polar B–N bond while the S-NICS data indicate a strong stable aromaticity for borazine (Anet and O'Leary, 1992).

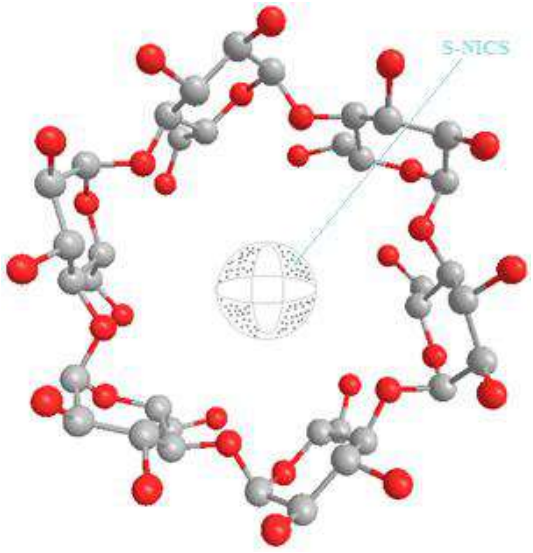
Cyclodextrins are natural nanoparticle that they are obtained by enzymatic digestion of starch. The α-, β- and γ- cyclodextrins contain respectively 6, 7 and 8 glucopyranose units, with primary and secondary hydroxyl groups located on the narrow and wider rims of a truncated cone shape structure (Boonyarattanakalin et al, 2012; Bhaskara et al., 2011). The steric arrangement of glucose units in the CD molecule brings in the shape of a hollow truncated cone with a hydrophilic external surface and a hydrophobic internal cavity, which permits CDs to form inclusion complexes with different guest molecules (Ibrahim et al., 2013).

The principal advantages of natural CDs as drug carriers are: (1) the availability of CDs of different cavity sizes, (2) a well-defined chemical structure, yielding many potential sites for chemical modification, (3) low toxicity and low pharmacological activity, (4) the protection of the included drug molecule from biodegradation (Fermeglia et al., 2003).

CDs are suitable compounds in supramolecular chemistries as receptors that are capable of including a range of organic, inorganic and biological compounds into their hydrophobic spaces in the non-covalent interactions (Del Valle, 2003; Ghatee and Sedghamiz, 2014). These non-toxic structures have interested not only in pharmaceutical industries, separation techniques, food industries, and molecule recognitions but also in environmental protections (Pan et al., 2011).

The objectives of these kind studies were to calculate the major components of Haeberlen's parameters and chemical shift anisotropies (CSA) for α-Cyclodextrin. Scheme-1 shows the sphere region of S-NICS in the structure of α-Cyclodextrin and it has been discussed those electronic properties in this structure for finding the reason

of relative stabilities in this rings in view point of isotropies and anisotropies. Finally, the electronic structure of α-Cyclodextrin has been studied by S-NICS method.



Scheme 1. The sphere region of S-NICS in optimized structures of α-Cyclodextrin.

1. Theory calculation

In using the CSA relaxation, anisotropy (CSA) means orientation dependence of the chemical shift and is described via a second-rank tensor, which includes six independent components (Mahdavian and Monajjemi, 2010).

It can be revised in its principal axis system, where it has a diagonal form. Where, the reduced anisotropy

$$\Omega_{PAS}^{(2)}=\frac{2}{3}\Delta\sigma\begin{bmatrix}-\frac{1}{2}(1+\eta) & 0 & 0\\ 0 & -\frac{1}{2}(1-\eta) & 0\\ 0 & 0 & 1\end{bmatrix}=\zeta_{(zz)}\begin{bmatrix}-\frac{1}{2}(1+\eta) & 0 & 0\\ 0 & -\frac{1}{2}(1-\eta) & 0\\ 0 & 0 & 1\end{bmatrix} \quad (1)$$

$$[\zeta_{(zz)}=(\sigma_{zz}-\sigma_{iso})=(\sigma_{33}-\sigma_{iso})] \quad (2)$$

and anisotropy ($\Delta\sigma$) with relation of $\Delta\sigma=\frac{3}{2}\zeta_{(zz)}$ including shielding asymmetry (η) can be defined as:

$$\Delta\sigma=\sigma_{zz}-\frac{1}{2}(\sigma_{xx}-\sigma_{yy}) \quad (3)$$

$$\eta=(\frac{\sigma_{yy}-\sigma_{xx}}{\zeta_{zz}})==\frac{3(\sigma_{yy}-\sigma_{xx})}{2\Delta\sigma} \quad (4)$$

The symmetric tensor in some cases, $(\sigma_{yy} - \sigma_{xx})$ will be 0 and then η=0, (Ilkhani and Monajjemi, 2015) therefore, $(0 \leq \eta \leq +1)$ and $\Omega = \Omega^{(0)} + \Omega^{(1)} + \Omega^{(2)}$. **(5)**

In spherical tensor investigated as Haeberlen and have estimated out, at fundamental stages in spherical styles.

$\sigma = \sigma^{iso(0)} + \sigma^{anti(1)} + \sigma^{sym(2)}$ **(6)**

Spherical tensors are generally involved the effects of tensor quantities on density matrix (Samiei Soofiand and Monajjemi, 2016) as follows: (Monajjemi et al., 2008 a)

$$\sigma_0^{iso(2)} = \sqrt[2]{\frac{3}{2}}\zeta_{zz} \text{ and } \sigma_{\pm 2}^{sym(2)} = \frac{1}{2}\zeta_{zz}. \quad (7)$$

The proportionalities of those equations exhibit the shielding anisotropy and asymmetry which can readily be associated with a spherical tensor as follows:

$$\sigma_{iso} = \sigma_{avg}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix} \quad (8)$$

The magnetic environment (Monajjemi and Chahkandi, 2005) of a spin is seldom isotropic. Hence, is described by a tensor of Span

$(\Omega) = \sigma_{33} - \sigma_{11} \qquad (0 \leq \eta \leq +1) \qquad (9)$

$$\kappa = \frac{3(\sigma_{iso} - \sigma_{22})}{\Omega} \qquad (-1 \leq \kappa \leq +1) \quad (10)$$

Based on the position of σ_{22} with consideration of σ_{iso}, the sign of κ is either positive or negative (Monajjemi et al., 2008 b). Based on our calculations α-Cyclodextrin, (κ) is negative.

Due to Herzfeld-Berger notation, (Herzfeld, 1980) three parameters have been defined with combination of the major components. Those are classified as; span (Ω), which describes the maximum width, $(\Omega \geq 0)$, skew (κ) of the tensor.

2. Result and Discussion

Total shieldings such as standard components, Haeberlen- Mehring, and Herzfeld-Berger parameters for α-Cyclodextrin have been calculated via density functional theory. This study aims to investigate a statistical method by using computing of nucleus independent chemical shifts (S-NICS) in a sphere of shielding and de-shielding

spaces of molecular rings. ONIOM method was applied to all calculation. CSA tensors and parameters for proton NMR in α-Cyclodextrin Fig 1-2 and Table 1 were calculated using the B3LYP method in conjunction with 6-31G**, 6-31G*and 6-31G basis sets.

In short distances from center, the asymmetric parameter (η), and the skew (κ), obey the Gaussian distribution on their fluctuation treatment, which is related to the distances of the molecular rings (Monajjemi et al., 2006, 2009, 2013, 2014). In the S-NICS methods, the best point of the shielding placed around the center of symmetric or non-symmetric aromatic molecules which indicates an aromaticity criterion. In this method the expectation of the (η*) and (κ*) have been calculated as the Gaussian curve functions around the center of the α-Cyclodextrin (Table 2). The isotropy (σ^*_{iso}) depending to (η^*) and (κ^*) and (Ω^*) and (ζ^*) are the best criterion for symmetric or non-symmetric aromatic molecules (Table 2) (Monajjemi and Mohammadian, 2015).

It has been mentioned, a large point's random numbers in the space of shielding are needed to gain the most exact data of isotropy criterion. Similar to the NICS method, in S-NICS, negative nucleus-independent chemical shifts denote aromaticity and positive values denote anti-aromaticity (Monajjemi and Mohammadian, 2015). Consequently the chemical shielding, electronegativity, hydrogen bonding, and magnetic anisotropy of π- systems would be changed due to the electrons around the proton which produce a magnetic field, countering the applied field. Furthermore via the S-NICS, it can be estimated the most accurate places for effective points as an aromaticity criterion (Ardalan et al., 2014). The chemical shielding is a vector orientation function for all of the shielding parameters that can change in various places inside the shielding area of the rings for aromatic compounds and also for each cycles, the (+) value denotes shielding and (−) indicates de-shielding (Yahyaei and Monajjemi, 2014).

S-NICS have been investigated via the Monte Carlo model through computation of nucleus-independent chemical shifts around the ring of α-Cyclodextrin. The asymmetry (η), and skew (κ) parameters fluctuate by the changing of tensors, while in the case of an axially symmetric tensor, σ_{22} equals either σ_{11} or σ_{33} and a = Ω/3, the span is κ= ±1 by changing asymmetry between $0 \leq \eta \leq +1$ and the span will be changed between

(-1 ≤ κ ≤ +1) and the parameter "κ" is zero when $\sigma_{22} = \sigma_{iso}$ and the details of the statistical data such as expectation of these parameters and S-NICS data for α-Cyclodextrin are shown Table 2.

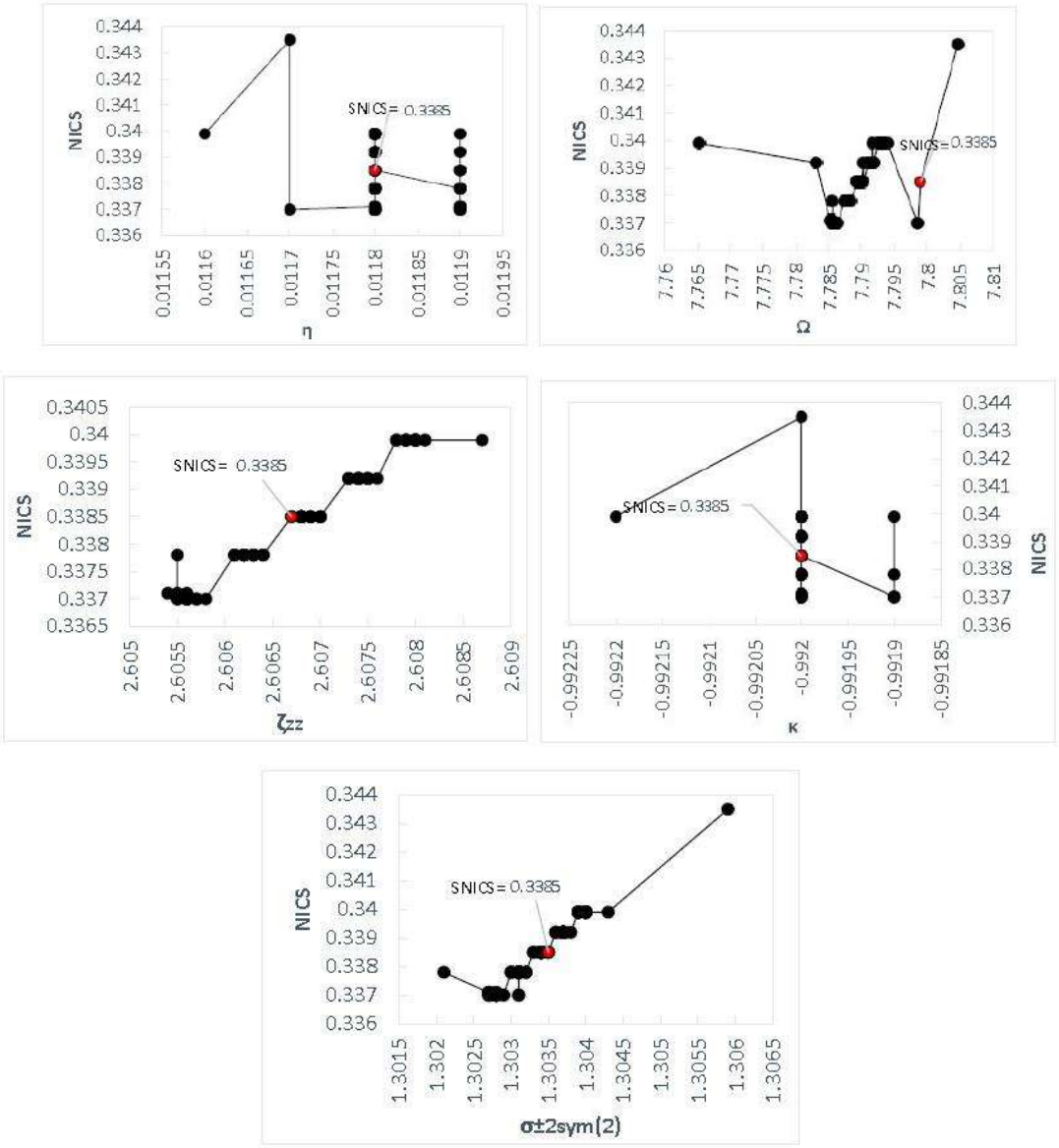


Fig 1. S-NICS (red point) from NICS calculation with 6-31G** basis set.

As it can be seen in the schems2 and figures2, symmetry of density electron on α-Cyclodextrin represents the regular rotation around the z axis. α-Cyclodextrin which accepts some molecular guests as hosts. Hamiltonian kinetics energy density G(r) of α-Cyclodextrin is shown in Scheme 3. The kinetics Hamiltonian represents a rotational direction and movement of the various segments of the α-Cyclodextrin.

Table 1. S-NICS parameters for α-Cyclodextrin by 6-31G* basis set.

R_{BQ}	η	Ω	κ	ζ_{zz}	$\sigma_{*2}^{sym(2)}$	R_{BQ}	η	Ω	κ	ζ_{zz}	$\sigma_{*2}^{sym(2)}$
0.17320	0.0117	7.8017	-0.9929	2.6118	1.3059	0.06708	0.0107	7.9603	-0.9927	2.6629	1.3314
0.12247	0.0105	7.9630	-0.9927	2.6637	1.3318	0.05477	0.0107	7.9527	-0.9927	2.6604	1.3302
0.01732	0.0107	7.9520	-0.9927	2.6602	1.3301	0.05744	0.0107	7.9548	-0.9927	2.6611	1.3305
0.02449	0.0107	7.9541	-0.9927	2.6609	1.3304	0.06164	0.0107	7.9568	-0.9928	2.6618	1.3309
0.03316	0.0107	7.9561	-0.9927	2.6616	1.3308	0.06708	0.0107	7.9587	-0.9928	2.6625	1.3312
0.04242	0.0118	7.7910	-0.9920	2.6073	1.3036	0.07348	0.0107	7.9605	-0.9928	2.6630	1.3315
0.05196	0.0107	7.7598	-1.0184	2.6628	1.3314	0.03316	0.0107	7.9522	-0.9927	2.6603	1.3301
0.02449	0.0107	7.9520	-1.0183	2.6602	1.3301	0.03771	0.0108	7.9544	-0.9927	2.6610	1.3305
0.03	0.0107	7.9542	-0.9927	2.6610	1.3305	0.04358	0.0107	7.9564	-0.9927	2.6617	1.3308
0.03741	0.0107	7.9563	-0.9924	2.6616	1.3308	0.05099	0.0107	7.9583	-0.9927	2.6623	1.3311
0.04582	0.0107	7.9581	-0.9927	2.6622	1.3311	0.05916	0.0107	7.9601	-0.9927	2.6629	1.3314
0.05477	0.0107	7.9599	-0.9927	2.6628	1.3314	0.03741	0.0107	7.9523	-0.9927	2.6603	1.3301
0.03316	0.0107	7.9522	-0.9927	2.6602	1.3301	0.04123	0.0107	7.9544	-0.9927	2.6610	1.3305
0.02	0.0107	7.9544	-0.9927	2.6610	1.3305	0.04690	0.0107	7.9565	-0.9927	2.6617	1.3308
0.04358	0.0107	7.9563	-0.9927	2.6616	1.3308	0.05385	0.0107	7.9583	-0.9927	2.6623	1.3311
0.0026	0.0107	7.9582	-0.9927	2.6622	1.3311	0.07937	0.0107	7.9601	-0.9927	2.6629	1.3314
0.05916	0.0107	7.9600	-0.9927	2.6628	1.3314	0.03741	0.0107	7.9525	-0.9927	2.6604	1.3302
0.04242	0.0107	7.9523	-0.9928	2.6603	1.3301	0.04123	0.0107	7.9546	-0.9927	2.6610	1.3305
0.04582	0.0107	7.9545	-0.9927	2.6610	1.3305	0.04690	0.0107	7.9566	-0.9927	2.6617	1.3308
0.05599	0.0107	7.9565	-0.9928	2.6617	1.3308	0.05385	0.0107	7.9585	-0.9927	2.6624	1.3312
0.05744	0.0107	7.9584	-0.9928	2.6623	1.3311	0.06164	0.0107	7.9602	-0.9928	2.6630	1.3315
0.06480	0.0107	7.9602	-0.9928	2.6629	1.3314	0.05099	0.0107	7.9526	-0.9928	2.6604	1.3302
0.05196	0.0107	7.9526	-0.9928	2.6604	1.3302	0.05385	0.0107	7.9547	-0.9927	2.6611	1.3305
0.05477	0.0107	7.9548	-0.9927	2.6610	1.3305	0.05830	0.0107	7.9567	-0.9928	2.6618	1.3309
0.05916	0.0107	7.9567	-0.9928	2.6617	1.3308	0.06403	0.0107	7.9586	-0.9928	2.6624	1.3312
0.06480	0.0107	7.9586	-0.9928	2.6624	1.3312	0.0707	0.0107	7.9605	-0.9928	2.6630	1.3315
0.07141	0.0107	7.9604	-0.9928	2.6630	1.3315	0.05916	0.0107	7.9529	-0.9928	2.6604	1.3302
0.02449	0.0108	7.9521	-0.9927	2.6602	1.3301	0.06164	0.0107	7.9550	-0.9928	2.6612	1.3306
0.03605	0.0107	7.9542	-0.9927	2.6610	1.3305	0.06557	0.0107	7.9570	-0.9928	2.6618	1.3309
0.03753	0.0107	7.9563	-0.9927	2.6616	1.3308	0.07071	0.0107	7.9589	-0.9928	2.6624	1.3312
0.04582	0.0107	7.9582	-0.9927	2.6622	1.3311	0.07681	0.0107	7.9606	-0.9928	2.6630	1.3315
0.05477	0.0107	7.9599	-0.9927	2.6628	1.3314	0.04242	0.0108	7.9525	-0.9927	2.6604	1.3302
0.03	0.0107	7.9522	-0.9927	2.6603	1.3301	0.04582	0.0108	7.9546	-0.9927	2.6611	1.3305
0.03464	0.0107	7.9543	-0.9927	2.6610	1.3305	0.05099	0.0108	7.9566	-0.9927	2.6618	1.3309

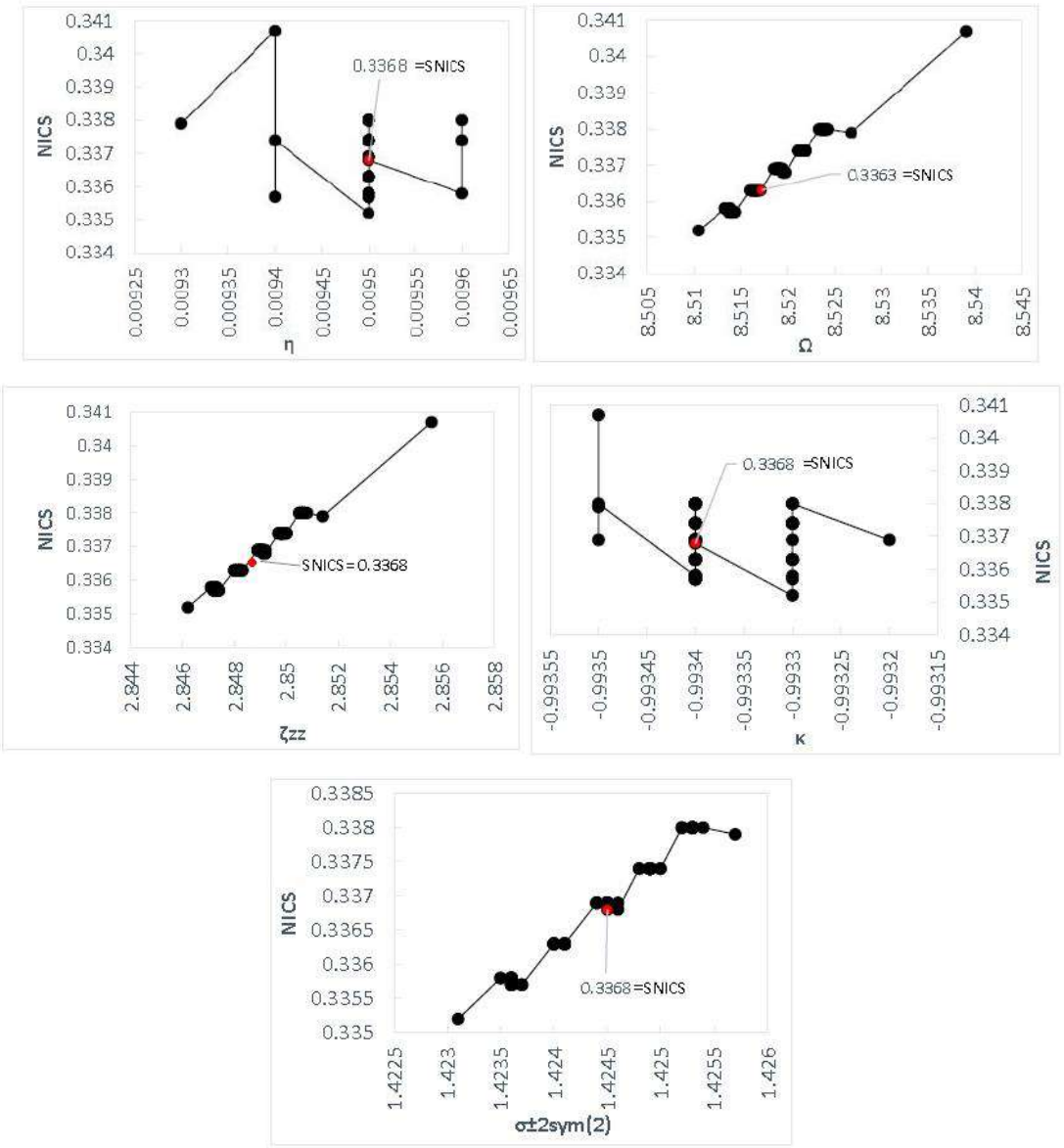
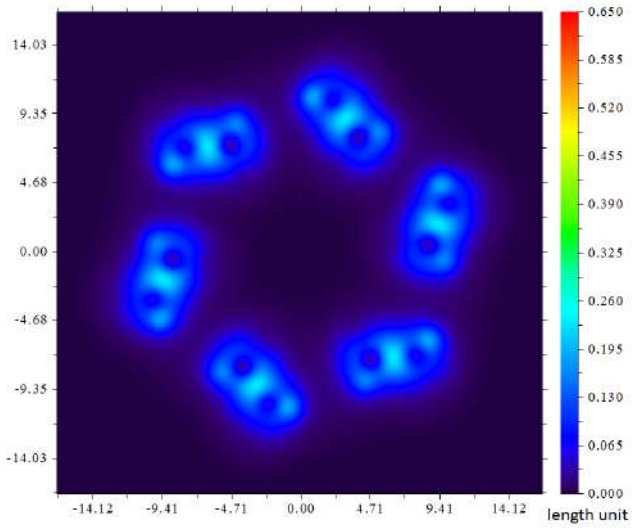


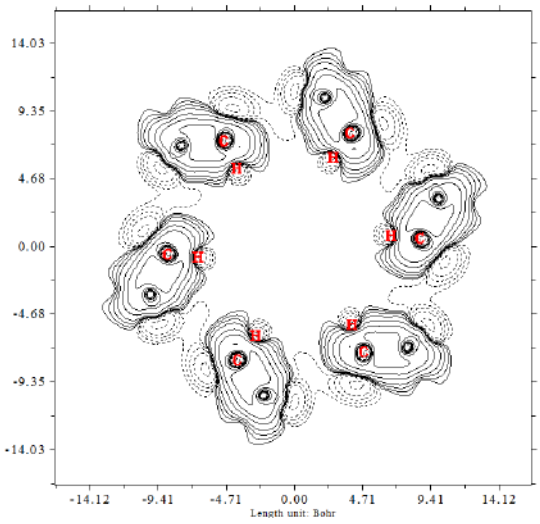
Fig 2. S-NICS (red point) from NICS calculation with 6-31G basis set.

Table 2. NICS and S-NICS parameters for α-Cyclodextrin in different basis sets

α-Cyclodextrin									
Basis set	ζ*	η*	Ω*	κ*	S-NICS	NICS	R_{Bq}	(aniso)*	(NICS)*
6-31G**	2.6068	0.0118	7.7294	-0.992	+0.338	+0.336	0.0531	3.9103	+0.338
6-31G*	2.8490	0.0094	8.5198	-0.9937	+0.336	+0.335	0.0531	4.2736	+0.337
6-31G	2.6603	0.0107	7.9516	-0.9932	+0.3236	+0.3213	0.0531	3.9909	+0.3253



Scheme 2. Electron density of α-Cyclodextrin.



Scheme 3. Hamiltonian kinetics energy density G(r) of α-Cyclodextrin.

Conclusion

At the ring centers of the shielding spaces of aromatic molecules, the absolute magnetic shielding computed at ring centers are applied as an aromaticity and anti-aromaticity criterion by the NICS method.

We have concentrated on statistical calculation through Monte-Carlo for the asymmetry (η) and skew (κ) parameters. The expectation of these parameters such as (η*), (κ*) exhibited maximum abundance in the areas of the shielding spaces.

The isotropy analogous with modified parameters of asymmetry, span, anisotropy and skew is called Modified isotropy " σ^*_{iso} " this isotropy is most considerable as an aromaticity criterion because it's miles arises from the maximum abundance of states, and it's stable value that is independent of the symmetric or non-symmetric structures of the molecules. In contrast to the NICS, the S-NICS calculations would be lengthy without the use of any simplifying software.

The results revealed that positive S-NICS and NICS values for α-Cyclodextrin indicate anti-aromaticity. It was observed from the values of (η^*), (κ^*) based on our calculations for α-Cyclodextrin is negatives.

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Comparison of neural networks and genetic algorithms to determine missing precipitation data (Case study: the city of Sari)

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ABSTRACT

Neural networks and genetic programming in the investigation of new methods for predicting rainfall in the catchment area of the city of Sari. Various methods are used for prediction, such as the time series model, artificial neural networks, fuzzy logic, fuzzy Nero, and genetic programming. Results based on statistical indicators of root mean square error and correlation coefficient were studied. The results of the optimal model of genetic programming were compared, the correlation coefficients and the root mean square error 0.973 and 0.034 respectively for training, and 0.964 and 0.057 respectively for the optimal neural network model. Genetic programming has been more accurate than artificial neural networks and is recommended as a good way to accurately predict.

KEY WORDS: neural networks, genetic algorithms, prognostic data, Sari.

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Comparación de redes neuronales y algoritmos genéticos para determinar datos faltantes de precipitación (Estudio de caso: la ciudad de Sari)

RESUMEN

Redes neuronales y programación genética en la investigación de nuevos métodos para la predicción de precipitaciones en el área de captación de la ciudad de Sari. Para la predicción se utilizan varios métodos, como el modelo de series temporales, redes neuronales artificiales, lógica difusa, Nero difuso y programación genética. Se estudiaron los resultados basados en los indicadores estadísticos de error cuadrático medio y coeficiente de correlación. Se compararon los resultados del modelo óptimo de programación genética, los coeficientes de correlación y la raíz del error cuadrático medio 0.973 y 0.034 respectivamente para entrenamiento, y 0.964 y 0.057 respectivamente para el modelo de red neuronal óptima. La programación genética ha sido más precisa que las redes neuronales artificiales y se recomienda como una buena forma de predecir con precisión.

PALABRAS CLAVE: redes neuronales, algoritmos genéticos, datos de pronóstico, Sari.

Introduction

Factors affecting water resources systems analysis, including precipitation predicted in one of the major issues in the design, operation and studies relating to these sources is considered. For this purpose, various methods such as artificial neural networks, fuzzy logic, Genetic programming and time series.

Circulating among the genetic programming algorithm is a method that is based on Darwin's theory of evolution is based on. Mentioned algorithm to define an objective function in the form of quantitative criteria and then mentioned function to compare different solutions to solve the problem in a step by step process to apply correct data structure and finally, providing the perfect answer. Genetic Programming is a recent development in the methods of evolutionary algorithms due to sufficient accuracy, the application is more (Feuring and Golubski, 2000).

Khu and colleagues (Khu ST, 2001) in a study on the catchment Avrgval in France, Genetic programming used to predict runoff and results with observed data and calculated values were analyzed by classical methods. The result indicates the accuracy of genetic programming is acceptable.

Lee Jung et al (Liong SY, 2002) studied the relationship between rainfall-runoff that concluded that the use of genetic programming algorithm to predict the behavior of precipitation - runoff in watershed will cause fewer errors. (Aytek and Kisi , 2008), a study on the phenomenon of sediment transport in streams, genetic programming as a suitable approach for modeling of suspended sediment were introduced. According to research (Aytek and Kisi, 2008; Aytek, Asce and Alp, 2008). Genetic Programming a suitable method and the action is in anticipation of rainfall-runoff relationship (Liong et al., 2002). Genetic Programming with incomplete data to estimate the height of waves in the Gulf of Mexico found the method of accuracy in the prediction of time series is very good.

A parallel processing system using artificial neural networks mimic the human brain are very simple biological nervous system. This emulation is based on a mathematical configuration, so that consists of several layers of neurons in each layer. The performance of these networks is thus an input layer, and acting inappropriately. And layers (layers) between the data processing and finally, the output layer to output resulting from application of its models.

(Abrahart and See, 2000) in a research area Wi-Vavs a comparative study of artificial neural networks method and ARMA model to predict the flow of the river is dealt. Comparative benchmark results show that the neural network capable of simple results than ARIMA model with the same input data generated. Kisi (2004) in a research Gvsvdr basin located in the State Issaquah Japan of artificial neural network and multiple regression to predict the monthly flow. The results showed higher accuracy than regression models were artificial neural networks (Kisi, 2005) in an investigation into Blackwater and Gila basin using artificial neural network models to predict the flow of the river's Atoregrsion. The results showed higher accuracy than the artificial neural

network approach is Atoregrsion. Dogan et al (2006) in a research on Sakarya basin of two artificial neural networks and Atoregrsion used to predict the flow of daily revolt. The results show high accuracy recurrent neural network model to predict the course of daily revolt. (Firat M, 2007) in a study on watershed in Turkey's Cihan neuro-fuzzy methods, artificial neural networks feedforward neural network generalized multiple regression to predict daily river flow data can be used. Results showed superiority over the other two methods are neuro-fuzzy approach.

The aim of this study was to predict rainfall data at the basin city of Sari using genetic programming and artificial neural network model and compare the results of one of the most accurate method is common as is.

1. Methods

1.1. Genetic Algorithm

In genetic algorithm, first available block that includes the purpose and function of the input variables and connecting them, defined and reasonable structure model and its coefficients are determined. It involves a link between input variables and output equation and thus able to automatically select the appropriate variable and remove the variable is unrelated This will reduce the size of input variables. Select the appropriate inputs one of the most important things that need to be addressed in this way. It is also used in the absence of secondary input data, it will be more important; Because they provide unbiased input data, reduces the accuracy of the model and create more complex models That interpretation is faced with more difficult.

In engineering applications, the genetic programming is widely used in modeling to determine the structure of the phenomenon comes into action.

Genetic Programming for process step by step the following steps (Willis et al, 1997):

1. An initial population of combined functions of predictive models, considered to be random.

2. Any member of the population using the fitting functions, are evaluated.
3. In each production, the following steps will be taken to select a new population:

a) A cross operator, mutation and selection can be copied.
b) A good number of people in the crowd are selected.
c) The selection operator is used to produce offspring.
d) Son is mentioned in a new population.
e) The model is evaluated using different brushes.

4. The third step is to achieve the maximum number of publications, will be repeated.

In this way at the start of any relationship is not intended function and this method is able to optimize the structure of the model and its components.

Genetic Programming for Computational step by step flowchart shown in Figure 1.

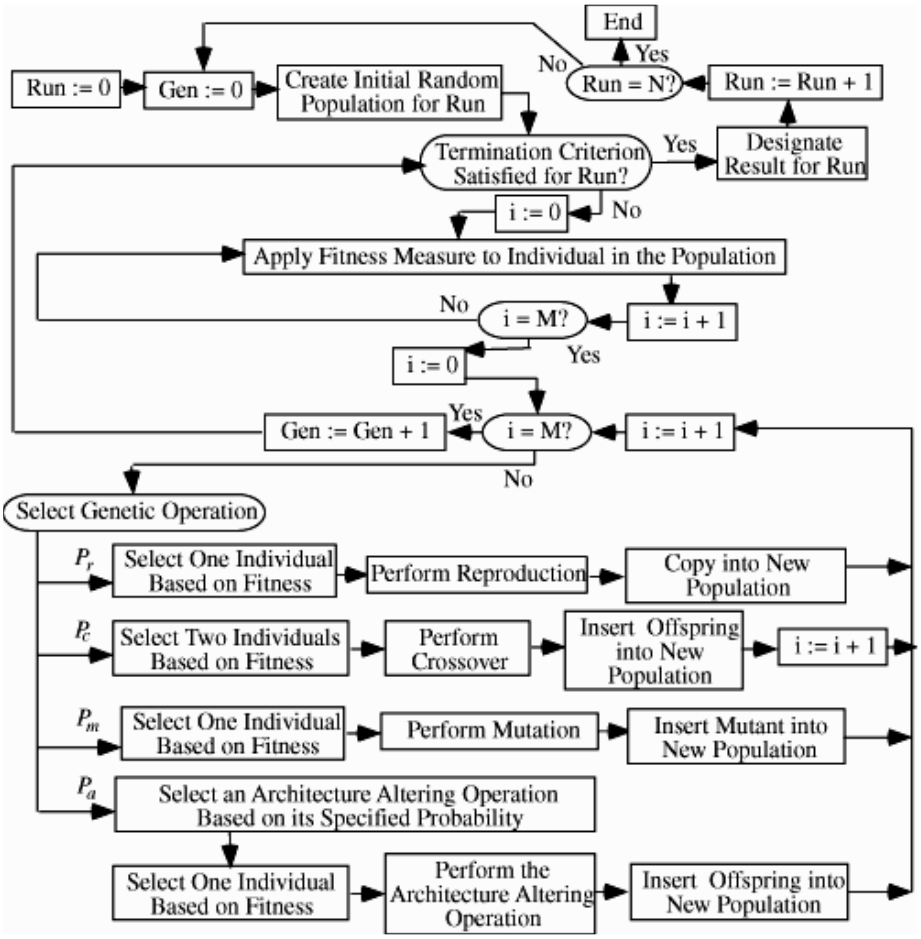

Figure 1. Flowchart genetic programming (Kozo, 1992)

1.2. Artificial Neural Networks

These networks mimic the neural networks in organisms and using a large number of artificial neurons are interconnected to perform the necessary calculations. A neural network consists of several nodes or compute nodes and In cases where the weighted inputs is used, The nodes are able to produce appropriate outputs will be using functions. Each layer may be formed from multiple neurons and neural network also includes one or more layers will be connected together. A three-layered structure of a network that consists of an input layer I, a hidden layer H and an output layer O. The above description is given in Figure 2.

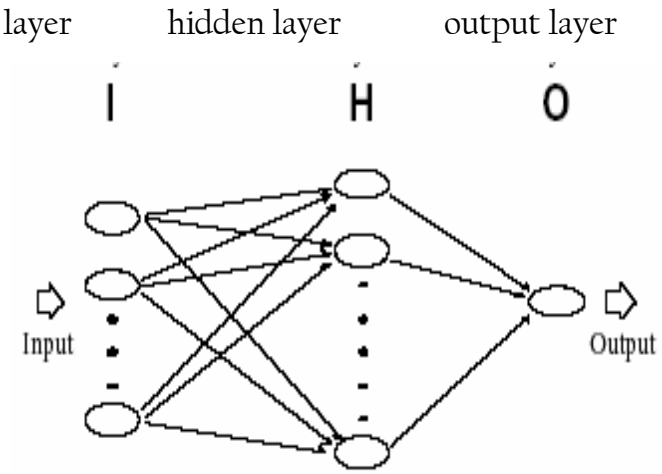

Figure 2. Structure of an artificial neural network (Alvisi et al., 2005)

The main elements of a neural network, or artificial neurons are nerve. Input pattern to a node dendritic cells is biologically similar That it can be a vector with N elements as indicated whit $X=(x_1,x_2,....,x_n)$. Sum of the weights of fellow inputs can be scalar quantity S displayed.

$$s=\sum_{n=1}^{N} w_n x_n = W^T X \qquad (1)$$

Where $W=(w_1,w_2,....,w_n)$ is the weight vector of the neuron. Quantity s Then f is a nonlinear function to output result:

$$y = f(s) \quad (2)$$

Non-linear transfer function is usually in the form of sigmoid function is defined as follows:

$$f(s) = (1+\exp(-s))^{-1} \quad (3)$$

The output can be the result medal, or input is the next layer multi-layer network.Various algorithms to calculate the optimal weights of the algorithms presented in the "propagation" which is the most widely used. Networks that were used in this study process modeling is a Multilayer Perceptron network. The leading network for action and the Structural optimal design as much as possible try to take a middle layer. Multilayer Perceptron network training using back propagation algorithm was used.

Import of raw data to reduce network speed and accuracy. For authentication of such circumstances and in order to equalize the value data for the network, the normal practice was that this would shrink the excessive weight and early saturation is inhibiting the neurons. Frequently, data normalization in the range (0.9 and 0.1) takes place. In this study, all data input before applying to the network were normalized using the following equation:

$$X_{normal} = 0.1 + 0.8 * \left(\frac{X_0 - X_{\min}}{X_{\max} - X_{\min}} \right) \quad (4)$$

In this relation X_{normal} is the normal amount, X_0 is real amount, $X_{\max}$ and $X_{\min}$ The data are the maximum and minimum values respectively. The artificial neural network model data for training and testing are divided into two categories, In this study divided into two categories: training and testing patterns, respectively, 75 percent and 20 percent considered.

The performance of these networks is thus an input layer, action to accept data and layers (layers) between the data processing and finally, The output layer to output

resulting from the application of the model. During the modeling coefficients related to errors in nodes for trial and error corrected which in most cases mean error profile data is used. It does so by comparing output model the performed with data input observations.

$$R = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2}} \quad (5)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - x_i)}{N}} \quad (6)$$

In the last equation, R is the correlation coefficient, $RMSE$ is Root Mean Square Error, x_i is The observed value at time step, y_i is The amount calculated in the same time, N is The number of time steps, the mean of observations and $\bar{y}$ The mean values is calculated.

1.3. Case study

Sari in Mazandaran province in northern Iran, the largest and most populous city in Mazandaran province. Sari, located in the foothills of the Alborz mountain range has two parts is mountainous and plain In longitude and latitude 36 degrees 53 degrees 5 minutes and 4 minutes. Tajan River passes through the City of Surrey. The river flows in East Surrey. Zaremrod of 3 main branch of the river in the north and the main branch of Tajan in central and southern branch of the White River basin is formed and, moreover, they are on their way tributaries such as the Valley Babrcheshmeh, Pelaroy, ShirinRood, Salar Dareh, Tirjari water and one of them receives. The study and forecast data on precipitation is very important.

Figure 3. Location city Sari

2. Results

According to various studies done on the effectiveness of artificial neural networks and genetic programming models predict precipitation data, Clearly, the ability of these techniques according to different patterns and structures and The nature of the problem we solve is different.

Surrey city station rainfall data from 1971 to 2014 and was used for this study. In Table 1, comparable statistical indicators related to the results of the application of genetic algorithm to predict rainfall data is given.

Table 1. Statistical analysis accuracy capability

Test			Training			
RMSE	R^2		RMSE	R^2	Run number	Input pattern
0/043	0/925		0/045	0/937	200	1
0/035	0/969		0/038	0/971	200	2
0/033	0/971		0/034	0/973	200	3

From the above results it can be concluded that the results are gradually improving and is a convergent answer.

In the present study to investigate the accuracy of genetic programming, artificial neural network model with the same input patterns with input data were normalized. For each input pattern by changing the number of hidden layers and the number of hidden layer neurons, Different neural networks were trained and finally a structure that has the fewest errors, was chosen as the most suitable structure.

Table 2 shows the most appropriate structure for each input pattern. For each input pattern, Structure with five neurons in a hidden layer and an output layer neurons in the best structure has been sigmoid function of the type of stimuli used. In between these structures, such as genetic algorithms to improve with fewer errors and higher correlation coefficient is the fourth structure.

Table 2. Statistical analysis of the accuracy of artificial neural networks

Training		Test			
RMSE	R^2	RMSE	R^2	Structure	Input pattern
0/048	0/945	0/049	0/948	2-6-1	1
0/051	0/958	0/055	0/956	3-6-1	2
0/055	0/960	0/057	0/964	4-6-1	3

Following the results of the two methods is shown as a graph.

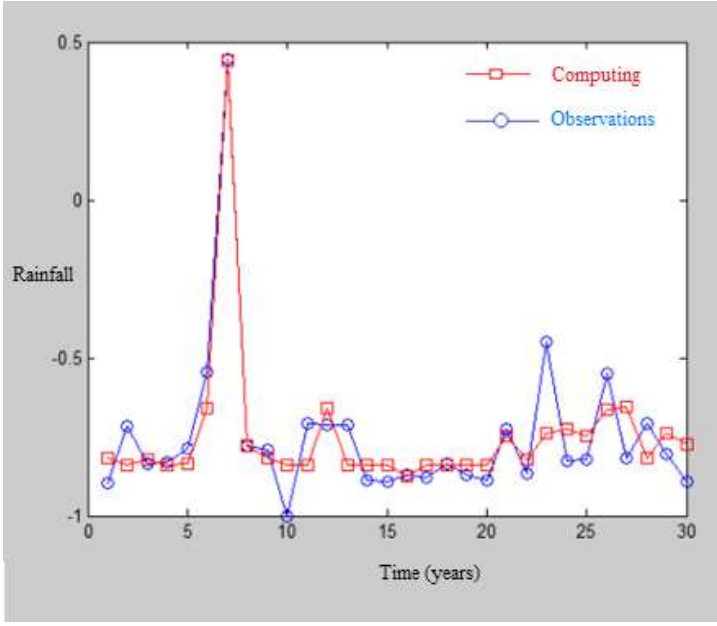

Figure 4. Results related to neural networks (Training)

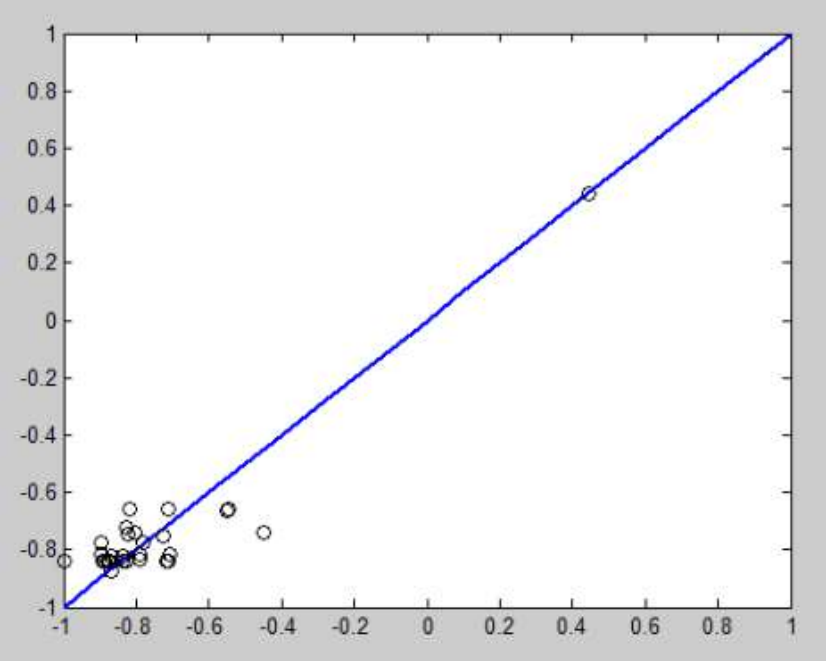

Figure 5. The regression line for Training mode in the Neural Network

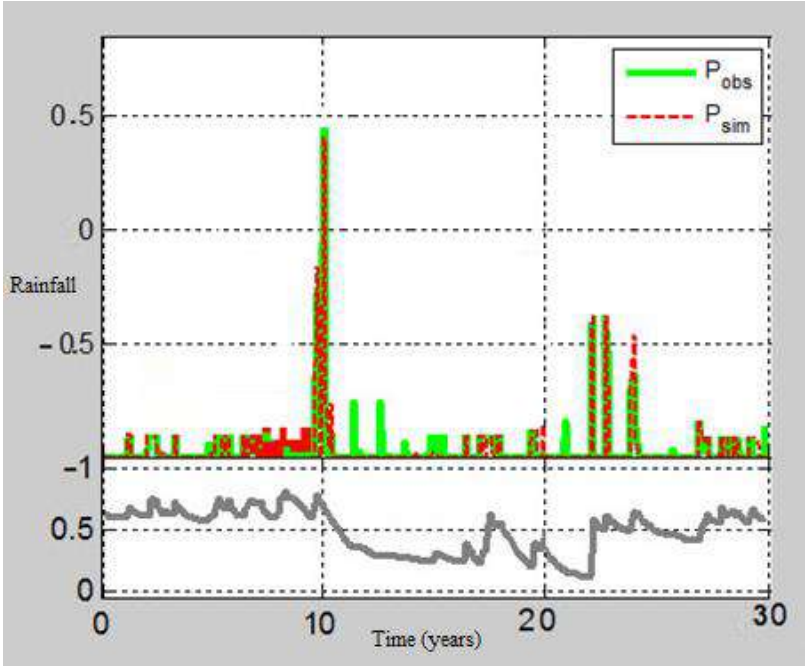

Figure 6. Results of genetic algorithm

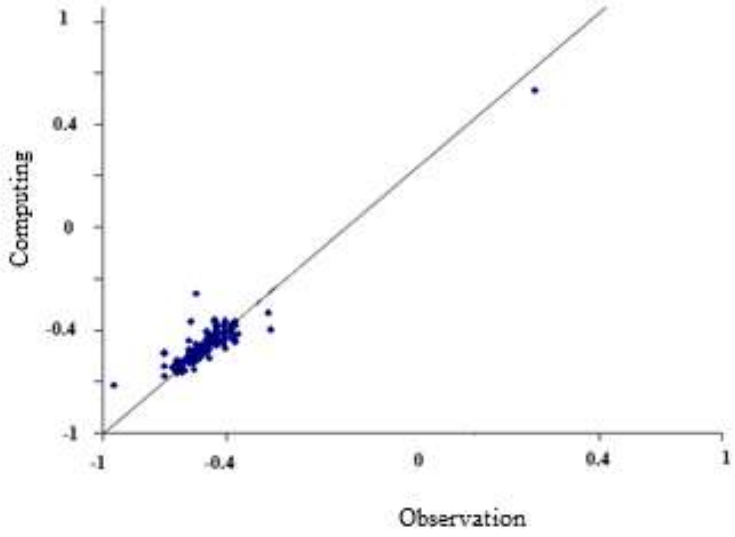

Figure 7. The regression line for the training in Genetic Algorithm

In Figure 8 Comparison of Two Methods used in the study are shown in the diagram.

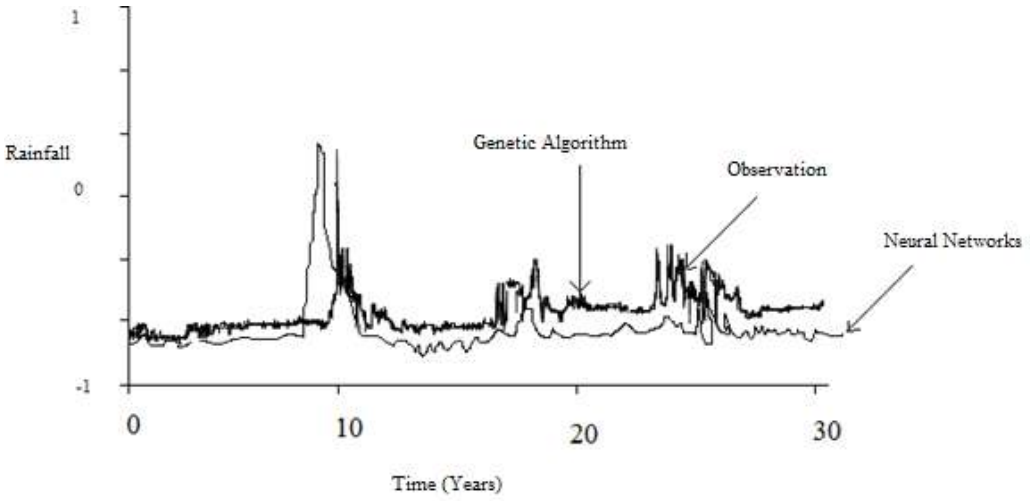

Figure 8. Compare computational methods with the observed data

The results showed that in terms of the values in Table 1 and 2 respectively genetic algorithm is more accurate than using artificial neural networks. In Figure 9 correlation coefficient for the two methods that reflect the above explanation is given for comparison.

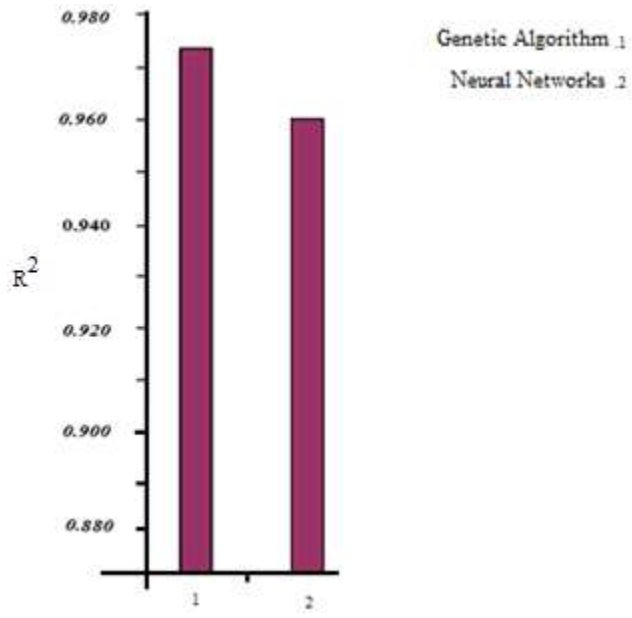

Figure 9. The correlation coefficient for the methods used

Conclusion

Given that in this study, two methods were used to predict after calculating the correlation coefficients and root mean square error of the results of both methods are acceptable. For genetic algorithm correlation coefficient and root mean square error 0.973 and 0.034 respectively for training and artificial neural network model for optimal 0.960 and 0.055 respectively were obtained. According to the results we can say that genetic algorithm is more accurate than using neural networks.

In a study of (Aytek and Kisi, 2008) conducted a genetic programming in modeling sediment extremely high accuracy relative to the regression model showed and Khu et al. (2001) took advantage of genetic programming for runoff prediction and results with observed data and calculated values were compared by classical methods. The result is an expression of ultra-high precision genetic programming. The results with respect to the accuracy of model genetic programming is consistent with the results of the above studies.

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(4n +2)π Huckel's rule of $B_n N_n C_{(8-2n)} H_8$ as anti-cancer heterocyclic systems

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ABSTRACT

Replacing of Boron and nitrogen atoms in [8] annulene molecule help us for explaining the details of mentioned magnetic mechanism concerning the ring currents of the carbon disappearing in the isoelectronic azabora-hetero-cycles variants ($B_n N_n C_{(8-2n)} H_8^{2-}$,n=0,1,2,3 and4 The (4n+2)π systems aromatic on variants of BnNnC(8-2n) H8 (n=0, 1 ,2,3 and 4) via the localized orbital by considering the current density induced have been studied. It has been predicted a four-electron dia-tropic (aromatic) ring current for (4n+2) π azabora-hetero-cycles variants of BnNnC (8-2n) H8(n=0,1 ,2,4) and a two-electron para-tropic (anti-aromatic) current for (4n) π. HOMO and LUMO energies and also HOMO/LUMO overlapping in whole space have been calculated. Two forms can be considered, first the HOMO–LUMO transition leads to a para-tropic contribution, and second HOMO–LUMO+1 transitions to the dia-tropic contributions. In addition, the NICS and SNICS values confirm the amounts of aromaticity and anti-aromaticity in those rings.

KEYWORDS: Aromaticity, LOL, ELF, Annulene, current density induced, azabora-hetero-cycles.

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(4n +2) π Regla de Huckel de Bn NnC (8-2n) H8 como sistema heterocíclico contra el cáncer

RESUMEN

El reemplazo de los átomos de boro y nitrógeno en la molécula de anuleno [8] nos ayuda a explicar los detalles del mecanismo magnético con respecto a las corrientes anulares del carbono que desaparecen en las variantes isoelectrónicas de azabora-heterociclos (Bn Nn C (8-2n) H82- , n = 0,1,2,3 y4. Los sistemas (4n + 2) π aromáticos en variantes de BnNnC (8-2n) H8 (n = 0, 1, 2,3 y 4) se ha estudiado la densidad de corriente inducida a través del orbital localizado. Se ha predicho una corriente de anillo dia-trópico (aromático) de cuatro electrones para (4n + 2) π aza-bora-heterociclos variantes de BnNnC (8-2n) H8 (n = 0 , 1, 2,4) y una corriente para-trópica (antiaromática) de dos electrones para (4n) π. las energías HOMO y LUMO y también la superposición de HOMO / LUMO en todo el espacio. Se han calculado dos formas, primero, la transición HOMO-LUMO conduce a una contribución para-trópica, y la segunda transición HOMO-LUMO + 1 a las contribuciones dia-trópicas. Además, los valores NICS y SNICS confirman las cantidades de aromaticidad y anti-aromaticidad en esos anillos.

PALABRAS CLAVE: Aromaticidad, LOL, ELF, Annulene, inducida por densidad de corriente, azabora-heterociclos.

Introduction

1,3,5,7-Cyclooctatetraene (COT) is known as "Annulene" and in contrast of benzene structure, COT follows a nonplanar conformation with alternating double and single bonds via D_2d symmetry (Willstätter and Waser, 1911; Willstätter and Heidelberger, 1913). $C_8H_8^{2-}$, is an aromatic ring with high resonance energy in the aromatic reactions. This molecule is both planar and octagonal in the shape and aromatic with the Huckel electron count of (4×2) +2=10. Huckel's long-standing "4n+2" rule indicates mono aromatic rings from anti-aromatics, and correlates the electronic structures of those systems with their magnetic properties (Gellini and Salvi, 2010). Through the interaction between alternating bonds it has been confirmed that the structure of COT involves a planar transition state of D_{4h} symmetry (Wu et al., 2012). Moreover the NMR experimental data indicate that COT^{2-} also adopts a D_{8h} symmetry structure (Naor and

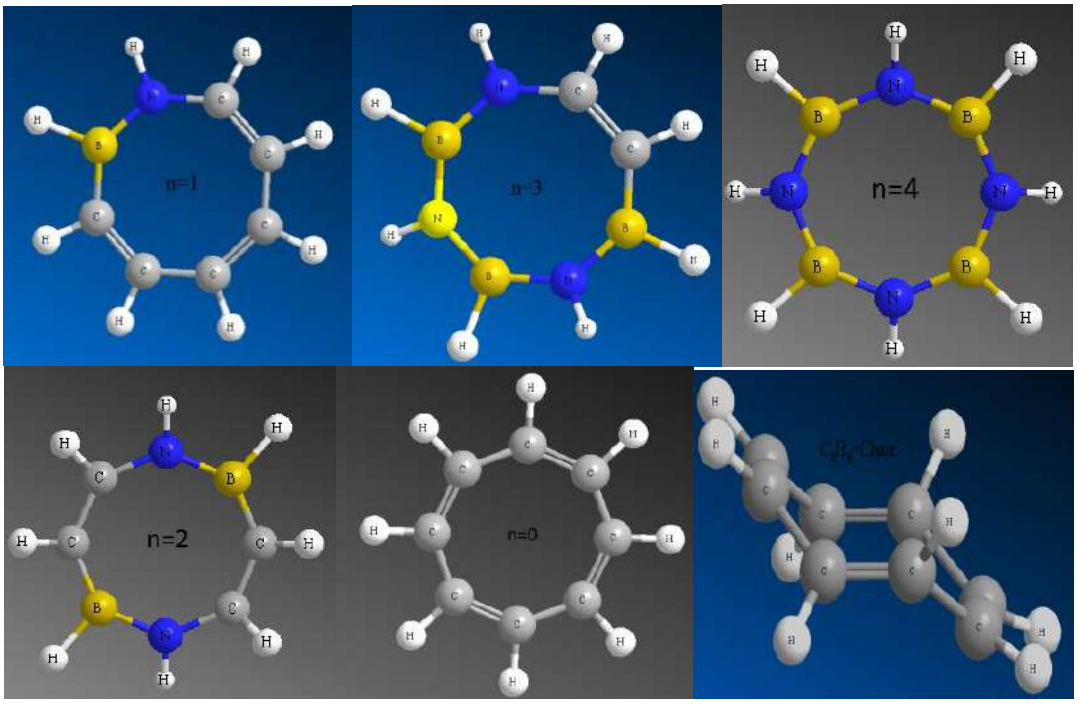
Luz, 1982). Although the planar D_{4h} structure for the ring inversion of COT has a transition state (TS) with around 12 kcalmole^{-1} barrier energy (Nishinaga et al., 2010), the D_{8h} bond switching TS lays a few kilo calories per mole higher. Actually, COT has three fundamental structural changing including 1- ring inversion, 2-bond shifting and 3- valence isomerization (Schild and Paulus, 2013).

Planar conjugated COT^{2-} exhibit a strong link between p-electrons. Coupling between COT^{2-} charge state and its mechanical conformation creates new opportunities for COT^{2-} as an aromatic molecule including electromechanical converter treatment (Wenthold et al., 1996).

Replacing of Boron and nitrogen atoms in COT help us for explaining the details of mentioned magnetic mechanism concerning the ring currents of the carbon disappearing in the isoelectronic azabora-hetero-cycles variants ($B_nN_nC_{(8-2n)}H_8^{2-}$,n=0,1,2,3and4 scheme.1 (Wu et al., 2012) and (Stevenson et al., 1998) . Steiner and coworkers investigated a model via frontier-orbital contributions which yields an accurate account of p ring currents in benzene, COT^{2-} and suchlike planar rings (Schild and Paulus, 2013). London, Pauling and Pople investigated the concept of aromaticity and anti-aromaticity in view point of magnetic criterion, diatropic (Planer of 4n+2 systems) and paratropic currents (planar of 4n systems) (Yoshida et al., 2015). Recently, it has been shown that the ring currents are a consequence of the HOMO–LUMO transition depends on symmetry properties (Andrés et al., 1998). For the 4n+2 hetero-cycles, $B_nN_nC_{(8-2n)}H_8^{2-}$(n=0,2,4), densities maps, exhibit the "p" electrons with the localized circulations around the electronegative nucleus (Hrovat and Borden, 1992).

In this work we exhibited that an extension of the figurative orbital model is able to account for both the currents in carbocyclic aromatic rings and their B-N analogues such as $B_4N_4H_8^{2-}$. Although it is generally agreed that $B_3N_3H_6$ is not aromatic (due to localized of p electrons on the more negative nitrogen atoms), they have suitable resonance energies for aromatic reactions. Although a few derivatives of the homologues rings of $B_nN_nC_xH_y$ such as diazadiboretane and borazoin have been synthesized, some compounds

of $B_nN_nC_{(8-2n)}$ H_8^{2-} (n=0,2,4) have not been prepared yet. Therefore any theoretical calculation and detailed discussion might be useful for understanding in the area of aromaticity and also physical chemistry mechanism of these kind compounds.



Scheme.1: $B_n N_n C_{(8-2n)} H_8$, including n=0 ,1, 2,3 and 4

1. Theoretical background

1-1. Aromaticity & ring current

Current-density's map can be estimated through theoretical methods without any gauge-dependence problem by vector potential generating of the magnetic field. Meanwhile from occupied to unoccupied orbitals, the total current densities are evaluated which are modulated and governed by energy denominators and symmetry rules respectively. Aromaticity can be also defined through magnetic criteria (Longuet, 1967) and is a trustworthy account of the currents induced by an external magnetic field capability. In addition chemical shift, isotropy, anisotropy, span, asymmetry and other properties are all integrals of these current densities . For the magnetic criterion, the

resultant of all such components explains the aromaticity or anti-aromaticity which is related to the net dia-tropicity and para-tropicity of the ring current respectively.

1.2. Anticancer properties, heterocyclic rings and Aromaticity

Cancer is one of the important causes of death in the new century. This work is done for developing of modern anticancer drugs. Many of heterocyclic compounds are known as anticancer drugs such as alkylating agents which have targeted cell DNA causing cell death. Heterocyclic structures are composed by atoms other than carbon, where the most times substituents are sulfur, oxygen, Boron and nitrogen. The model size of heterocyclic ring such as $B_n N_n C_{(8-2n)} H_8$, with the substituent group of the core scaffold, impact tightly on the chemical and physical properties while among the clinical applications, heterocyclic compound has an active role as anti-bacterial, anti-viral , anti-fungal , anti-inflammatory and anti-tumor drugs. Traditional drugs for anticancer such as alkylating agent has targeted cell DNA causing cell death. Generally, chemical-physics and biochemical properties like donor-acceptor capability, hydrogen bond, π-π stacking interactions, van der Waals, co-ordination bonds with metals and in total hydrophobic forces have caused the increasing interest in anticancer studies for such compounds $B_n N_n C_{(8-2n)} H_8$. These properties are important of understanding for their reactivity enable derivatives to readily bind with various nucleic acids, enzymes and biological structures.

1.3. Isotropic and anisotropic parameter

Spherical tensors can be noted as $\sigma_0^{iso(2)} = \sqrt[2]{3/2}\,\zeta_{(zz)}$ And $\sigma_{\pm 2}^{sym(2)} = \frac{1}{2}\zeta_{(zz)}$ **(1)**

Where, $\zeta_{(zz)}$ is the reduced anisotropy and can be calculated through $[\zeta_{(zz)} = (\sigma_{zz} - \sigma_{iso}) = (\sigma_{33} - \sigma_{iso})]$**(2)**. Haeberlen and Mehring (Haeberlen, 1967) have investigated fundamental tensors as $\sigma = \sigma^{iso(0)} + \sigma^{anti(1)} + \sigma^{sym(2)}$ **(3)**. This parameter is related to the anisotropy $(\Delta\sigma)$ with $\Delta\sigma = \frac{3}{2}\zeta_{(zz)}$ **(4)** and (η) shielding which can be estimated via

:$\Delta\sigma = \sigma_{zz} - \frac{1}{2}(\sigma_{xx} + \sigma_{yy})$ **(5)** *and* $\eta = \left(\frac{\sigma_{yy}-\sigma_{xx}}{\zeta_{(zz)}}\right) = \frac{3(\sigma_{yy}-\sigma_{xx})}{2\Delta\sigma}$ **(6)** (Anet and O'Leary, 1992).

Since the magnetic resonance of a spin is seldom isotropic, therefore they have to represent by new tensors by Herzfeld-Berger notation. These tensors are known as Span (Ω) Ω ≥ 0, which describes the maximum width of the model and the skew (**κ**) of the tensor which is a magnitude of the values (Ω) $= \sigma_{33} - \sigma_{11}$ **(7)** *and* $\kappa = \frac{3(\sigma_{iso}-\sigma_{22})}{\Omega}$ **(8).** Moreover the orientation of asymmetry tensor is given by $\kappa = \frac{-3\Upsilon_{(yy)}}{\Omega}$ *or* $\kappa = \frac{3(\sigma_{1so}-\sigma_{22})}{\Omega}$ **(9)** (-1≤ κ ≤ +1), and$\Upsilon_{(yy)} = \sigma_{22} - \sigma_{iso}$. Asymmetry (η) indicates that how much deviation can be appeared from an axially symmetric tensor, therefore the region of η is between zero and one (0 ≤ η ≤ +1) and in some cases η = 0.

1.4. ELF and LOL functions

Electron density can be written as $\rho(r) = \eta_i \left|\varphi_i(r)\right|^2 = \sum_i \eta_i \left|\sum_l C_{l,i}\,\chi_i(r)\right|^2$**(10)**. Where "χ" is the basis function of orbitals and η_i is occupation number. *C* is also a coefficient matrix. The unit of electron density in atomic scale is e/Bohr^3. Bader exhibited that the regions with having large electron localization must have a large magnitude of Fermi-hole integration. Becke and Edgecombe cleared that spherically averaged like-spin pair has direct correlation to the Fermi hole. Consequently, they introduced a new function as "electron localization function" (ELF) (Lu and Chen, 2012).

ELF(r) = $\frac{1}{1+[D(r)/D_{0(r)}]^2}$ **(11)** where

D(r) = $\frac{1}{2}\sum_i \eta_i \left|\nabla\varphi_i\right|^2 - \frac{1}{8}[\frac{|\,|\nabla\rho_\alpha|^2}{\rho_\alpha(r)} + \frac{|\,|\nabla\rho_\beta|^2}{\beta(r)}]$ **(12)** and $D_{0(r)} = \frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}]$ **(13)** for close-shell system, since $\rho_\alpha(r) = \rho_\beta(r) = \frac{1}{2}\rho$, *D* and D_0 terms can be simplified as D(r) = $\frac{1}{2}\sum_i \eta_i \left|\nabla\varphi_i\right|^2 - \frac{1}{8}\left[\frac{|\nabla\rho|^2}{\rho(r)}\right]$ **(14)** and $D_{0(r)} = \frac{3}{10}(3\pi^2)^{\frac{2}{3}}\rho(r)^{\frac{5}{3}}$ **(15)** .

Savin *et al.*, indicated which $D(\mathbf{r})$ reveals the excess kinetic energies densities caused by Pauli repulsion, while $D_0(\mathbf{r})$ can be noted as Thomas-Fermi kinetic energies densities. In other words they reinterpreted ELF in view point of kinetic energy through Kohn-Sham DFT's wave-function. Therefore ELF would be in the range of [0, 1] and a large ELF value indicates that electrons are strongly localized. ELF has been widely used for a wide variety of systems, such as organic and inorganic small molecules, atomic crystals, coordination compounds, clusters.

LOL or Localized orbital locator is another function for locating high localization regions likewise ELF, invistegated by Schmider and Becke. $LOL(r) = \frac{\tau(r)}{1+\tau(r)}$, where $(r) = \frac{D_0(r)}{\frac{1}{2}\sum_i \eta_i \ |\nabla\varphi_i|^{\ 2}}$, (16) $D_0(r)$ for spin-polarized system and close-shell system are defined in the same way as in ELF. LOL has similar expression compared to ELF. Actually, the chemically significant regions that highlighted by LOL and ELF are generally qualitative comparable, while Jacobsen pointed out that LOL conveys more decisive and clearer picture than ELF. Obviously LOL can be interpreted in kinetic energy way as for ELF; however LOL can also be interpreted in view of localized orbital. Small (large) LOL value usually appears in boundary (inner) region of localized orbitals because the gradient of orbital wave-function is large (small) in this area. The value range of LOL is identical to ELF, namely [0, 1].

2. Computational details

Geometry & electronics structures have been accomplished using the m06 groups in (DFT) functional. This methods are based on an iterative solution of Kohn-Sham equation (Kohn and Sham, 1965) of DFT in the plane-waves with the projector-augmented wave pseudo-potentials. The Perdew-Burke-Ernzerhof (PBE) (Perdew et al, 1996) exchange-correlation functional of the generalized gradient approximation (GGA) is adopted. The geometry of each part of ions was optimized at the various methods including M062x/cc-pvdz, M062x/cc-pvtz and CASSCF methods. For obtaining ab-initio amounts on the currents in BN analogues of the 4n and 4n+2 carbo-cycles, calculations

were performed for $C_8H_8^{2-}$, BNC6H8, $B_2N_2C_4H_8$ and $B_4N_4H_8$ and currents were calculated by using the ipsocentric approach. At this level of theory, C_8H_8 and $B_4N_4H_8$ have planar structures with D_{4h} symmetry. To draw the contour line maps of Current-density for both the constrained planar and the fully optimized structures Multiwfn software have been used. We have plotted the contour line corresponding to electron densities=0.001 a.u., which are defined by R. F. W Bader (Bader, 1990). This is useful for analyzing distribution of the electrostatic potential on potential surfaces. Such contour lines have also been plotted in gradient lines and vector field's maps through the same options.

The relief maps were used for presenting the height data at each point. If these values are too large, they will also be truncated in those graphs. Therefore, it can be chosen for scaling the values with a factor for avoiding truncation. Shaded surfaces maps with and without projection are used in our representation of height values at each situation. For confirmation the data several extra calculation including MP4 (SDQ)/6-31+G(d'), QCISD(T)/6-31+G(d') and CAM-b3lyp/6-311g have also been done. The charges transfers were also evaluated using the Merz-Kollman-Singh, chelp, or chelpG . Those methods are based on molecular electrostatic potential approaches (MESP) fitting which are suitable for small molecules (in large molecules some of the innermost atoms are located far away from the points at which the MESP is computed). Obviously the representative atomic charges for molecules should be computed as average values over several molecular conformations. A detailed overview of the effects of the basis set and the Hamiltonian on the charge distribution can be found in.

The electron densities (Both of Gradient and Laplacian), values of orbitals and LUMO, HOMO wave-functions, electrons spin densities, electrostatic potentials from nuclear atomic charges, electrons localization functions (ELF), localized orbital locator (LOL) and total electrostatic potential (ESP), as well as the exchange-correlation densities, correlation holes and correlation factors, and the averages local ionization energies using the Multifunctional Wave-function Analyzer have also been calculated in this work. Among the various methods and basis sets (both large and medium) which have

been used in this study, the cc-pvdz and cc-pvtz basis sets exhibit the most favorable results for electrostatic potential (ESP) fitting. The cc-pvdz is a double-ζ basis set with a single set of polarization functions for B to F and cc-pvtz is a triple-ζ basis set including diffuse functions, double d-polarizations, and a single set of polarization functions. The active space for the CASSCF method was composed of all valence electrons and orbitals of B, N and C atoms. A Quadratic CI calculation including single and double substitutions has been used to evaluate various one-electron properties including NBO, bonding analysis, atoms in molecules (AIM), natural population analysis, multipole moment, electrostatic potentials, and electrostatic potential-derived charge using the Merz-Kollman-Singh, chelp, or chelpG (Besler et al., 1990).

The AIM keyword is also used for computing the atomic charges of atoms in molecules, covalent bonds, localized orbitals, and critical points for any further properties predication of atoms in molecules (Chirlian and Francl, 1987). In addition Polarizabilities and hyper-polarizabilities have been calculated through CISD, QCISD and CASSCF methods. CHELPG charges (Martin and Zipse, 2005) can also be computed using the well-known ab initio quantum chemical packages such as Gaussian or GAMESS-US. In this study, it is indeed difficult and at some points not important to use the large basis sets and demanding methods such as MRCI for CHELPG and ESP calculations due to the large number of calculations in various situations of MESP simulation. Therefore, with medium methods in terms of computational cost, we have found the accurate results for our approach. All the calculations were performed using the Gaussian program package and the optimization were done along with the frequencies calculation for confirming that the geometries were real minimum without any imaginary frequencies.

3. Result and discussion

The compounds of $B_n N_n C_{(8-2n)} H_8$, (n=1,2,3 and 4) have not been synthesized, although many derivatives of the homologues such as di-aza-di-boretidine and borazocine have been prepared.

Although 8p-electron of $B_nN_nC_{(8-2n)}H_8$, (n=2,4) were originally called "an inorganic Compounds" and believed to have a resonance energy similar to that of Annulene, they were soon recognized that they took part in few reactions typical of aromatic systems. Geometries and energies of $C_8H_8^{2-}$ in various methods have been listed in Table.1. It has been exhibited(Table.1) that m062x/cc-pvTz method has more accurate results compare to other methods, therefor this method has been considered for investigation and calculation on variant of $B_nN_nC_{(8-2n)}H_8$, (n=0 ,1,2,3 and 4). It is now generally agreed that homologues rings of $B_nN_nC_xH_y$ such as diazadiboretane and borazoin are not aromatic.

In contrast to benzene or $C_8H_8^{2-}$, the p electrons are localized on the more negative nitrogen atoms, even if a few chemical behaviors are reminiscent of that of aromatic rings. ELF current-density map from ab initio calculations on COT^{-2} and $B_4N_4H_8^{2-}$, are shown in (Fig.1) and the currents are dominated by HOMO contributions Table 2.

Table.1: Geometry and energy of $C_8H_8^{2-}$ in various methods

Methods	Energy (Hartree)	C-C &C-H in resonated ring (Å)
MP4(SDQ)/6-31+G(d')	-308.46562	1.415, 1.100
QCISD(T)/6-31+G(d')	-308.52139	1.415, 1.08
CAM-b3lyp/6-311g	-309.24996	1.413, 1.099
m062x/cc-pvdz	-309.33567	1.415, 1.05
m062x/cc-pvTz	-309.43505	1.409, 1.094

Table.1: continue: HOMO/LUMO and Aromaticities

C-C-C and H-C-C angle in resonated ring	LUMO/HOMO Gap Energy $kJmol^{-1}$	Aromaticity	
		NICS	S-NICS
135.0, 112.5	519.06	-14.95	-15.85
135.0, 112.5	519.13	-15.11	-15.83
135.0, 112.5	519.05	-14.87	-15.87
135.0, 112.5	547.1	-17.59	-15.88
135.0, 112.5	493.43	-15.90	-15.82

Table 2. HOMO/LUMO and Aromaticities

Molecule	LUMO/ HOMO Gap energy	% composit for HOMO	% composition of atoms for LUMO
$B_4N_4H_8^{2+}$	3.34 eV	23.0(B1+B4 +B6+B7)	7.8 (B1+ B4 + B6 + B7) +10.5 (N2+N3+N5+N8)
$B_4N_4H_8^{2-}$	3.54 eV	25.0(B1+B4 +B6+B7)	6.8 (B1+ B4 + B6 + B7) + 11.5 (N2+N3+N5+N8)
$B_4N_4H_8^{0}$	3.14 eV	26.0(B1+B4 +B6+B7)	7.1 (B1+ B4 + B6 + B7) + 12.1 (N2+N3+N5+N8)
$B_2N_2C_4H_8^{2-}$	4.055 eV	30.0(B1+B7) + 4.0 C3+ C5) + 15.9 (C4+C6)	9.0 (B1+B7)+ 19.4 (N2+N8)- 4.7(C3+C5) + 34.6(C4+C6)+9.1B7
$BNC_6H_8^{2-}$	4.59 eV	7.0N1+8.6B2 +1.2C3+23.0 (C4+C8)+0. 6C5+33.4C 6+0.9C7	1242B2-43N1-1580C3+99 C4+4205C5+5610C6+15 207 C7

In a ring with "4n+2" electrons, the HOMO and LUMO are related to "n+1" and "n", but for a ring with "4n" electrons, the HOMO and LUMO are derived from a split degenerate (λ=n). For n=4 or $B_4N_4H_8$ λ is zero and meanwhile dia-tropic contribution arises from a transition in which $\Delta\lambda$ =+1 and a para-tropic contribution arises from a transition in which $\Delta\lambda$ =0 .

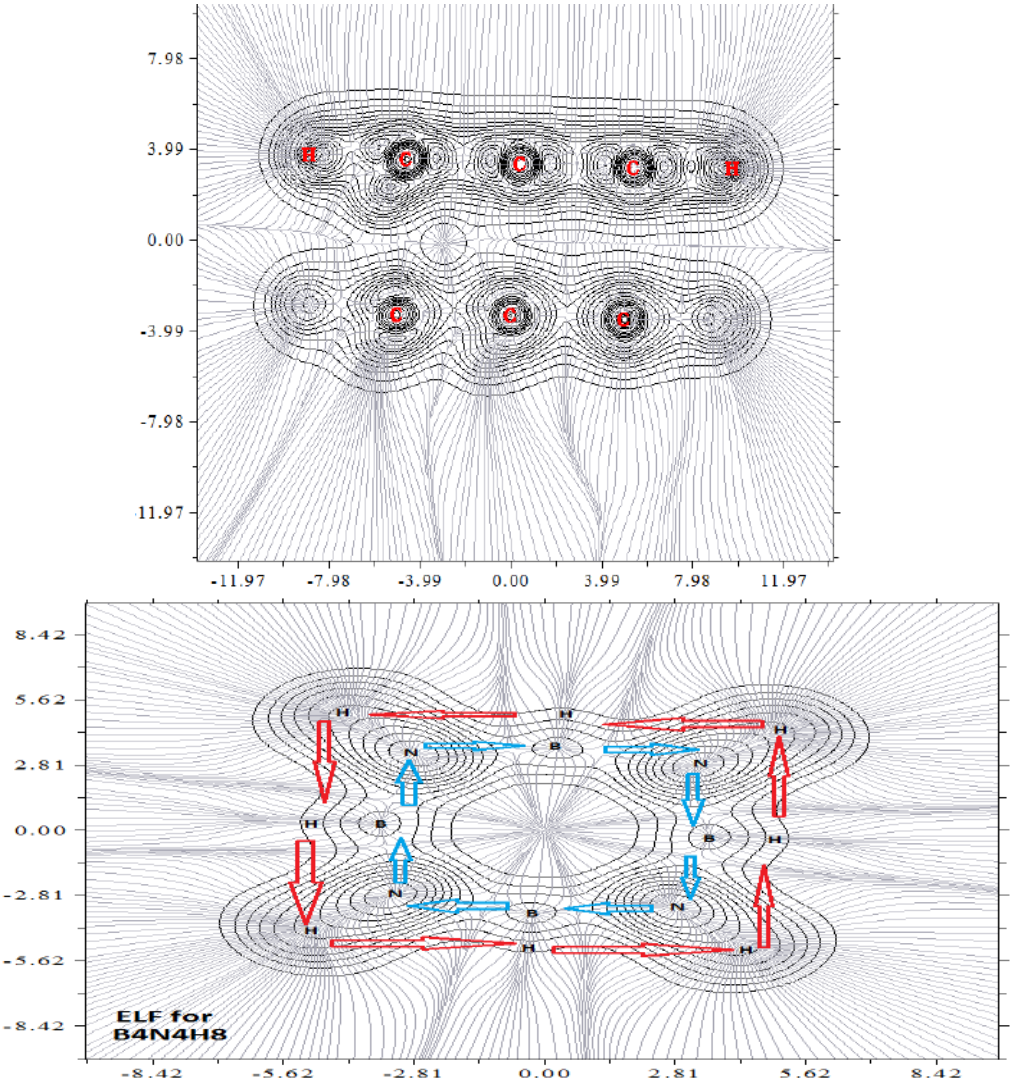


Fig1: Gradient lines map of ELF and current density induced in cyclooctatetraene ($C_8H_8^{2-}$) and boron nitride in cyclooctatetraene ($B_4N_4H_8^{2-}$) by a perpendicular external magnetic field.

Calculated by the Cam-B3lyp/ 6-31G**. Anticlockwise circulations are Dia-tropic, clockwise circulations Para-tropic

% composition of atoms for (HOMO-1)	HOMO/LUMO overlap in whole space	HOMO/HOMO -1 overlap	Molecule
23(N2+N3+N5+N8)	0.314	0.323	$B_4N_4H_8^{2+}$
25(N2+N3+N5+N8)	0.348	0.338	$B_4N_4H_8^{2-}$
26(N2+N3+N5+N8)	0.316	0.344	$B_4N_4H_8^{0}$
0.02B1+15.3N2+28.9C3+5.7 C4+28.8C5+5.7C6+0.01B7+ 15.3N8	0.333	0,554	$B_2N_2C_4H_8^{2-}$
13.4N1+1.1B2+2.5C3+21.3C 4+16.8C5+0.5C6+23.7C7+1 5.4C8	0.152	0.718	$BNC_6H_8^{2-}$

Therefore for the 4n+2 systems (with higher symmetry) only the HOMO–LUMO transitions are consider (dia-tropic current) and for the "4n" ring (lower symmetry) two forms can be considered , first the HOMO–LUMO transition leads to a para-tropic contribution, and second HOMO–LUMO+1 transitions to the dia-tropic contributions (Table.2)(Monajjemi et al, 2010; Monajjemi and Khaleghian, 2011; Monajjemi, 2012). In Huckel theory it is needed to rearrange the Coulomb and resonance integral parameters as: (1) boron and nitrogen are zero- and two- electron.

Table.3: HOMO and LUMO characteristics in several molecules

Therefore in structure of $B_nN_nH_n$ with the differing electro-negativities of boron and nitrogen a symmetric changing to the Coulomb parameters yield $(\alpha-\gamma\beta)$ and $(\alpha+\gamma\beta)$ energies which γ is a correlated parameter in various $B_nN_nH_n$ structures and varied between $0\leq\gamma<1$. Solution of the Huckel equation via considering the γ parameter with a simple modification gives molecular orbitals $\{\emptyset\}$ and related energies $\{\varepsilon\}$ from which the Consequences for cycle currents can be deduced. Canonical molecular orbitals (Streitwieser, 1961) $(\Psi_{\lambda,c})$ are delocalised set with $(\gamma=0)$ and in each position of $\gamma\neq0$ a linear combinations of these set can be written for orbitals.

In the full symmetrical systems of carbocyclic, the degeneracy of $\Psi_{2,c}$ and $\Psi_{2,s}$ can be stabilized through several ways such as distortion to D_2d and D4h geometries of "clamped"-substituted COT systems. Due to its bond alternation, planar D4h COT keeps delocalized orbitals and the cycle current of the equilateral carbocyclic, as Fig.1 exhibits. In the heterocyclic systems or $(\gamma\neq0)$ $\Psi_{2,c}$ and $\Psi_{2,s}$ are bonding and antibonding wave function, respectively, and are belongs to the B1u and B2u symmetric on the setting of D4h within D8h. It is notable wave functions $\Psi_{2,c}$ and$\Psi_{2,s}$, is the HOMO and LUMO, for all amounts of γ, which is completely localized, the HOMO on the nitrogen atom and the LUMO on the boron atom. Obviously,$\emptyset_{0,c}$, $\emptyset_{1,c}$, $\emptyset_{1,s}$, $\emptyset_{3,c}$,$\emptyset_{3,s}$ and $\emptyset_{4,c}$, become strongly localized on the electronegative atom. In the $\gamma=1$ the nitrogen and boron atoms Obey from Huckel's population as $1\pm\frac{1}{2}(\frac{1}{2}+\frac{1}{\sqrt{3}}+\frac{1}{2\sqrt{5}})\approx 1.66$ and 0.36 electrons, respectively. In the Huckel–London approach the ring current of the eight-membered ring in small amount of γ, HOMO–LUMO contribution overcome to the bond–bond polarizability. By increasing the γ from the planar-constrained of COT (where $\gamma=0$) to the B4N4H8 planer (where $\gamma=1$), the eight-membered ring has still net para-tropic circulation. The symmetry conclusion to deduct the line currents in 4n π position includes several steps; firstly $(\gamma\approx0)$, those currents are overmatched via the HOMO–LUMO transitions amongst small gap energies. This situation $(\Delta\lambda=0)$ generates an intense, para-tropic intensities.

In other words the symmetry reasoning for deducing the currents in 4n systems consist of several levels from (γ =0), which the current is under HOMO–LUMO transition with a small energy gap towards γ =1which, the HOMO–LUMO gap opens, and the intensity of the current falls but remains paramagnetic. Here the separation of HOMO-1 and LUMO as well as HOMO and LUMO+1 increase slowly and the para-tropic or anti-aromatic cycle current is reduced Significantly.(Tables2-4), Current-density maps, ELF and LOL from ab-initio calculations on the $B_nN_nC_{(8-2n)}H_8^{2-}$, are shown in Figures1-3 and are listed in tables 4,5.

Aromatic fluctuation index (FLU) & De-localization index (DI)	Para delocalization index(PDI)	Para linear response indexes (PLR)	Molecule
FLU=0.002 DI for all B-N atoms pair in the ring =1.24	PDI=0.041	PLR=0.18	$B_4N_4H_8^0$
FLU=0.001 DI for all B-N atoms pair in the ring =1.30	PDI=0.031	PLR=0.16	$B_4N_4H_8^{2-}$
FLU=0.000 DI for all atoms pair in the ring =1.46	PDI=0.035	PLR=0.14	$B_3N_3C_2H_8^{2-}$
FLU=0.003 DI for B1-N2 atom pair= 1.370 and for N2-C4=1.4 And for C4-C5=1.6	PDI=0.029	PLR=0.15	$B_2N_2C_4H_8^{(0)}$
FLU=0.003 DI for N1-B2 =1.32	PDI=0.014	PLR=0.04	$BNC_6H_8^{2+}$

Table.4, 5: continue Localization index (LI), Ring perimeter, Aromatic fluctuation, PDI and PLR for variants of $B_n N_n C_{(8-2n)} H_8$, (n=0 ,1,2,3 and4)

Molecule	Ring perimeter(Å) & area(Å^2)	No. Pi Orbitals & No. Pi electrons	Localization index (LI)
$B_4N_4H_8^0$	11.41& 10.12	20 & 10	For all B atoms=3.24 For all N atoms=5.44
$B_4N_4H_8^{2-}$	11.56 & 10.04	22 & 10	For all B atoms=3.195 For all N atoms=5.567
$B_3N_3C_2H_8^{2-}$	11.41 & 9.73	24 & 8	B1 to B3=4.102 N1toN3=3.22 All H atoms=0.345
$B_2N_2C_4H_8^{(0)}$	11.40 & 9.94	16 & 10	B1,B7=3.27 & H9, H15=0.49 N2,N8=5.4
$BNC_6H_8^{2+}$	11.42& 9.84	8&8	N1=5.45, B2= 3.13, C3=4.4, C4=4.33, C5=4.137, C6=4.412, C7=4.5,C8=4.33,

For each molecule, the maps indicate total p and s contributions for inducing current densities. As expected, the currents arising from the p electrons are, respectively, strongly dia-tropic in benzene and strongly para-tropic in COT. The currents are dominated by HOMO contributions in both cases. An angular-momentum analysis shows how the symmetry rules account for these features. At each successive energy level, the

quantum (Daudel et al., 1959) number, l (=0,1...,N/2), increases by one. In a cycle with N=4n+2 electrons, the HOMO and LUMO correspond to l=n and n+1, respectively. It is notable that that photo-excited cyclooctatetraene relaxes toward the planar *D8h*-symmetric and its structure appears to be identical to the thermal double bond shift transition state. This is the typical π-delocalized structure expected to characterize for a Huckel anti-aromatic [4*n*] system. As it can be seen in the Table.3 the some electrons are localized and some other is not on the aza-bora-hetero-cycles variants. For benzene the low energies may only involve one delocalized allyl radical and three adjacent unpaired electrons while , in cyclooctatetraene, due to its larger size, a new and more stable tetra-radical-type configuration might be possible.

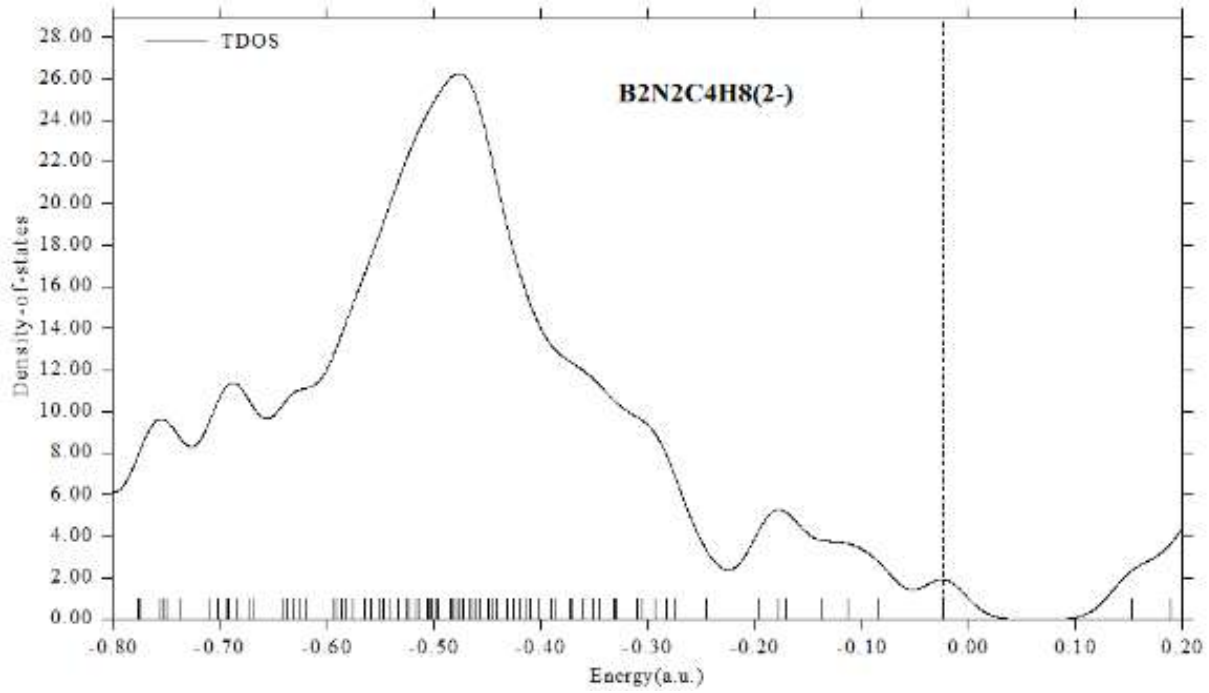
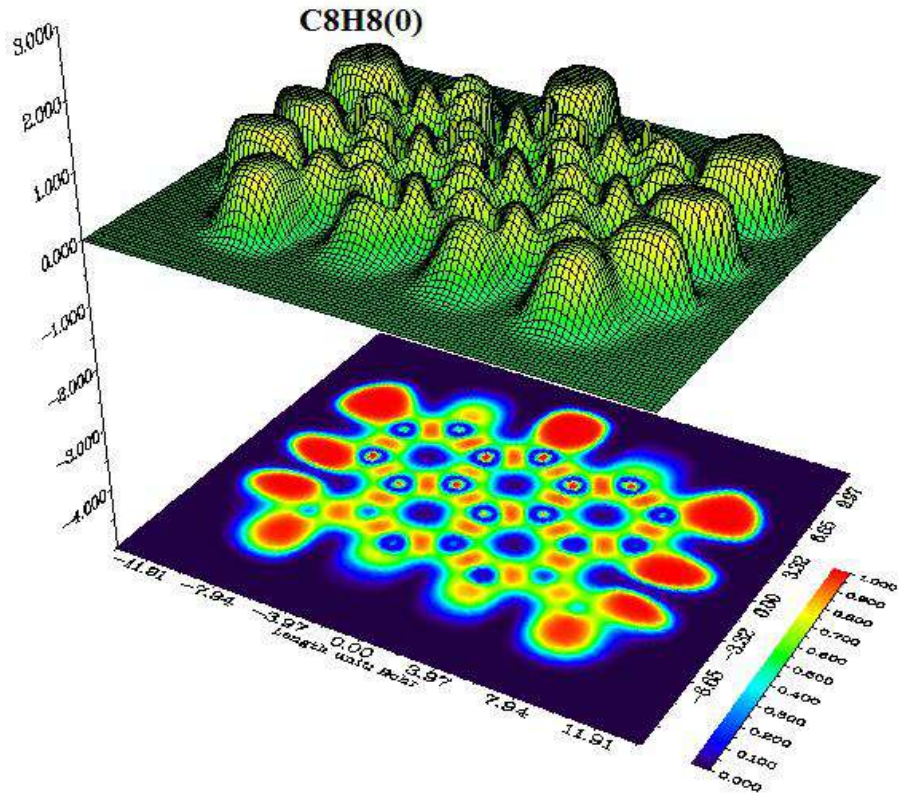


Fig.2: Density of states for π electrons in the rings

Table.5: Various calculations of charges for $C_8H_8^{2-}$ and $B_4N_4H_8^{2-}$

(MK)Merz-Kollman ESP fitting Sum of values=-2	Mayer's valance	Wiberg's bond order
-0.868949, -0.154367 0.430606, 0.092885 0.428573, 0.094883 -0.866058, -0.155198 0.421720, 0.094818 -0.868144, -0.154232 -0.851509, -0.160690 0.417617, 0.098044	3.35, 0.86 2.98, 0.90 2.98, 0.90 3.35, 0.86 2.98, 0.90 3.35, 0.86 3.35, 0.86 2.98, 0.90	B1-N2: 1.244 B1-N3: 1.244 N2-B4: 1.244 B4-N5: 1.244 N5-B7: 1.244 B7-N8: 1.244 N8-B6: 1.244 B6-N3: 1.244

Fig.3: ELF for variants of $B_n N_n C_{(8-2n)} H_8$, (n=0,1 ,2,3 and4)



COTs have extended delocalized structures (i.e., identical 1.40 Å π-bonds and planarity, recalling an aromatics system). Therefore, it can be image that COT as being

stabilized by a kind of aromatic effects which plays against the out-of-plane deformation needed for reaching both the boat and the kink structures due to those motions which break delocalization. The total electrostatic potential for variants of $B_nN_n C_{(8-2n)} H_8$, (n=0 ,1,2,4) are plotted in Fig.4. As it can be seen in the Fig.4 the stable electro static for those variant are started in positions 1.40 Å, 1.45 Å, 1.48 Å,1.50 Å for CH_8H_8, $B_4N_4H_8$, $B_2N_2C_4H_8$ and BNC_6H_8 which is correspond to bond length and they will be ended in the positions around 5.5 for CH_8H_8 and 10.5 for other variants.

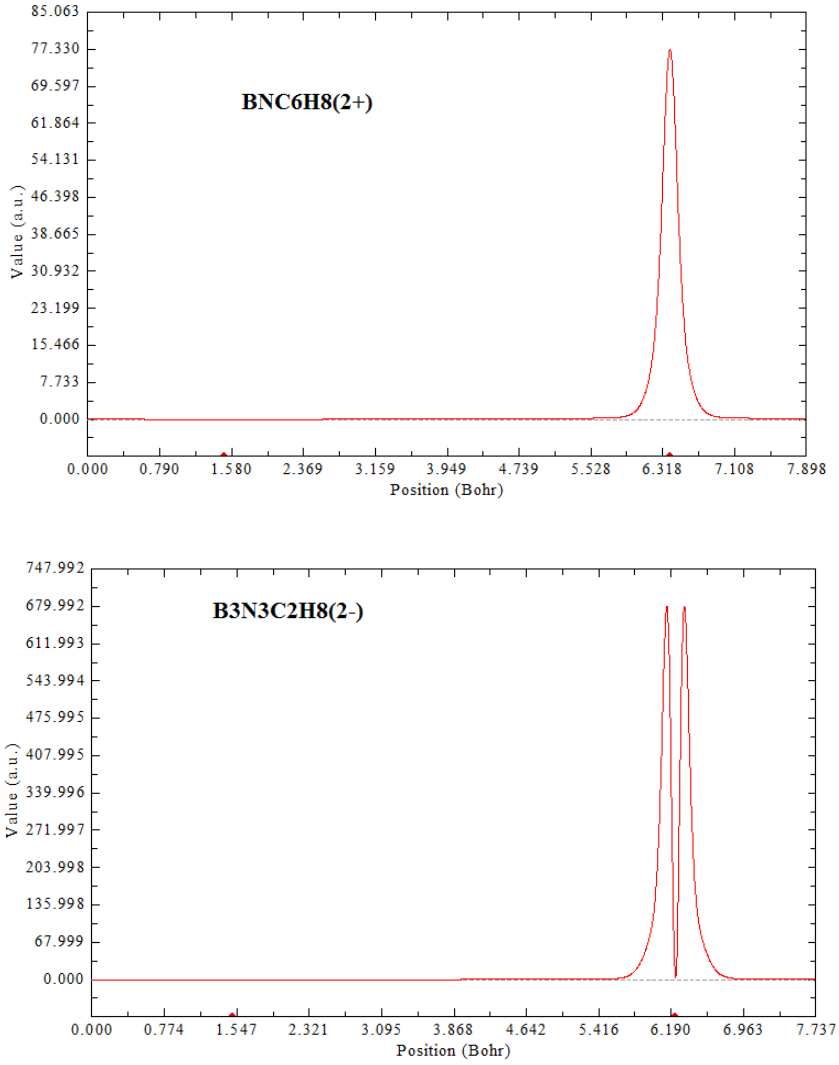


Fig4: Total electrostatic potential for variants of $B_n N_n C_{(8-2n)} H_8$, (n=0,1 ,2,and 4)

Conclusion

Current-density maps, ELF and LOL from ab-initio calculations on the $B_nN_nC_{(8-2n)}$ H_8^{2-}, are investigated as a novel method for understanding the aromaticity and anti-aromaticity in heterocyclic compounds by this work. For each molecule, the maps indicate total p and s contributions for inducing current densities. As expected, the currents arising from the p electrons are, respectively, strongly dia-tropic in benzene and strongly para-tropic in COT. The currents are dominated by HOMO contributions in both cases. An angular-momentum analysis shows how the symmetry rules account for these features.

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The concept of flexibility in the formation of contemporary biological spaces

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Mahsa Soltani **

ABSTRACT
Flexibility in architectural spaces makes it possible to adjust the living conditions associated with human settlements and adapt the residential unit to human behavior. Today, due to the lack of a correct statement about the proper placement of spaces, biologic neighborhoods in relation to geographic location and the neglect of the true concept of comfort in modern buildings, seems necessary to provide appropriate solutions to this problem. What is the concept of flexibility and how to create and achieve solutions for the reconciliation of the human environment in the climate of own habitat? All of this research seeks to provide a solution to the creative design of flexible spaces, with goals such as: improving and increasing the performance of residential spaces, developing creative design solutions in residential spaces, introducing theoretical foundations and criteria for flexible spaces, and taking advantage of in today's design of housing. The study of theoretical concepts of flexible spaces will help residents to create comfort in the living space of contemporary buildings. This research proposes, through deductive reasoning, appropriate solutions to the positive effects of physical, functional, social and functional characteristics, on increasing the comfort of living in resident settlements. This research is of qualitative and descriptive-analytic method for elaboration of the issue of flexibility and promotion of biological comfort in contemporary habitat. In the discussion of theoretical foundations, a library research has been used including specialized sites, books and scientific articles that use Results and data aggregation can be found in effective physical solutions appropriate to the conditions of the construction of contemporary buildings in Iran.
KEYWORDS: Flexibility, Settlement, Space, Biocompatibility.

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El concepto de flexibilidad en la formación de espacios biológicos contemporáneos

RESUMEN

La flexibilidad en los espacios arquitectónicos permite ajustar las condiciones de vida asociadas con los asentamientos humanos y adaptar la unidad residencial al comportamiento humano. Hoy, debido a la falta de una declaración correcta sobre la ubicación adecuada de los espacios, los vecindarios biológicos en relación con su ubicación geográfica y el descuido del verdadero concepto de confort en los edificios modernos, resulta necesario proporcionar soluciones adecuadas a este tipo de problemas. ¿Cuál es el concepto de flexibilidad y cómo crear soluciones para la reconciliación del entorno humano con su propio hábitat? Esta investigación busca proporcionar una solución al diseño creativo de espacios flexibles, con objetivos tales como: mejorar e incrementar el rendimiento de los espacios residenciales, desarrollar soluciones de diseño creativo en espacios residenciales, introducir fundamentos teóricos y criterios para espacios flexibles, y tomar ventaja del diseño actual de la vivienda. El estudio de los conceptos teóricos de los espacios flexibles ayudará a los residentes a crear comodidad en el espacio habitable de los edificios contemporáneos. Esta investigación propone, a través del razonamiento deductivo, soluciones apropiadas a los efectos positivos de las características físicas, funcionales, sociales y funcionales, para aumentar la comodidad de vivir en asentamientos residentes. Esta investigación es de método cualitativo y descriptivo-analítico para la elaboración del tema de la flexibilidad y la promoción del confort biológico en el hábitat contemporáneo. En la discusión de los fundamentos teóricos, se ha utilizado una investigación bibliográfica, que incluye sitios especializados, libros y artículos científicos que utilizan resultados y datos que pueden emplearse para soluciones físicas efectivas apropiadas a las condiciones de la construcción de edificios contemporáneos en Irán.

PALABRAS CLAVE: Flexibilidad, Asentamiento, Espacio, Biocompatibilidad

Introduction

Flexibility in biological spaces is one of the most important concepts that the minds of humans have been focusing on for a long time and have sought a systematic approach to creating improved spaces, not only in terms of function but also in terms of the principles of aesthetics. As a result, by testing and utilizing these strategies, humans were able to identify biocompatible components by creating constant and semi-constant flexible spaces. Flexibility in architectural spaces creates a variety of variations that make it possible to adjust environmental conditions dependent on

human settlements and create a comfortable environment and adapt a residential unit to human behavior. By measuring their needs, these humans over time have come to understand the concept of flexible space.

1. Problem statement

Today, due to the lack of attention to the proper location of biological spaces and neighborhoods in relation to the geographical location, as well as the neglect of the real concept of comfort in the habitat of residents of contemporary buildings today, providing appropriate solutions to this issue seems necessary. What is the concept of flexibility and how it is created and how to achieve solutions to reconcile the environment of human life in the climate of one's own habitation is one of the issues that a person can always identify with and create these flexible spaces, effective communication between man and space, the opportunity for people to communicate with each other, with the context of their surroundings and the formation of everyday events, qualitative needs, access hierarchies, safety, and comfort.

2. The importance of research

Looking at the past and receiving the concepts of space and functional architecture of the era before, including residential buildings, we can actually conclude that the most prominent feature of the architecture of each settlement is the need for flexible spaces with the ability to evolve space in functional, physical, social and functional fields. In fact, the creation of space expresses what he wants to bring to man's mind, using functional forms, and on the other hand, observing the aesthetic principles. As a result, flexible and variable spaces can be changed over time and will create human needs.

3. Litreture Review

The idea of flexible design of residential units has been introduced since the beginning of the twentieth century as part of the modern movement by architects such as Le Corbusier, Mises and Huberakan. With common methods, various solutions, such as folding furniture, moving partitions, etc are offred. The possibility of overlapping of spaces in the interior composition of the building was provided. In the 1990s, flexibility became an effective means of solving the multiple and varied applications of housing in

rapidly changing societies, shifting from the idea of structural flexibility and functional flexibility, meaning that withoutthem the form of flexibility in the form of space, was able to accommodate various activities (Borhani, 2006).

In traditional Iranian homes influenced by the habitat and climate tradition, a summary of nature with regular geometry is organized in the inner courtyard of the house and all the original spaces of the house are opened to the human handmade nature, while traditional houses of Iranian building with fixed elements and slab walls was formed and the flexibility was created by moving the day and the person in different directions of the house. The most important spatial feature of the Shiraz houses is the visual and sensory connection of the main room of the house with the evergreen courtyard. Most of the houses in the old style of Shiraz are the main room of the main room of the house that this room is located on the northern front and the water pool facing it is to portray the lush green space of the courtyard with its dense water that illustrates the sky and trees are one of the most suitable tools. This large wooden bay, with the help of its various perceptions that can be moved to use, has many features. When the bottom of the whole understanding, interior spaces are completely separated from the space of the courtyard, the light passes through the colorful glasses a pleasant atmosphere.

With all the perceptions, the room turns into a porch that faces the courtyard. And by raising one of the perceptions, the communication is controlled by the yard (Memar, 2010; Rasooli Sani Abadi, 2017),). In the study of resilience in this research, from specialized books such as "A Yen Bentley" entitled "Responsive Environments" and architectural aesthetics from "Jorg Corrupt Grotter", an example of flexible housing cases on a scale and microclimate and flexibility of multi functional spaces have been used, and John Huberakan's paper, "Design for Flexibility (2008)" and from existing research in Iran, can also be found in articles such as a template for Flexibility, written by Alireza Einifar, who has been selected from a research project of the same name at Tehran University, which lists the types and factors Flexibility in traditional housing, in all of these sources, is flexible in adapting to housing changes to suit the current and future needs of users.

4. Purposes

In fact, flexible spaces in biological spaces are considered as a solution to prevent the collapse of people interactions with their habitat and the possibility of adapting housing to their physical and psychological needs, changing their audience and having flexibility with the ecosystem and the qualitative needs of each user. The aim of this research is to help improve the living space of residents by creating a comfortable environment for residents through a flexible way of creative design of flexible spaces. Therefore, the following goals are:

Develop a creative design approach in residential spaces. To introduce theoretical foundations and criteria for flexible spaces and the possibility of using it in today's housing design.

Address the theoretical study of the concepts of flexible spaces for creating comfort in contemporary buildings.

5. Hypothesis

Due to the inadequacy of the proper placement of biological spaces and the lack of consideration of the biological comfort in people's daily lives and the interactions of residents, as well as the lack of correct answer to the question of how to create spaces with greater flexibility in the design of contemporary residential buildings, the hypothesis of this research is that through deductive reasoning. It is able to offer a suitable solution for contemporary constructions by providing a positive impact on the physical, functional, social and functional features, increasing the comfort of the inhabitants' settlements, and able to organize the built spaces features for definition of the possible needs of its comfort.

6. Theoretical Foundations

Space in the design of architects is an attempt to create desirable and useful spaces for human beings that determine how to use it and generally consider the qualitative and quantitative dimensions of human behavior within each space of the scenario of space. According to Louis Kahn, "space particles open space that wants space." Charles Moore says: When a room is made of a floor and a ceiling and four walls, a sixth element alongside the six elements has a seventh element that is space, and this element has more effect than the physical elements that space has been made by them.

But the quality of space in the first place is dependent on the elements and the relation of these elements (Grother, 2004). This is where the organization of human space is constructed and changed in order to achieve the conditions, needs, and applications of a new term with a new dimension called the human space, with the definition of such a "human environment" of the metaphors of literary texts for achieving a concept which one calls the unconscious geometry of human space.

His analysis reveals a huge shift from the imagined space of the Renaissance, which is geometric and rational, to emphasize the "sense" of space, and in fact, the concept of space requires more displacement and from beyond the boundary of vision to a very sensory atmosphere going deeper "and, as a result, creates a flexible environment has been used to a large extent in traditional Iranian architecture from the earliest times. Flexibility is an applied concept for optimal use of residential spaces. Changes in life and human desires, executive needs such as the need to strengthen the relationship between designer-user and the transformation of lifestyle over time are the main reasons for this concept (Hall, 1996).

6.1. Siri in the concept of flexibility

To explain the concept of flexibility, research has been carried out and numerous definitions have been presented, some of which are further elaborated by the authors.

Table 1: Siri in the Concept of Flexibility

Thinkers	definitions
John Lang	Some environments provide many activities without changing or reorganizing. Some environments can easily be modified to provide various activities. Environmental designers have used different terms to define these two situations. Here, the first "adaptable" And the latter is called "flexible".
Robert Venturi	The postmodern architect is concerned with expressing the quality of the flexibility of the functionality of a space and believes that this building has several decent functionalities. A room can have different functions at one time or at different times.
Bentley	Places that can be used for a variety of purposes offer more choices to users than those designed for a limited, user-friendly environment. The environments that have the capability to offer such options are of a quality that is flexible. We call it

Rapport	The flexibility of a building is primarily related to its ability to be broadened (reproducible) or, conversely, to a smaller extent to meet a newer or wider need.
Grotter	When it comes to a system without having to compromise the principle of the system or its main elements and allow the space to be adapted to the need, it is talk of flexibility, and since the space constructors are defining that space, then it must inevitably be for Space flexibility These factors are also flexible
Hobrakan	The concept of flexibility is defined as building capability for physical change and adaptation with respect to changing conditions. Flexibility is "a new kind of challenging architecture"
Edward Hall	Since the building blocks of architectural space are defining it in its entirety, in order to achieve a flexible space, these elements of the components of the component must be flexible too.
OVEN	In the architecture and design of the environment, the concept of the flexibility of organizing the human space is made and changed in order to meet the conditions, needs and new applications.

Based on the studies carried out and the definitions of the term on theoretical foundations, one can express: Reflecting the concept of flexibility in designing a space architecture, responding appropriately to changing the needs of the audience and changing the functional patterns in accordance with the wishes of people and living environments that they are formed. Accordingly, by creating flexible spaces in traditional habitats and using them in the system of contemporary living environments, effective factors can be considered: increasing social interactions, regulating human relationship with man and nature with man, improving the quality of space, grading Suitable hierarchy of access to spaces, the ability to adapt and expand the spaces, and consequently to increase the comfort of the living can be helped.

6.2. Reasons for Flexibility

Explaining the need for flexibility in housing can clearly help the research question. Given the need for flexibility to change over time and with changing human needs, one can only generalize the factors that make effective payments. The need for flexibility in the residential unit can be classified into social-economic and economic functional areas. The requirements for functioning with changing family and household size, lifestyle changes, changes in activities and changes resulting from the aging process of household members and changes in the use of equipment, home appliances and furniture. The psychological and social effects of each of these changes

make residential space more flexible. The financial and human resources of the people can contribute to the creation of space flexibility if the impact of the functional factors and its social and psychological outcomes is well known.

6.3. Flexible variety

In a book on architectural planning, Perchal et al, 2015 have considered flexibility to include multifunctional architectural features, variations in internal spaces, and externality, and argue that each of these concepts alone can not replace the concept of flexibility. The important point to be taken from past experiences and its subsequent uses is that all the concepts of flexibility are not of a single species and on a scale. Identification of species and the scale of flexibility will help to better understand the concept. Variants of flexibility are defined as diversity (multifunctional concepts), adaptability (daily seasonal displacement), and versatility (segregation) (Perchal et all, 2005).

6.4. Adaptability (seasonal and daily displacement)

The versatility or the ability to coordinate a space with new conditions is required. In the new housing, adaptability is the ability to provide new needs by changing the interior walls and installing parts in residential units, provided that these changes do not change the area of the residential unit. In practice, the versatility of all internal changes, such as changing personality and structure, micro elements, and composition of spaces, are included. In planning of new residential complexes, the most effective way to achieve versatility, are the lack of internal implementation and the possibility of their various combinations. In traditional Iranian housing, following the map, the facade and the house spaces, a general pattern of formation and the establishment of fixed spaces, the adaptation of daily and seasonal life by adjusting the horizontal and vertical relationships of the house and the use of different spaces at different times of the day and in different seasons are possible. Spaces such as summer, winter, basement, and roof make it possible to adapt a home to different living conditions. The organizer of flexibility on this scale is the central element of the house, the courtyard (Einifar, 2003; Hobraken, 1986).

Table 2: Types of Flexibility (Versatility)

Flexible species		Iranian house
Adaptation	operational	The connection of the rooms by opening the doors, the connection inside and outside the house by opening in the curtain window
	Structural	Pimon is a modular with longitudinal divisions, with a pivotal function of roof covering with heavy and fixed walls
	Spatial	A room is used in the Iranian house around the room.

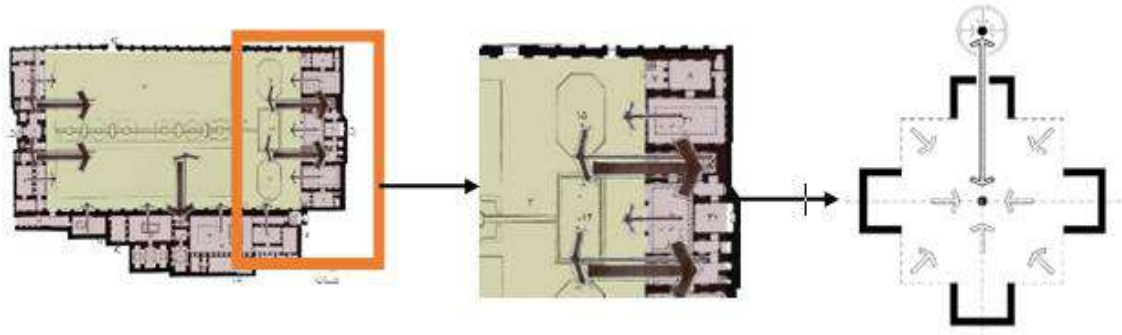


Figure 1: Types of Flexibility (Versatility)

1. B. Diversity (Multi Functional Space)
2. Variation is the ability to provide various uses of space.
3. This flexibility is affected by two variables of space and time.
4. Residential space can be used for several functions simultaneously, and for different functions at different times.
5. Variance can be achieved by designing a map with a regular geometric structure, easy and readily accessible access to housing equipment or by adjusting the size of the rooms.
6. Variation is the most basic and effective way to achieve flexibility in the design of traditional Iranian honey.
7. The reason for this is the ability to replace the working space over time.
8. The most important properties of spatial diversity are:
9. Easy and legible accessibility to the rooms
10. Integrating functions in a space and reducing waste in communication spaces
11. Usefulness of the access, so that the functions can be converted
12. Follow building facades from the general pattern of house formation

Table 3: Types of Flexibility (Diversity)

Flexibility Scales		Iranian homes
Variation	operational	The room responds to different functions at one time or at different times, such as the three doors and the five doors, summer and winter
	Structural	The structure of heavy structures and walls and ceilings are fixed
	Spatial	The porch and the interiors doors allow the flow of fluid between the spaces. The height of the room and the opening of the hall will help to distinguish between public and private spaces.

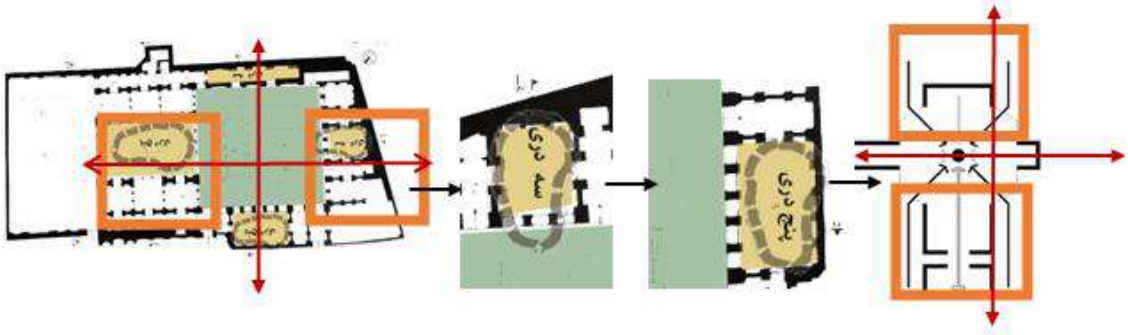


Figure 2: Species of Flexibility (Variability) - Source: Writer

6.5. Variability (segregation and aggregation)

In the design of housing flexibility, it is said to increase and decrease a little or the separation and aggregation of spaces and the possibility of returning to the initial design of a residential unit after its expansion or reduction. In this case, flexibility means the ability to respond to the growth of the household at different stages of life. In other words, this feature makes it possible to resize the residential unit either in the direction of its smaller size or in the direction of enlargement. The need for such flexibility may be due to long-term or short-term needs. The type of long-term, with changing the size of the household and the need for more space for life, and the type of short-term, space change is due to other reasons. Variability can be achieved in two ways by adding to the existing home infrastructure, and by separating its spaces (without changing the area).

This case has been applied to the horizontal or vertical expansion of traditional Iranian homes and the separation of multi-courtyard houses and their use for the extended family life in different stages of life (Einifar, 2003).

Table 4: Types of Flexibility (Separability)

Flexibility Scales		Iranian homes
Variation	operational	Self-propelled and single-span and fixed-span and single-span houses
	Structural	Fixed blood unit allows for more space than fixed
	Spatial	Native and small niches with each nest in the basement of the house make it possible for new entrants to have a stable home

Flexible species of Iranian house

Functional variation of the vertical and horizontal expansion of the house and the ability to separate and integrate multi-courtyard houses. The structure of a repeatable Peyman unit allows the use of a variable of a fixed structure space. Space change of the public and private space with the vestibular intermediate element on the threshold of the house. Possible to create a new entry for the house segregated sections.

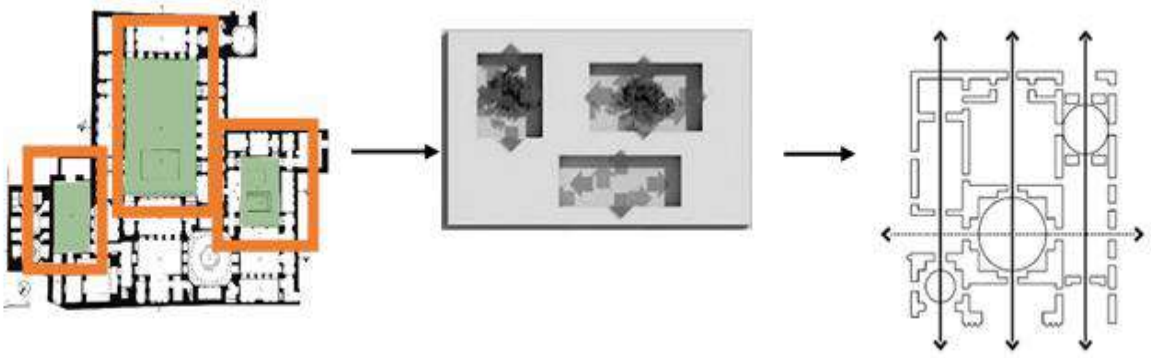


Figure 3: Types of Flexibility (Separability)

Different parts of space have different potentialities for influencing or interacting in flexibility. Two types of these sectors require special attention:

Soft and hard parts: In the form of buildings, there are spaces that offer common facilities such as stairways, elevators and ducts. In their place. These spaces are often considered to be part of the "hard" building. The probability of functional change in

these parts during the useful building is very low. This hard part should be deployed in places where the rest of the space can not be restrained. (Bentley et al., 2006).

Active and Inactive sections: Within an important range of productivity and potential, flexible exterior spaces depend on activities or organizations that occur in areas or adjacent areas. For some indoor activities, the ability to develop in adjacent outer public spaces may be beneficial. If such a process occurs, they will be involved in public space activities. (Bentley et al., 2006; Demaria, Colorado, 2015).

Table 5: Potential Impact Sectors on Flexibility

Potential Affecting Sectors	the part	Space	Change User	Location
	Soft and hard	Stairs, elevators, ducts	is low	Do not have any restrictions on other spaces
	Active and inactive	The adjacent parts of the outer exterior are flexible, such as edges	Relative to the life of the building can be changed	There is no limit to other spaces

Types of Flexibility Scales

Flexibility is defined in the dimensions and spatial and functional components of the home of the service spaces and the spaces of the recipient and the spaces of communication.

Small-scale flexibility: Micro-scale flexibility involves smaller and smaller design decisions, so it is critical to users and can be considered at the latest stages or in later stages. (Bentley et al., 2006).

Table 6: Flexibility Scales (Small Scale)

	Flexibility Scales	**Iranian homes**
Small scale	**Fixed space**	(Three doors, five doors, a hall, a windproof, a sash, a chest and a porch, a niche, a raft, etc., a tatami room, a closet, fixed doors
	Semi-stabilized space	Rugs, pillows, mattresses, tablecloths, etc.
	Shapeless space	A multi-functional space whose relations between elements are provided through interfaces such as the porch and the floor and the gate of the circle

Intermediate scale flexibility

This scale is related to the flexibility of a residential unit in how spaces are grouped to respond to household needs, and deals with the main pattern and home-based activities of the home. The functional layers of the building and the use of natural light and natural ventilation are very important in this regard. Also, the internal and external views of the house and their adherence to the general pattern of formation are also significant points. (Bentley et al., 2006)

Table 7: Flexibility Scales

Flexibility Scales		Iranian homes
Medium scale	Fixed space	The courtyard of the house and the communicator of the functional elements in the periphery of the yard
	Semi-stabilized space	Elements shaping the green space of the house and the bed on the pond and so on
	Shapeless space	The intruder courtyard is the place of all the home events. The relationship between the house's inhabitants and the fluid space between the inside and outside through the porch and elements such as the in-window

Macro-scale flexibility

The macro-scale flexibility is about the ability of variability in the use of the whole building as a single unit or major parts of the building. (Bentley et al., 2006).

Table 8: Flexibility Scales (Macro Scale)

Flexibility Scales		Iranian homes
Macro scale	Fixed space	Consolidation and separation of outer and inner courtyards and indirect communication with overstone interfaces with outer space
	Semi-stabilized space	Elements such as the cover of the courtyard ceiling that is used in certain times
	Shapeless space	The changing external and internal social environment of each

Flexibility is trying to answer a wide range of practices used in an environment. In this approach, by exploiting the potential for development, change, and multiplicity of the environment, the quality of the project designed to interact with the needs of its audience will increase. In general, the space created by the flexibility approach can be considered as a plan that responds to a variety of locations designed for specific and limited functionality in order to fit different needs of the audience, and the right to offers a greater choice for its users. Locations that have the ability to create such spaces can be examined and evaluated with the above features and behavioral characteristics. (Einifar, 2007). In the meantime, we examine the flexibility approach by analyzing the three key factors of "variability", "versatility" and "changeability:"

1) Depth of building: The use of buildings requires light and natural ventilation. Buildings with a very large depth or length can not easily respond to user changes in this regard.
2) Access: They need some communications and connections to the outside world. So the number of access points can be made by one of the users. The key elements of the organization are to facilitate the adaptation of the diversity of use in a building.
3) The height of the building also affects the importance of access to the height of the building. In high-rise buildings, the higher the floors go, the greater the limitations of access to the outside. Hence, the upper classes take a more inappropriate position for a wide range of applications. (Bentley et al., 2006).
4) Flexibility in the design of a residential home: In the traditional Persian house, the ordering base is the Paymun home, used in the form of a large, small pyramid, used by the architects of time. It is relying on that system, the highest task of the architect of cognition, the perception and visualization of the living and moving forces in the building was carried by the building, and with the aristocracy created in the design, and the proportions and dimensions of the perimeter sections were determined. (Abolqasemi, 1986).

Figure 1: Effective Flexibility Factor in the Long Term

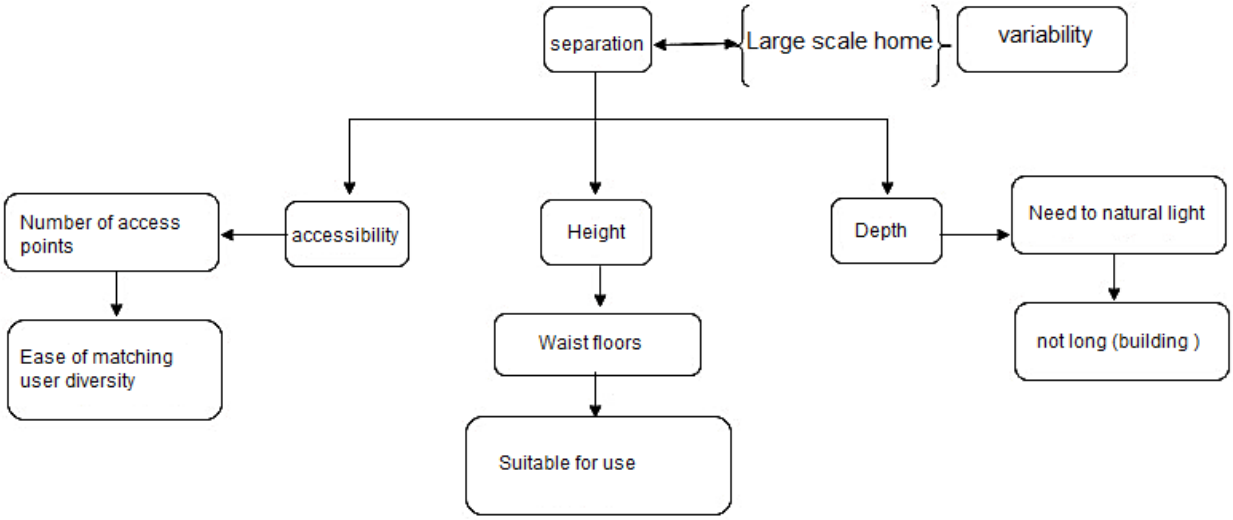
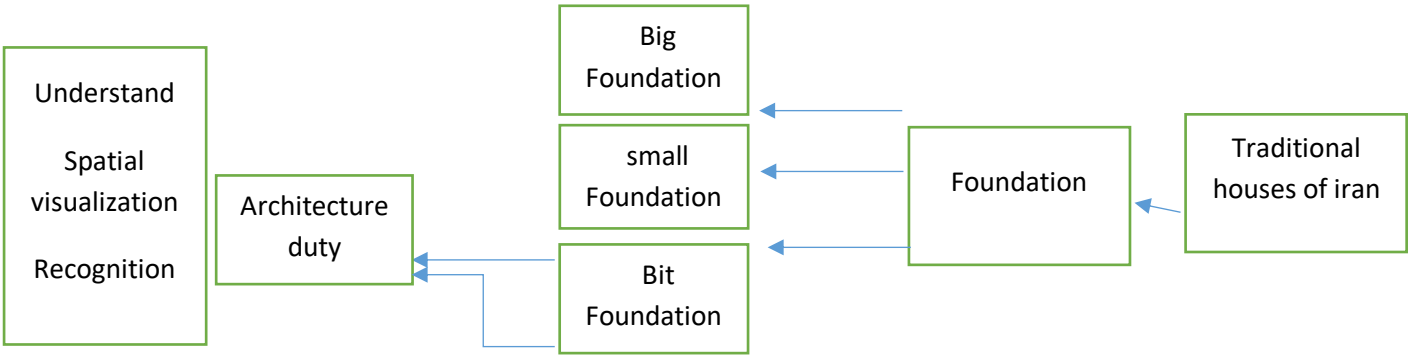


Chart 2: The Basis of Order in Iranian Traditional Homes



6.6. Contexts of adaptation of concepts and structures in the organization of space

In order to select an appropriate case study, to obtain an analytical result among the examples of the concept of flexibility in the current habitat of ones, among the houses of the Qajari of Shiraz, one of the factors is the way of creating the comfort of a home made up of large houses over 100 square meter is a relatively healthy home, where accessibility and field observations are available, for a case study.

House of Qavam

Table 9: Specimen Specifications: House of Qavam

Profile of the building	The direction of the building	Course and Area	Sample name
1. The Narenjestan's buildings are made up of two parts: the northern part with an adjoining porch and one underground floor, and two upper floors used for office and ceremonial use, and the south part with four rooms in the southeast corner and Southwest where the crew were present	Northeast to the southwest, the main entrance of the garden, opens to the south	An area of 3500 square meters and a 940 square meter substructure located at Lotf Ali Khan Zand Shiraz Avenue	House of Narenjest Qavam

Fig 4: Plan and showcase the house of Narenjestan Qavam

Forogh ol Molk House

Table 10: Specimen Specifications: Forough Al-Mulk Home

Name	Course and Area	The direction of the building	Profile of the building
Forogh ol Molk House	AN AREA OF 1020 SQUARE METERS LOCATED IN THE BLACK STONE SHIRAZ NEIGHBORHOOD	Northeast southwest	It has four main parts: exterior, interior, furnishings, baths and stalls. The exterior of the building is connected by the corridors to the courtyard of the mansion and an interior for the use of family members. The Indoor Mansion has a main lounge, such as a reception room and a number of rooms in the east and west. The mirror room is located in the south of this same area. Materials used in the construction of wood, stone and bricks are covered with gypsum mortar, soil, and some spit dots. In two parts, north and south, there are two five-door rooms, three floors with basements, all floors are connected by a basement used as a warehouse.

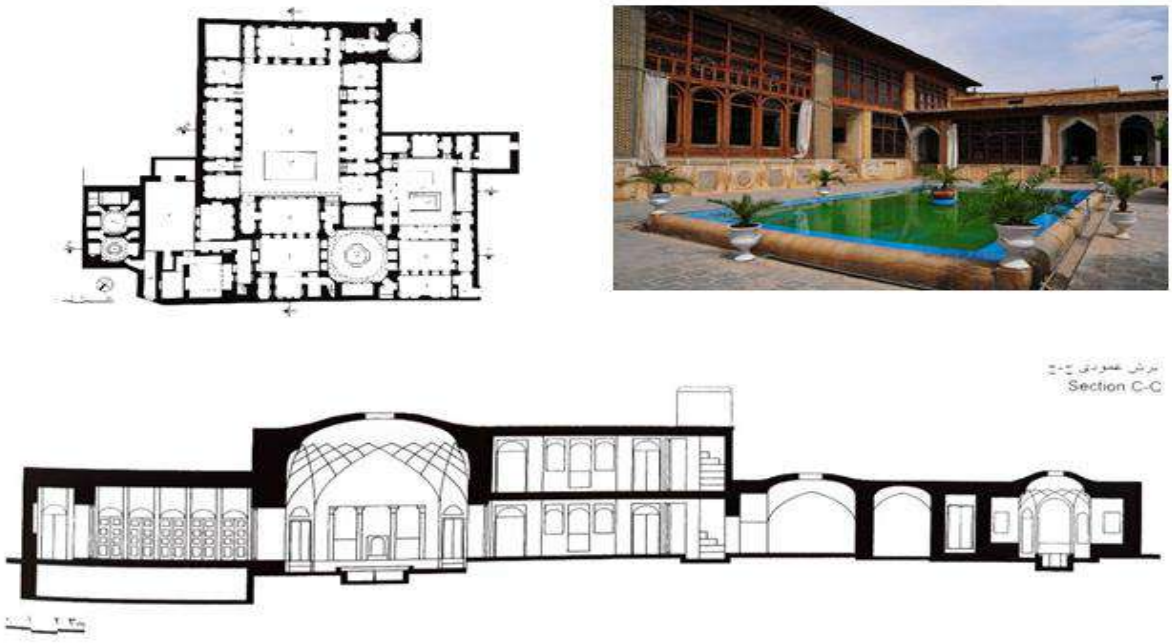


Fig 5: Plan and cut the house forogh al-Milk

Nasir ol molk house

Table 11: Specimen Specifications: House of Nasir ol molk

name	Course and Area	The direction of the building	Profile of the building
Nasir ol molk house	THE TOTAL AREA OF NASIR AL-MOLK COMPLEX IS 2890 SQUARE METERS AND THE INFRASTRUCTURE IS 2216 SQUARE METERS	Northeast southwest	What's left of Nasir al-Mulk's home now includes the main hall, part of the inner courtyard, the exterior and the basement. The hall of the mirror is made up of symmetrical shapes, and on both sides there are two sashs (a kind of old that has a special frame and has been opened and closed up and down) A large country with a subtle Chinese knot and colored glass that is connected to the inner and outer courtyards, as well as a large five-leaf arches in the middle of which are two floors with high ridges and a basement with bolts with arches And the rocky skylights are beautiful.

fig 6: Plan and Cut the House of Nasir ol molk

Define levels of complexity

In order to create a hierarchy in the analysis of samples and given the complexity of different projects is not the same in terms of flexibility. In this study, the complexity levels and order of examining case examples on the basis of the adjustment of the role of communication spaces at each level is also analyzed to find that various levels of complexity contribute to flexible understanding, and facilitates familiarization with simpler levels of complex design process. Several branches are involved in determining the complexity of a project. One of the most stable indicators is the ability to change the use of indoor spaces, and it may be said that the creation of flexibility in a plan is based on these characteristics, and it can be claimed that this feature is more or less present in all flexible projects.

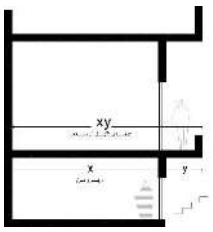
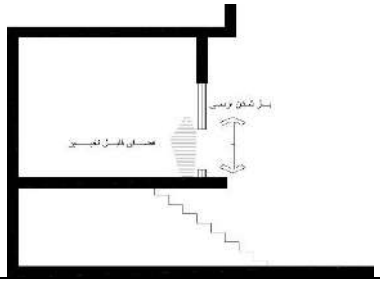
Table 12: Flexibility solutions from the perspective of contemporary houses and traditional elements at levels of complexity.

Sample Traditional Elements	solutions	Levels of complexity
lporches -high home -basement	Definition: Ability to change user is one of the most important features of all types of flexibility and the most basic level that specially deals with multi-purpose rooms. The purpose of the design of the room is to accommodate different functions and to change the user of each room according to their needs.	Level 1: Multipurpose Rooms
-Injection or Tucker or Summer House -the hallway	Definition: refers to a room that is usually floated between two residential units and can be assigned to either of these two units. The purpose of the room design is to make the room an independent space	Level 2: Shared rooms
lArsy -Three Doors - five doors	Definition: In these plans, flexibility is often achieved through the multi-functional spaces and their change of use in a short time. The purpose of the room design is to have rooms in direct communication.	Level 3: Rooms with folding compartment

-Central courtyard -Eight -old man room	Definition: One of the ways that ensures the ability to change in a space defines the freedom of space, ie the use of separators with space constraints, applications, and activities. The purpose of the design is that the space is usually an open room with a head that can be made with different layers with light blades.	Level 4: Raw spaces

Analysis of the findings

In this regard, looking at the past and receiving the concepts of space and functional architecture of the era before, including residential buildings, we can conclude that the most prominent feature of the architecture of each settlement is the need for flexible spaces with the ability to evolve space in functional, physical, social and biological function. In fact, the creation of space expresses what he wants to bring to man's mind, using functional forms, and on the other hand, observing the aesthetic principles. As a result, flexible and varied spaces can be created over time with a view to changing human needs, and as a solution to prevent the collapse of individual interactions with their habitat and the possibility of adapting housing to the changing physical and mental needs of their audience.

		Multipurpose Rooms
		Shared rooms
		Rooms with folding compartment

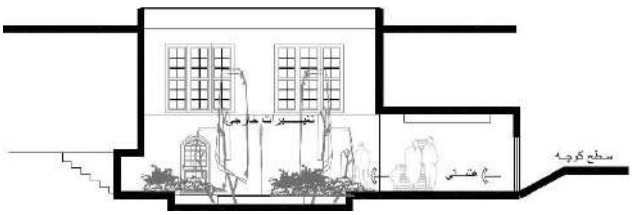
		Raw spaces

Table 13: Flexibility solutions in traditional homes and their use in contemporary.

Conclusion

The main findings from the conclusion in this study can be argued that flexible space includes varieties of designs that vary according to the short-term and long-term needs of users and, in response to their mental and psychological demands, are taken grfadually. Accordingly, the main domains of flexibility and its mode of operation in the contemporary and past times related to the differentiation, diversity, adaptability to the habitat of ones, by presenting variable and fixed solutions of a building, are described throughout the research. Obviously, full flexibility can not cover all of the changes, but by providing appropriate solutions, the use of past experiential factors, as well as significant changes in some parts of the building on a small scale, can be made to an acceptable level of environments with the appropriate response to the changing needs of people. The information and discussion presented in this study can be used as a background for further research on the issue of flexibility in designing contemporary homes. In addition, we can consider bio-comfort as a result of meeting the different needs of users with a variety of lifestyles, and finally it can be stated that "what distinguishes flexible spaces in terms of the comfort of biological spaces of particular rank."

It seems that designers of space patterns in the Iranian architectural tradition focus on the majority of mental and psychological conditions and everyday physical behaviors while at the same time creating a homogeneous environment, with a huge amount of responses for the needs of users and providing users who put it. In fact, by explaining the types of flexibility and concepts, each one provides a systematic and comprehensive analysis that helps in thinking space in the concept of flexibility. Based on the results, it seems that the conceptual value of the type and flexibility of operation are more effective than industrial solutions and developments in building technology in

housing design. Based on the fact that, with a better understanding of the concept of flexibility, we can make optimal use of the design spaces. In this way, the quality and quantity of houses, with the change in each of the factors of creativity, creates a significant impact on physical and physical functioning. By creating an internal relationship and relying on flexible concepts, a conceptual relationship can be found. Creating a better place in design and creativity.

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Recognition of architectural patterns in the houses of the Niakie neighborhood in Amol

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Jamshid Mirhadi**
Ali Asgharzadeh***

ABSTRACT

Traditional housing fabrics are an obviously valuable heritage to be reviewed and analyzed, as they present the right pattern for native architecture because it is considered the main core in the creation of cities, as well as the architectural elements and buildings located in them. The objective of this study is to review and recognize the physical and social behavior patterns of these buildings to improve these valuable fabrics and save them from their presence of unusual buildings. First, this study would review the key problems on the design of patterns in the architecture of the house, obtaining an analytical-descriptive point of view; This research first reviews the key issues of the patterns in the architecture of the house, and then identifies the physical components that are effective in traditional buildings, contrasting with the theoretical foundations obtained. The next step has been the identification and physical review using the field research method to physically identify and review the case study buildings in the historical fabric. After the analysis, the most effective physical components would be prioritized by hierarchical method. Finally, considering the results obtained, not only the principles of native architecture are identified, but also some approaches are introduced to improve the relationship between physical behavior environments in the Niakie neighborhood in Amol.

KEY WORDS: Behavior pattern, recognition of traditional fabric, native residential home, Niakie neighborhood in Amol.

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Reconocimiento de patrones arquitectónicos en las casas del vecindario de Niakie en Amol

RESUMEN

Los tejidos de vivienda tradicionales son un patrimonio obviamente valioso para ser revisado y analizado, pues presentan el patrón adecuado para la arquitectura nativa porque se considera el núcleo principal en la creación de ciudades, así como los elementos arquitectónicos y los edificios ubicados en ellas. El objetivo de este estudio es revisar y reconocer los patrones de comportamiento físico y sociales de estos edificios para mejorar estos valiosos tejidos y salvarlos de su presencia de edificios inusuales. Primero, este estudio revisaría los problemas clave sobre el diseño de patrones en la arquitectura de la casa, obteniendo un punto de vista analítico-descriptivo; esta investigación primero revisa los temas clave de los patrones en la arquitectura de la casa, y luego identifica los componentes físicos que son efectivos en edificios tradicionales, contrastando con los fundamentos teóricos obtenidos. El siguiente paso ha sido la identificación y revisión física mediante el método de investigación de campo para identificar y revisar físicamente los edificios de estudio de caso en el tejido histórico. Después del análisis, los componentes físicos más efectivos serían priorizados por método jerárquico. Por último, considerando los resultados obtenidos, no solo se identifican los principios de la arquitectura nativa, sino que también se introducen algunos enfoques para mejorar la relación entre los entornos de comportamiento físico en el vecindario de Niakie en Amol.

PALABRAS CLAVE: Patrón de comportamiento, reconocimiento de tejido tradicional, hogar residencial nativo, vecindario de Niakie en Amol.

Introduction

In one hand, home has such an importance in setting down, relaxing, self-referring, growth and human movement. On the other hand, these are mess, vast and non-identical spaces in today's life. So, there should be thinking and meditating about this issue. These days, from the quantity point of view, the housing usage has been mostly specialized to the urban buildings including the historical_traditional tissues. The space border and spritlessness is usually because of lack in types of fixed behavioral patterns in the environment. The most important point is the need to get the balance, make the matching and adjustment of a behavioral pattern with its physical environment, in which the behavior occurs. This feature causes for some places to be in

more suitable relationship with some behavioral patterns and have more capability (Rivas, 2018). Among these, Amol is one of the historical cities of Iran in which there are some valuable and architectural houses in its traditional tissue. The target of this study is to review and recognize the behavioral and social patterns of these buildings to improve these valuable tissues and to save them against her presence of unusual buildings. The planner has relied on the her context knowledge from presented buildings patterns, urban patterns and other environmental patterns to get a theory about the behavioral patterns, This matter can predict about the future environmental. This paper is considered descriptive analytic according to the method and one of the partical researches according to the target. The question that is answered at the end of the study are the patterns of physical behavior, the most important in Amol. Historical traditional housing spaces, " Niakie neighborhood ": so, in addition to knowing the related concepts, selecting the method and suitable analysis, at the end of the research, there would be some solutions to connect the behavior and physical environment around Niakie neighborhood.

1. Research Background

1.1. Pattern

Pattern does not judge about the special ideas, targets or values. The pattern result can let the things be alive and this is much better than conquering every artificial valued systems. To define all the existing forces is the only way in which the pattern can practically help to make a situation live honestly. Then the world would be found in witch the forces can get far from each other, the pattern gets a part of the nature and finally, when we can deeply look at the pattern which is made by human, so deeply without any shadow of idea and image, we have found a part of the nature which has the same validity and eternity (Alexander, 2011).

Norman has been applied a significant change in Gibson's theory. He has substituted the expression of conceptual capability instead of view capability instead of view capability because according to him, the designers care about what is done by user understanding more than something which has the possibility of correctness.

Considering this issue, knowing the concept of capability is followed to make it clearer in building a theoretical farm to define a theoretical investment to form it in a paternal method.

1.1.1. The definition of behavioral pattern

Behavior is the most observable and human reaction to the environment where he is situated in. so, the person can issue a message or contact with the others only by showing their behaviors in the environment without using any word but by using the behavior identity as a nonverbal tool. The way of doing any activity is behavior .The human behavior is the process of human's motivation and demands, the environment capability, the person's mental image from the utter world causing from his understanding and the meaning of image for him. Although the behavior is touchable and definite, it has a kind of complicated mechanism. Environmental behavior predication is the one of the main questions for behaviorists for which it makes many years study to find the answer for the behavioral experts. Even, some researchers introduce the behavioral science as the beginning of environmental psychology (Shahcheraghi & Bandarabad, 2015).

On the other hand, Alexander says that a building prides itself quietly and gracefully based on the panguage effect of common patterns which makes it and every presented part and activity which has leaded it. All the huge buildings in the history are built like this; by languages. So a rich pattern is a collection of patterns adjusted to the deep consideration about what ever makes a building more beautiful. According to Etelson, the information coming from the environment has symbolic and meaningful features; they have traits which present the mental reactions and have messages which motivate the demands. The values and aesthetical properties are transferred to the environment by people because human being needs to experience the environment as a model from meaningful relationships.

The previous experiences are the base of to understand the new condition. According to the studies of the reaction approaches, people describe their understanding both in an experienced from and in a structural type.

1.1.2. Designing the behavior pattern

The process of environment adjustment with behavior pattern include the physical environment designing would be defined by behavior patterns they need. Maybe, experts who have the related fields to designing can also define these objectives. These experts including the time and movement researchers, the ease planners or the people like these, know both activity systems and the manner of effect on the built environment on behavior. This process is formed more imaginatively and it is usually due at the time of decision making on spaces unconsciously (Alexander, 2011).

As Shahrokhabadiet et al, have written; the spaces names can show the activities which one done in them. The architects and planners use the more improved technologies of behavioral sciences to make the process easy be more objective of course the patterns and different in every culture and in every period. However, all of them are all man-made and dependent to the culture. In every period and everywhere, the structure of our world is necessarily the result of the patterns collections which are repeated (Shahrokhabadiet al., 2019).

John Lang (2002) believed that the designing process cannot be totally scientific, any way but it can be describe and explained by using the scientific and semi scientific methods. The abilities of the specific patterns for the made environment can be achieved by its designing manner, the materials used in it and its installation way results from the special group of people. In the known meaning levels (such as understanding), defining the environment abilities seems to be a performance from the human's biological features and on the symbolic meaning level, these abilities are performance of people's culture and social experience (Lang, 2002).

According to Maier and Fadel, then should be a kind of ability before a capable ability can occur (Maier & Fadel, 2009).

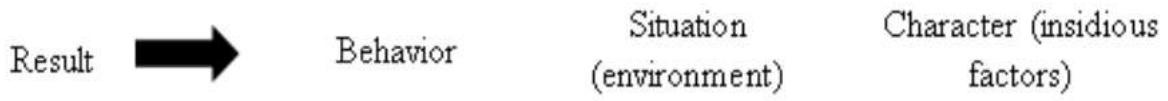


Figure 1. A diagram of human's behavior

Attention to human behavior and its role in the environment have been brought into the realm of behavioral geography using psychological thought and theories. The spatial behavior of the people is almost affected by the mental images from the environmental structure and can impact a lot on people's direction finding through the buildings, neighborhoods and cities.

1.2 Architectural ancient pattern experiences

The city surrounding tissue has various buildings falling images. As well as wide's pread trench like spaces full of sleeping cats. This mentioned city tissue has been surprisingly situated against its pure and empty interior. The city complete silence made by light and darkness wrapped may in arms by abstract of the interior and exterior. These ancient pattern experiences are neither the sensational facing nor severely logical and scientific but the pure 3 and 4-dimensional concepts. Perception considering the concept is like a model for architectural thinking in which every architectural student tries to be an observer. The art of observing is especially enjoyable because it is involved with the world's discovery. However, it remains in a perspective through which we from our paternal views (Holl et al., 2006).

1.3 The identical features of a traditional neighborhood according to the recognizing occurrence

1.3.1 Recognition

Atkinson (2005) says, defining the nature of the gained information is the first thing that our conceptual system should do to make the information meaningful. As a matter of fact, recognizing something is relating it to an issue. There are a lot of things to help us to recognize things but the shape is the most important factor. The shape importance in recognition is because of this fact that we can recognize a lot of objects by seeing the general line and the simple line patterns in which only the objects shape is remained safe and it is true even when they are black and white or they are not situated in a situation as they are always in.

1.3.2. Recognition of the traditional tissues

The traditional tissue is the synthesis of all physical parts and general organic streets and blocks that can be known as different manners of neighboring, the full and empty spaces in various combinations as well as segmentation of the specific lands. The features related to the neighborhood recognition field are the basic feature which is the infra-structure to the occurrence of a local system .these features are reviewed based on 3 analytical orientations in traditional neighborhood.

- Boarding the neighborhood socially and culturally
- The hierarchical spatial and performing system
- Following the scale, unity and coordination in
- Physical tissue and appearance, in neighborhood center and the neighborhood services (Falamaki, 2015).

1.4. The behavioral patterns in an Iranian house

1.4.1. The traditional houses in Iranian architecture

The traditional houses in Iran show the living methods and the people's thought in different ages. The spatial types of these houses are defined based on the existence or lake of the physical components. The opened spaces are occurred by defining the floor and wall. The semi opened spaces are distinguished by the concept of floor, ceiling and a specific definition of wall, although the closed spaces completely present all 3 element of floor, ceiling and wall.

The constructors of these native units have tried to make the living spaces more human through making a friendly connection among living environment culture and the architectural forms (Falamaki, 2015).

1.4.2. The house privacy

A house is not only the person's identification reflex ion and base but also the family one. The house is the mysterious carriage of a private life hidden from the public, even though it forms the social life. The house describes the private and public limits of life (Palasma, 1992).

Rappaport knows the houses as an organization which is more than a materialistic concept through complicated targets and their performance. According

to Moore, the house is the center of universe for its residents and for its neighborhood the most prominent building in the place standing. Both Rappaport and Palasma (1992) believe the house is the first grade of every organization which is existed for a lot complicated targets not a structure (Palasma, 1992).

1.4.3. Changing in architectural patterns in recent houses

In the past the housing space followed kinds of geometrical rules. However, it is now affected by the land geometry.

Also there is the change from the multipurpose spaces, multipurpose combination including the opened spaced, closed spaces and semi-opened spaces which caused the spatial variety to the recent closed living spaces.

According to Lang, one of the main targets of the recognition stage is to edit the patterns need for environment to response to the psychological and aesthetic demand. This stage cannot be forceful. Maybe the modern architect has made more mistakes in this issue rather than any other matters. It seems these architects have predicted wrongly about the behavioral patterns and the made environment ability to make specific behaviors. This revolution architects have decided based on the incomplete models of human and the human's behaviors (Lang, 2002).

1.5. Reviewing the case studies done

Christopher Alexander and Donald Iliyard have performed the role of behavioral patterns in forming the human oriented urban spaces. They have considered the human demands and motivations in forming the spaces in recent years and both of them have confirmed the progressive actional and behavioral patterns in spaces some of most important issues favorable for both of them are considering the micro spaces and defining the space based on the human activities the relationship between the micro spaces and macro spaces (Sadeghzadeh & Pourmohammadi, 2013).

The analysis of socialization in physical environment comes from the nature understanding in human made environment as well as the nature understanding manner in human made environment which have meaningful effects on patterns socialization and physical spaces.

This study has reviewed the behavioral science theorist emphasis on studying the life routine spaces in residential samples (Daneshgar Moghaddam et al., 2011).

Environment perception (the role of psychological relativism in understanding the environment) works on analyzing the rules and laws of getting the better environmental designs and patterns according to the people (Barati & Soleimannejad, 2011).

The architectural teaching models are based on Gibbon's theory of environmental capability which has reviewed the theories and the approaches related to it. They also have defined the hidden and evident angles of the capabilities, have found the theoretical structures coming from the behavioral ideas to improve the teaching method for architectural designing and have made the practical frames in the field of architectural teaching method (Naghdbishi et al., 2019).

There is recognizing the behavioral patterns in Enghelab square in Isfahan as well as reviewing the settlements and behavioral patterns in considering environment which has done by field observations. There is also the solution presented to improve the relationship between the behavior and physical environment (Delaket al., 2017).

As a consequence, the study background has got by reviewing the researches and studies. The patterns assessment, the physical factors recognition, the behavioral pattern recognition, architecture teaching model's based on Gibson's environmental capabilities, assessment for the impact of the environmental quality components on behavioral patterns, the behavioral patterns role on forming the urban, human oriented spaces according to Christopher Alexander and Donald Epilard and reviewing the theoretical foundations has been resulted through library studies. This history has helped a lot to cognitional analysis of behavioral pattern in historical houses in Niakie neighborhood. So, we in reviewed the patterns and their results (Latifi & Sajjadzadeh, 2015).

2. Study Methodology

To describe the methodology and gained results, in this study, firstly the research basic recognition has been done by analytical discretional methods and field studies the

required and basic information has been gathered. Also, according to the research approach based on physical components, the main related methods to the study title, the tables considering them, physical components and pattern recognition would be reviewed. The pattern elefinition in the previous architecture can help us in the modern designing especially in housing architecture. So, in this research, the pattern recognition has selected viewing the theoretical foundations, field studies as well as considering the physical view and practical approaches to the new diagrams. According to the mentioned principles, in this pattern recognition; some components are reviewed. These components include: the sectors tissues, the sectors tissue, the architectural elements, the natural elements, the architectural plans, the physical relation of the spaces, building direction in environment and the decoration pattern. There is also the architectural-physical analysis of the traditional houses in 3 spatial groups of open, semi-open and close studied in this study. The final result can be presented by the physical factors such as the space and masses system, geometry and form, spatial hierarchy, and functional system which are located in the new diagram frame to review the results.

3. Data Analysis

3.1. The study region and clime

Amol is one of Mazandaran cities. The old tissue has included 13 neighborhoods. The center is in two styles of linear and square from in Amol old tissue (Riahi, 2002). Because is located in the mild and humid region according to the climate elements, the annual temperature average is around 14.5 to 18 degree in this area and the annual temperature fluctuation is around 25 to 36 degrees (Kasmaee, 2003).

In this research, the study area is in the middle part of this historical traditional tissue called Niakie neighborhood in which there is significant building and can be reviewed as the remained art works from the ancient architecture. The architecture of Niakie houses is belonged to Qajar and Pahlavi era. Manuchehri, Malek, Darzi, Qurayshi, Ebadi and Moghimi houses are the oldest art works in this neighborhood and they are studied in this research.

Figure 2. South view of Qureshi House

3.2. The behavioral architectural patterns about the residential case study of traditional tissue in Niakie neighborhood, Amol, Mazandaran

According to the studies done and getting information from the architectural experts and cultural heritage office , at last 7 houses have been chosen among the valuabk houses in traditional tissue of Niakie neighborhood because of the limitation to get the documentaries and past information. The houses situation map has presented in figure 1-4 and the general feature and plans are shown in table 1-2-3.

Figure 3. Aerial photo of Amol, Niaki neighborhood, 1989

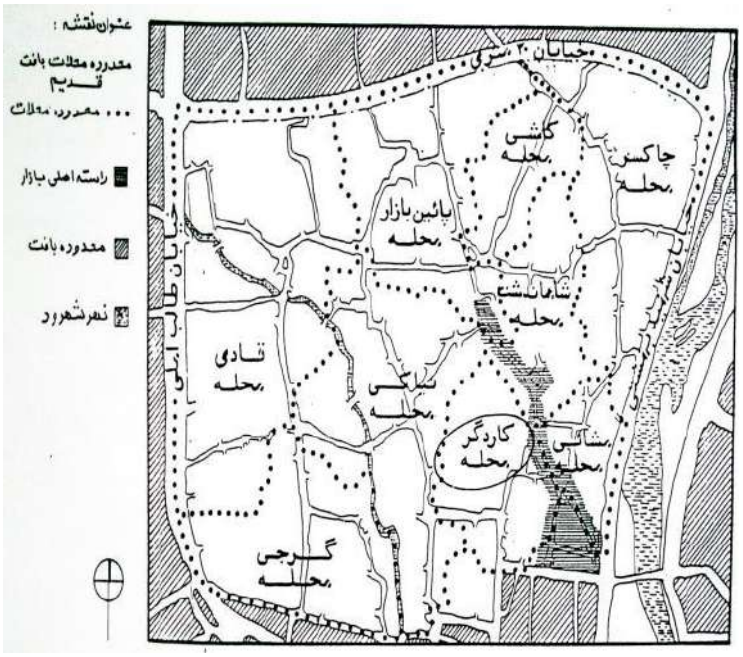


Figure 4. The general area and the neighborhood situations in the map of 50th decade about the old tissue of Amol city.

The historical tissue, accessibility, interlocking capability, the city cultural tissue, the descriptive plan sites, emptying, the view and the centralization in the city heart are really important.

The analysis of the used patterns in Mazandaran traditional houses –Amol- Niakie neighborhood According to theoretical concepts of this study (behavioral pattern) and knowing the architecture, the other factors should be studies including the spaces physical connections and the building direction pattern. In this section, there is the analysis of the introducing houses as the case study.

3.3. The spaces physical connections in houses

The studying houses are analyzed and then because of the discussing issue in each building, the physical connectional issues in these houses are reviewed in 3 general parts based on the locating position in each space. The 3 general parts are called the open space arena, semi open and closed arena, the elongation and climatic arena.

Table 1. The architectural definition of the selected historical houses in the traditional tissue of Niakie neighborhood, Amol

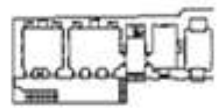
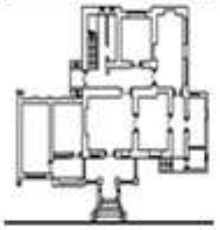
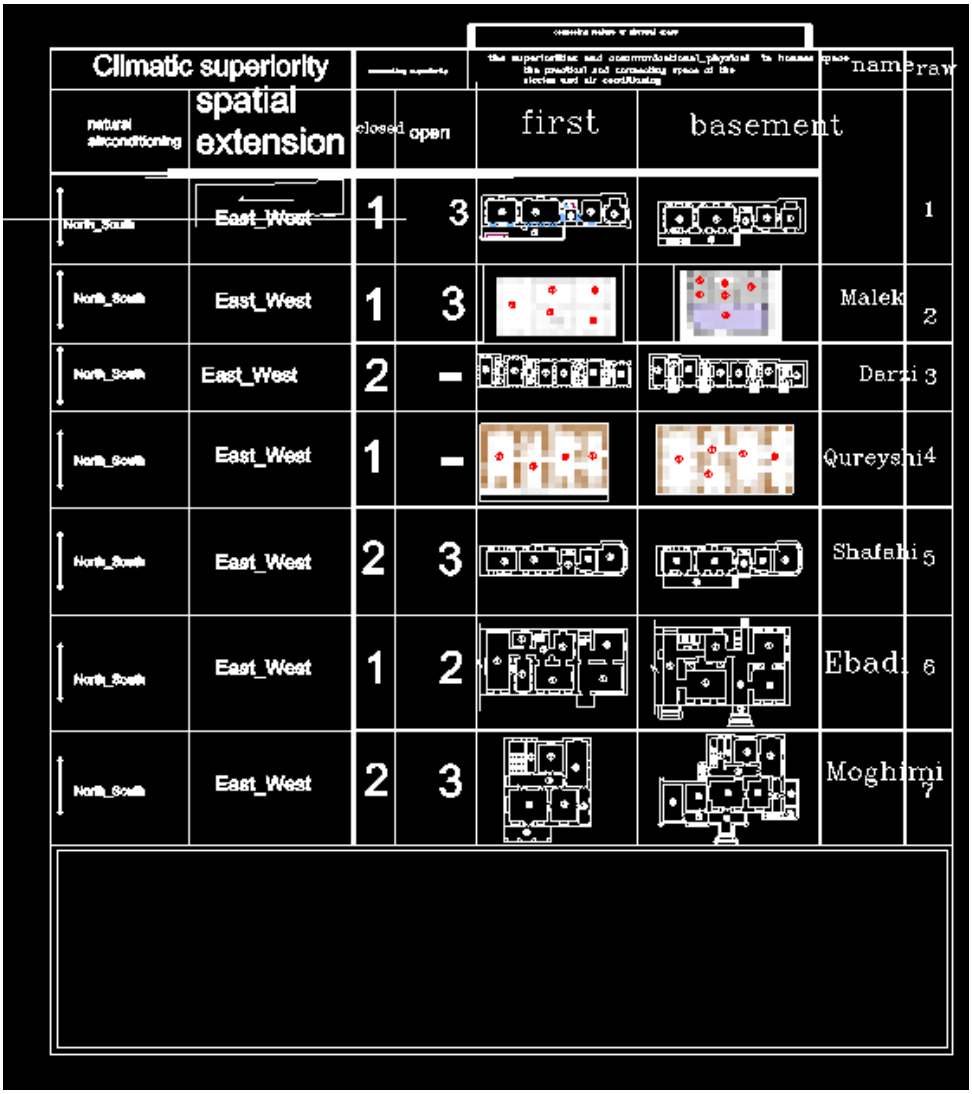
Raw	Name	Architectural features	Photo	Architectural plan
1	Manuchehri	Including entrance yard and 2-story, summerhouse with one entrance balcony and an interconnecting space porch, Extension: west to east		
2	Malek	Including entrance yard and 2-story, an interconnecting space porch, Extension: west to east		
3	Darzi	Including entrance yard and 2-story, summerhouse with 4 entrances between space porch with interconnecting space to the other rooms, Extension: west to east		
4	Oureyshi	Including entrance yard and 2-story, summerhouse with one entrance balcony and an interconnecting space called porch , Extension: west to east		
5	Shafahi	Including entrance yard and 2-story, summerhouse with 2 rooms which balcony of one is the entrance to the other one, Extension: west to east		
6	Ebadi	Including entrance yard and 2-story, summerhouse with the building ending into a porch which is the entrance for the other 2 rooms, Extension: west to east		
7	Moghimi	Including entrance yard and 2-story, there is one room with balcony with 3 entrances and a central core, Extension: west to east		

Table 2. The priority pattern and physical connectional issues is houses space (practical spaces and stores connections)



3.4. The testing process and the final patterns, analysis

In this part, the pattern recognition is reviewed in physical factors and would be tested through diagram drawing. Then finally the most effective physical featured would be selected based on the theoretical components, reviewing the subject history , getting the combined space patterns, getting the unity of a mixing pattern and combining the space orients. Then according to plans and architecture recognition, the line chart would be drawn for houses in Niakie neighborhood.

Table 3. The getting findings form the spatial behavioral criteria from the case studies in Niakie traditional tissue, Amol

The factor of spatial physical		Measurement	Classification		Notes
1	The relationship of mass and space	The most commonly used pattern	Including a yard	Developing front	All the yards located in front of the house
		The greatest amount of mass The least amount of space			
2	Space set up pattern	The majority of the placement	The balconies, kitchen, bed rooms, living room and the family room are on the North and South of the house/the entrance room: on the South which makes the division space		
3	Lifestyle	Private and public area	Independency/the connection between the availability space/the private spaces: on the first floor/the public spaces: on the basement		
4	Climate	The humid and mild climate	The houses extension: East to West both extraversion and introspection mood in the houses		
5	Functional relationship	Physical connection priority	Open space		The analysis of extraversion and introspection in the houses of Amol traditional tissue
			Closed space		

3.5. Investigation of spatial efficiency indicators

The convenience: this feature is dependent to the space flexibility and it is favorable when it has small amount of depth and a suitable convenience (Depending to the space) (Yin, 2003). So the achieving points can be some of the key factors to organizing, matching ease and usage varieties in a building.

The space depth or any other spaces part is related to another space according to its permeability measurement and integrity.

In this study, the private and half private spaces, permeability and their depth are reviewed in table 4. As a consequence, the spaces which would be in the less depth then entering spaces have optimum function and in this case, the spatial orbiting can be done more suitably and finally it promotes the function efficiency.

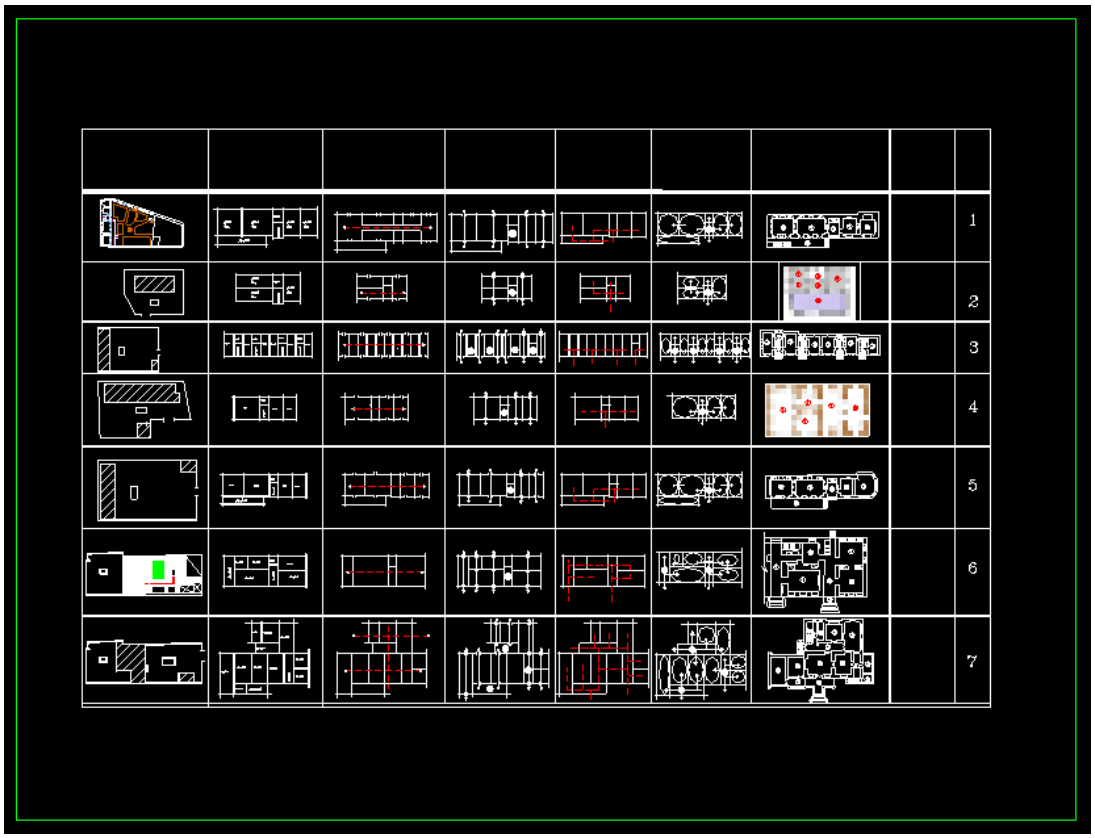
Conjunction: It means joining or separating of that space to the other existing spaces on that configuration and its concept is related to the depth that means the conjunct space is the one that the other environmental spaces are situated in rather lower depth than that. It has also direct and linear relationship to the connection index.

Access and connection: It is detected by space syntax technique from the perspective of visual and physical access. Also, connection is the connection among the links which are made between every space with the other space. Generally, functional performance indicators are calculated like the below table considering the previous contents.

Functional performance indicators the accessibility
The accessibility
Depth
Conjunction
Connection

To review and recognize the components and functional performance indicators is for making house desirability as well as assessment and reviewing the vestibule role and its influence on this spatial desirability of considered houses in old tissue of Niakie neighborhood. Based on the introducing the functional performance indicators and reviewing their role on vestibule in this physical spatial system, ever central closed space is not considered as the vestibule pattern. Vestibule means after passing the house head , we step to a space with the pausing possibility which is dimmer and colder than the trance and has gifted a kind of welcoming and relaxing manner to the user but from value point of view and national norms (hospital and respect to the person's understanding from the environment) , around the vestibule can be mentioned to make a suitable space from the guests to relax and wait and it also has the socialization and conjunction and people's gathering ability or at least the family gathering situation is included. The getting survey from these houses residents has proved this matter totally.

Table 4. Providing solutions related to extracted patterns influenced by physical structure and spatial behavior



Conclusion and Presenting the Solution

Recognition of the traditional tissue is to get the past identity maker native patterns and using it in today's architecture. So, according to the environment understanding, editing the environmental patterns is needed to answer the re-cognitive activities and requirements. The results show that the extroversion and interpose patterns in houses of Niakie neighborhood in Amol have Eastern-western elongation interest on the other hand, it can be shown by comparing the factors matching with the architectural features, mess and spaces, functional connection and building direction can be the priority of the house forming to get the continues behavioral pattern in the modern designing.

In order to continue the identity and modern building and structure to be united with the historical issue of Niakie neighborhood in Amol as well as using the

conclusions coming from research, there would be suitable solution to review the spatial and physical patterns which are presented by analyzing the archived diagrams in order to make the harmony with the traditional tissue using the traditional architectural components. We can use the archived diagrams in their updated from to present in today's building in Niakie neighborhood because they follow all the climate and situational factors. In Mazandaran climate, the houses are both extrovert and introvert. There are balcony and yard in all Mazandaran houses which is extroversion indicator and dividing space or vestibule and the connecting hall for rooms and space are introspection indicators. It is important to combine the spaces and their function in mild climate. By space recognition, a modern pattern will be achieved with the same function. So, a case with cultural pattern (hidden biological pattern) should be solved before considering the relationship between the values of space decoration and function in buildings and structures. This issue can be used as s designing pattern in the future.

The research results prove the correctness of research patterns recognition. So, the people's spatial behaviors can be more positively assessed if the physical environment includes suitable and adjusted organizing to the need of clients considering the effects of environmental making elements and the physical structures on people's spatial behaviors based on psychological, personal, identical, cultural and climatically features, people's social life and the way of their living. These things should have the ability of accessibility. After the analysis which is done, it is tried to present an effective design based on the psychological features and getting the people's sati's faction.

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Determination of the reasons for the lower injectivity of the injection wells

N. R. Krivova *

ABSTRACT

The injection of water into the formations to maintain their pressure is accompanied by loss of injectivity in the injection wells. It is necessary to determine the reasons for the loss of injectivity to apply various methods of regulation of the characteristics of the filtration tank in the area of the bottom of the formation, which will allow to restore the injectivity of the wells and increase the coverage of the formation by flooding. of water. The document presents the results of the determination of the alleged causes of a loss of injection well injection, the hypotheses to determine the causes of a loss of injection and the studies conducted to confirm or refute the causes mentioned.

KEY WORDS: Loss of injectivity, change in the salinity of the injected water, dilation of clay and rock particles.

Determinación de las razones para la menor inyectividad de los pozos de inyección

RESUMEN

La inyección de agua en las formaciones para mantener la presión de estas, se acompaña de pérdida de inyectividad en los pozos de inyección. Es necesario determinar las razones de la pérdida de inyectividad para aplicar varios métodos de regulación de las características del depósito de filtración en la zona del fondo de la formación, lo que permitirá restaurar la inyectividad de los pozos y aumentar la cobertura de la formación por inundación de agua. El documento presenta los resultados de la determinación de las supuestas causas de una pérdida de inyectividad de pozos de inyección, las hipótesis destinadas a determinar las causas de una pérdida de inyectividad y los estudios realizados para confirmar o refutar las causas mencionadas.

PALABRAS CLAVE: Pérdida de inyectividad, cambio en la salinidad del agua inyectada, dilatación de partículas de arcilla y roca.

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Introduction

Currently, when productive formations of large deposits have been significantly mined, commissioning of small deposits remote from areas of developed infrastructure is becoming very important. The commissioning of such deposits may be accompanied by a number of uncertainties and risks of non-conformity to estimated production and injection values (Pesotsky & Perovsky, 2015; Alvard et al., 2001; Alvard & Tokarev, 2002; Ahmadov, 2019). So, when commissioning one of the fields in Western Siberia, the problem of maintaining formation pressure became acute. The field in question is located in the Nizhnevartovsk region, it belongs to the category of small deposits and is located at a distance of 10.2 km from the nearest deposit.

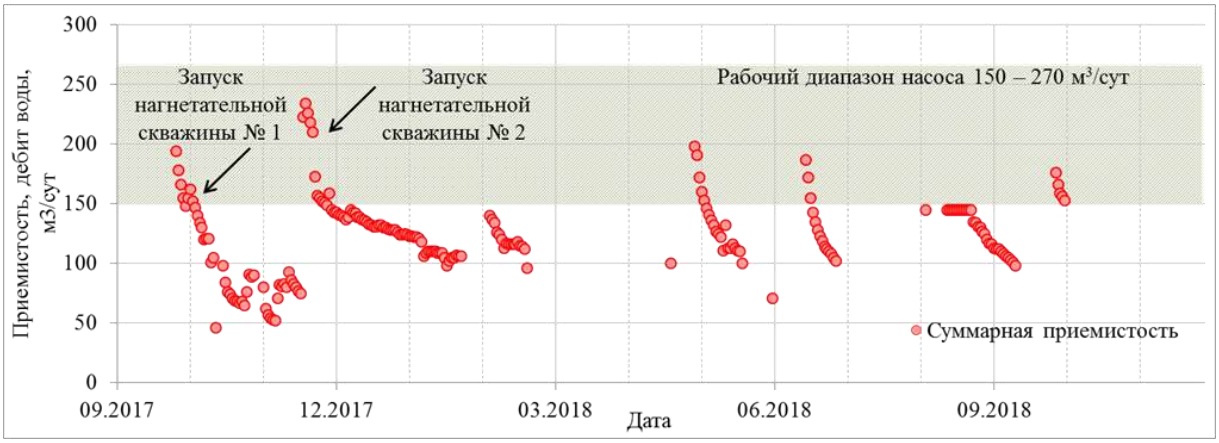
The exploited object UV_1 is represented by terrigenous reservoirs with a permeability of 8,5·10-3 μm^2 (the petrophysical dependence of a neighboring field was used to evaluate permeability, no own studies are available), porosity of 17% and initial formation pressure of 25,8 MPa.

As on 01.01.2019, 20 wells were drilled at the facility, 2 wells were transferred for injection. It should be noted that in order to maintain formation pressure, intra-cluster injection from a water well was organized, since it was less efficient to extend a 10 km high-pressure water conduit from a neighboring field for the pressure maintenance system.

When operating injection wells at the facility, an abnormal injectivity loss was registered with decrease from 150-200 m^3 / day to 40-50 m^3 / day in the first months of operation. Fig. 1 shows the operating modes of injection wells.

Total injectivity loss and, accordingly, the water flow rate in the well below 100 m^3 / day leads to a supply interruption, pump overheating and shutdown of the injection wells (the water well is equipped with an ECN-200 pump).

The article describes the suggested hypotheses, aimed at identifying the causes of injectivity loss, and studies conducted to confirm / refute them.



Injectivity, water flow rate, m³/day
Start of injection well №1
Start of injection well №2
Pump operating range 150-270 m³/day
Total injectivity
Date

Fig. 1. Operating modes of injection wells

The first hypothesis was put forward on the possible mudding of the bottomhole formation zone by reaction products of deposit and injected water, or by mechanical impurities. A description of the process of mudding and methods for its elimination is reflected in papers (Kuznetsov & Muzipov. 2010; Zakharova et al., 2016).

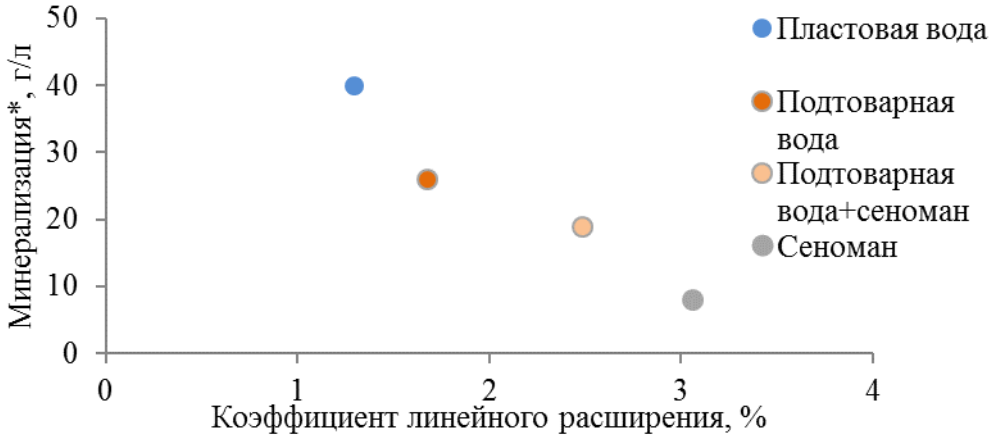
To test the hypothesis, samples of deposit and injected water were taken from the wells of the described object. The content of mechanical impurities in the samples of injected water was 3 mg / l (the limit of the content of mechanical impurities for reservoirs with a permeability of less than 0,1 μm² is 3 mg / l, which corresponds to the regulation OST 39-255-88 «Water for flooding of oil reservoirs. Quality requirements»).

Calculations for water compatibility were performed analytically based on an analysis of the water chemical compositions. For calculations, the specialized programs "CARBON" (Debye-Hückel method) and "ROSA" were used. According to the results of the assessment, it was found that the mixing of deposit and injected water in any proportions does not lead to precipitation in a volume exceeding the limit value in accordance with the requirements of OST standard (carbonate and calcium sulfate fall out in the amount from 0,013 mg / l to 0,77 mg / l).

According to the results of the analysis, the hypothesis on mudding of the bottomhole formation zone of injection wells was rejected due to its insolvency.

Next, a hypothesis was suggested about the possible dilatation of rock clay particles and a decrease in permeability in the bottomhole formation zone. The works (Kozhevnikov, 2016; Tang & Morrow, 2002; Stupochenko & Avanesov, 1991; Goldberg & Skvortsov, 1986; Mirchink et al., 1975; Kibalenko & Stupochenko, 1992; Buckley & Morrow, 2011), describe the process of reducing the injectivity of injection wells while reducing the salinity of the injected water.

To test the above hypothesis, core studies were planned and carried out on rock dilatation during the injection of water samples with various salinity. As the test solutions, there were used formation and bottom water, as well as a mixture of bottom and Alt-Alb water of the Cenomanian aquifer complex (AASVK). The results of the study of the samples are presented in Fig. 2.



Salinity*, g/l
- Formation water
- Bottom water
- Bottom + Cenomanian water
- Cenomanian water

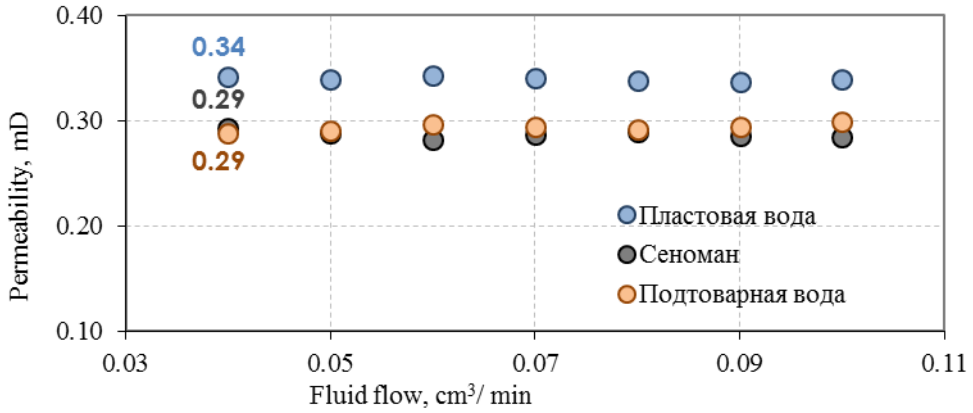
Expansion coefficient, %

Fig. 2. Dilatation of core samples during the injection of water samples with various salinity

With a decrease in salinity of water injected into the formation, clay dilatation is observed (a change in the coefficient of linear expansion is equivalent to a change in pore volume). According to the results of studies, the maximum dilatation of the rock / decrease in porosity can be achieved with the injection of Cenomanian water and will equal 2%.

During the second stage of research (for direct determination of permeability), a series of injections was carried out with a sequential decrease and then an increase in salinity (formation - Cenomanian - bottom) to assess the possible restoration of permeability and the subsequent decision to change the injection agent.

According to the results of studies, a change in salinity does not significantly affect the decrease in permeability and mobility. The decrease was 13,7% and 7,4%, respectively. The research results are shown in Fig. 3. With an increase in the salinity of the injected water, permeability recovery was not observed.



- formation water
- Cenomanian
- bottom water

Fig. 3. The dependence of the various water permeability on fluid flow (example for one sample)

Alongside with core research, an efficiency record was taken in one of the studied injection wells (studies were already conducted at the well during the period of production work).

Due to the fact that there is no clear exit to the radial mode (despite the long duration of the study, relative to the study in production at the same well), the

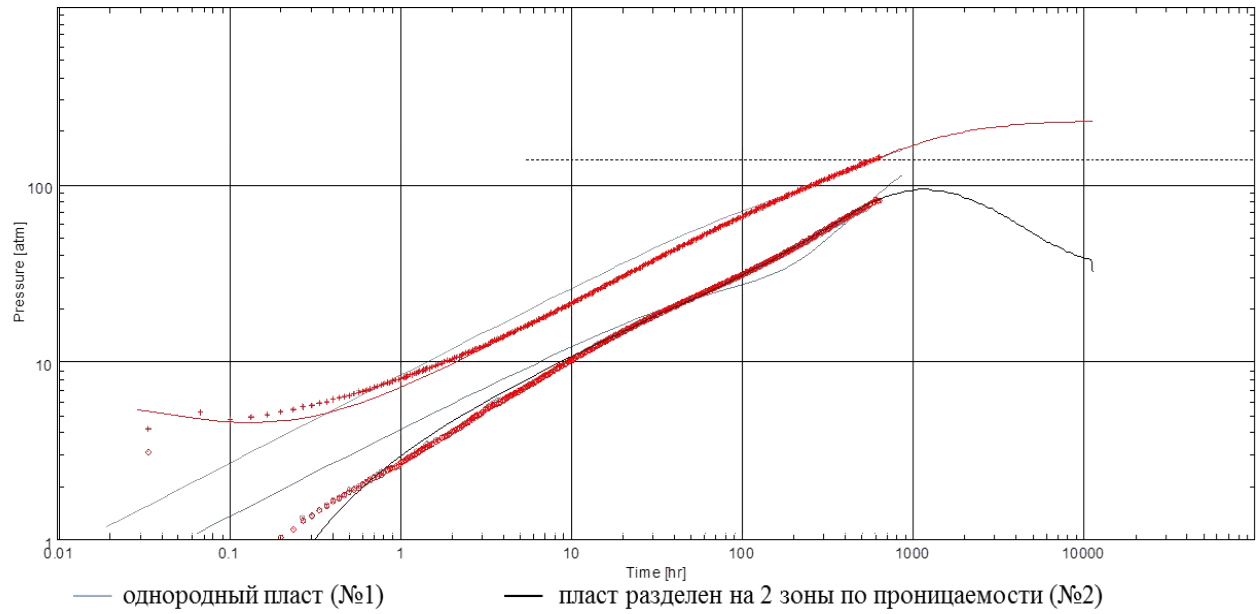
parameters obtained as a result of the interpretation can be considered as estimated figures, and the reliability of the study can be considered low.

The classical interpretation of the study (the accepted model of the well is a fracture with finite conductivity, a homogeneous formation, intersecting faults) does not provide acceptable convergence of actual and calculated data, therefore, a model of a radial composite formation was chosen for interpretation.

The selected model best describes the flows between the zone of low reservoir properties in the bottomhole formation zone and the zone of improved reservoir properties in the remote part of the formation. Fig. 4 and table 1 show the results of efficiency studies and comparison with the standard interpretation.

Table 1. Well test results for various options

Properties	Interpretation variant №1 – homogeneous formation	Interpretation variant №2 – formation is divided into 2 zones with various permeability
Formation	homogeneous	radial composite
Boundaries	intersecting faults	Infinite boundaries
Skin factor	-6.35	-6.05
Xf, m	125	124
Pi, atm	102.4	173.3
L1- non-permeable, m	32	-
L2- non-permeable, m	340	-
k*h, mD*m	1.45	2.07
k, mD	0.05	0.064 (closer zone) 0.233 (remote zone)
R of degraded zone, m	-	125



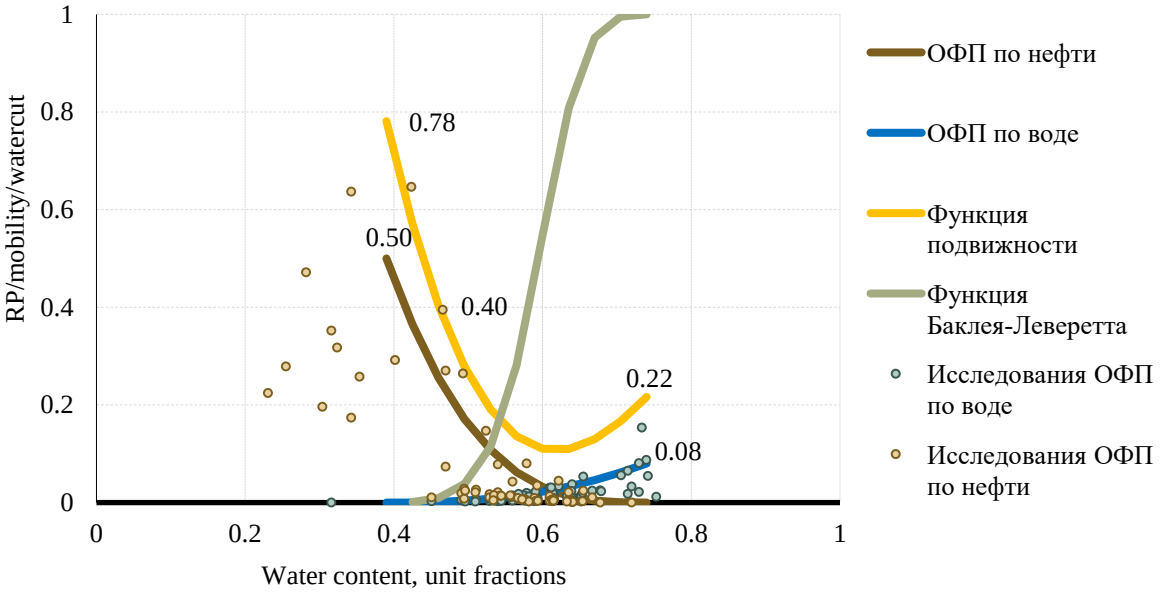
- homogeneous formation
- formation is divided into 2 zones with various permeability

Fig.4. Results of efficiency studies on injection well (diagnostic chart for different interpretations)

The radius of degraded zone was 125 m (the minimum value, it could increase with a longer study duration). According to the research results, the permeability in the degraded zone is 0,064 mD, permeability in the rest formation area 0,233 mD, a decrease equals 3,6 times.

The presence of a zone with degraded properties can be associated with both dilatation of the rock (the hypothesis is not confirmed by core studies) and degraded water permeability and hydrophilicity of the rock (natural causes) and can be partially described by the RP functions obtained in neighboring fields (Fig. 5).

Core studies conducted in October 2018 speak in favor of the assumption on RP deterioration. The porosity - permeability relationship significantly deviates from that adopted by analogues (2-3 times lower with average parameters). The results are shown in table 2.



RP to oil
RP to water
Mobility function
Buckley-Leverett function
Studies of RP to water
Studies of RP to oil

Fig. 5 Type of RP functions characteristic of UV_1 reservoirs (according to the analogic field)

Table 2. Core permeability assessment

Well №	Cpor, %	Relative permeability assessment, mD		Cperm (own data) / Cperm analogue, unit
		Analogic field	Own data	
1	13.1	1.9	1.2	1.5
2*	15.2	7.9	2.8	2.9
3*	14.6	5.7	2.3	2.6
4	15.8	11.1	3.4	3.2
5	15.5	9.9	3.1	3.1
6	15.5	9.6	3.1	3.1
7	16.0	17.5	4.3	4.1
8	14.9	6.1	2.4	2.6

9	14.6	5.1	2.1	2.4
10	15.4	8.7	2.9	3.0
11	15.5	9.9	3.2	3.1
Average	15.1	8.5	2.8	3.0

Note* - injection wells

To confirm the hypothesis of degraded reservoir properties, an analytical assessment of the well flow rate dynamics was performed during the period of work in production and injection.

For the calculations, the inflow equation for an unsteady operating mode (Basniev et al., 1993), was used (the calculations were performed in the corporate form for calculating the production rates of new wells taking into account the formation saturation and phase mobility, hydrophilic RPs from the analogic field were used):

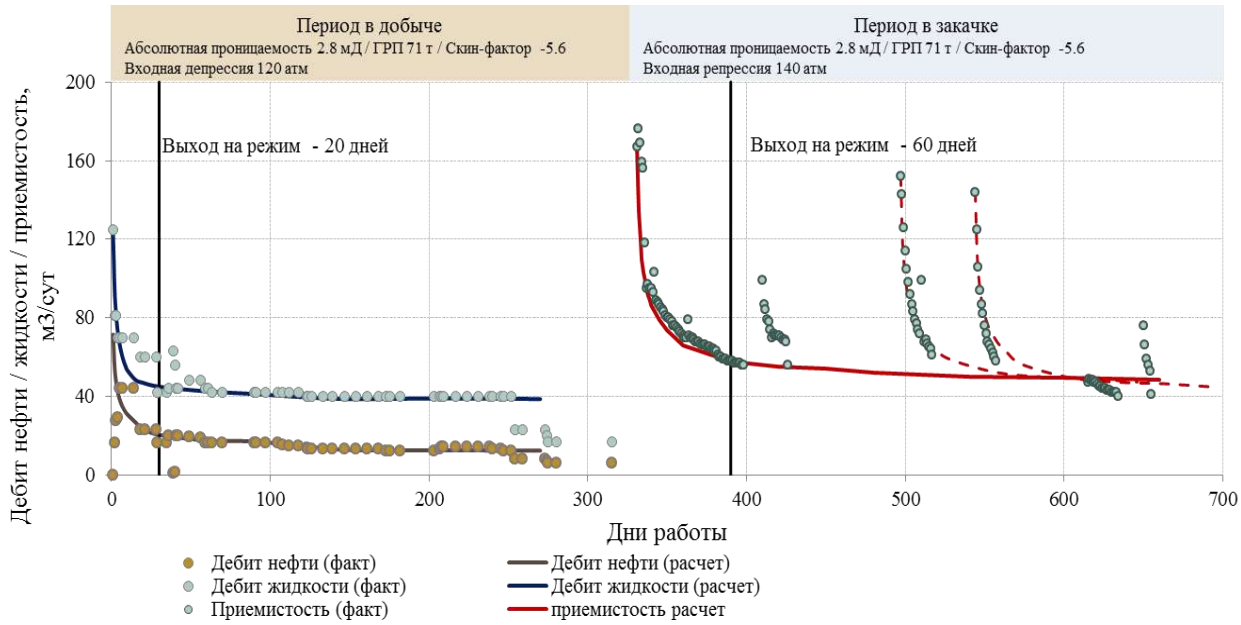
$$q = 2\pi \frac{kh(\overline{P} - P_{wf})}{\mu B(\ln\left(\frac{kt}{\phi\mu c_t r_w^2}\right) + S)}$$

Where k – formation permeability;
h – net thickness;
$\overline{P}$ – formation pressure;
P_{wf} – bottomhole pressure;
t – well operation time;
ϕ – porosity;
c_t – compressibility of pore volume;
r_w – well radius;
S – skin factor.

Analytical calculations show that with a changed permeability, a decrease in injectivity can be caused by a long response time of a well (a steady-state operation can be reached after 2-3 months of operation, Fig. 6), while the well's response time in production is much lower and equals 20 days. The injectivity of injection wells at a steady operating mode will be 40-50 m^3 / day.

According to the results obtained, a short-term work program has been developed, the main purpose of which is to confirm a new hypothesis (time for the well to reach steady-state operation). To do this, it is planned to put shutdown injection

wells into operation, change the pump in the water well to a less productive one (ECN-100), monitor the operation of injection wells in the first 4 months of work, and subsequently conduct flow test after the first months of work.



Oil rate/water rate/injectivity, m^3/day
Production period
Absolute permeability 2,8 mD/ FHF 71t/ Skin-factor -5,6
Incoming pressure-sink 120 atm
Response time 20 days

Injection period
Absolute permeability 2,8 mD/ FHF 71t/ Skin-factor -5,6
Incoming overbalance 140 atm
Response time 60 days

Operation days
Oil rate (actual) – oil rate (calculated)
Water rate (actual) – water rate (calculated)
Injectivity (actual) – injectivity (calculated)

Fig. 6. Analytical calculation of the injection well performance with account to the updated RP

Conclusion

In 2018 a series of research works has been carried out aimed at identifying the reasons for the injectivity loss of injection wells. The most likely cause is the low formation permeability and hydrophilicity of the reservoir, leading to a decrease in mobility when transferring wells for injection.

Based on the research findings it should be noted that:

• Change of the injection agent from the water of the AASVK group formations to bottom water is impractical.

It is necessary to consider the possibility of intensifying the injection using the following types of measures: bottom hole treatment, hydraulic fracturing, the installation of surface booster systems that allow implementing the auto hydraulic fracturing mode.

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Improvement of oil production in low permeability deposits with a system of horizontal wells

N.R. Krivova *

ABSTRACT

The article describes an approach to the production of difficult to extract oil, confined to deposits with low poroperm properties, using a system of horizontal wells and hydraulic multistage fracturing. The main problems that arise during the development of the well are analyzed. A conclusion is reached on the possibility of continuing to apply the method based on the analysis of pilot tests.

KEYWORDS: Upper Jurassic deposit, Horizontal Wells, production of reserves.

Mejora de la producción de petróleo en depósitos de baja permeabilidad con un sistema de pozos horizontales

RESUMEN

El artículo describe un enfoque para la producción de petróleo difícil de extraer, confinado a depósitos con bajas propiedades de poropermo, utilizando un sistema de pozos horizontales y fractura hidráulica de etapas múltiples. Se analizan los principales problemas que surgen durante el desarrollo del pozo. Se llega a una conclusión sobre la posibilidad de seguir aplicando el método basado en el análisis de pruebas piloto.

PALABRAS CLAVE: Depósito del Jurásico Superior, pozos horizontales, producción de reservas.

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Introduction

Today, Russia's oil industry tends to have more reserves, which is associated with a greater number of discoveries and production targets being developed with difficult geological and physical indicators. Traditional production methods used in recent years do not always lead to the expected result.

There is a fairly large number of borehole systems for developing oil and gas fields known, characterized by the usage of vertical and directional wells. Studies on Horizontal Well (HW) development systems are not enough for now (Grachev & Samoylov, 2015).

Therefore, special attention should be paid to studies and introduction of effective production methods. One of such methods is horizontal directional drilling, which has been playing an essential part in the exploitation strategy of various deposits over the past decade. But in conditions of low-permeable reservoirs, even HWs have insufficient oil production for its profitable recovery.

One of the first works in this area considers the placement of HWs and MHHWs (Kolesnik, 2009). The basic principles of placement and calculation of vertical wells development systems are used therewith. Alternative development plans are proposed in that take into account the nature of filtration flows to HW systems (Borisov & Tabakov, 1962; Brekhuntsov et al., 2004). The following systems (process models) for development of oil and gas fields with HWs were recommended as a result of the research:

- linear (single-row and multi-row) systems, when the rows of production and injection wells are parallel, there is a certain distance between the rows;

- block-linear system uses the principle of a parallel-linear system with development blocks;

- radial systems ("fan", "ring") are effective for massive deposits.

It is necessary to increase oil production in a cost-effective way to achieve commercial productions. One of these methods is the use of Multi-Stage Hydraulic Fracturing (MSHF) in wells with horizontal tailing-in.

The article gives consideration to experience of using this technology on the example of Upper Jurassic deposits of the Western Siberia field.

1. Oil production in low permeability deposits from a system of horizontal wells

The field was discovered in 1976 and was brought into pilot development in 1988. The main production target of the considered field is the UV_1 producing layer. Horizon UV_1 refers to complex geological objects characterized by significant lithological and facies variation, expressed both in significant number of beds and frequent change of individual permeable partings with non-permeable varieties, very low poroperm properties, and "stairstep" water-oil contacts (WOCs).

The production target includes UV_1^1, UV_1^{2+3} layers. During the analysis of all the available material it was established that the upper UV_1^1 layer is isolated from two layers below, that is ensured by a mature shale break between them. The latter circumstance served as the basis for distinguishing it as an independent reserve estimation target. The UV_1^2 and UV_1^3 layers were included in the second common reserve estimation target, since the thickness of the shale break between them did not exceed 2 m, which does not ensure their isolation during joint development.

The reservoirs of the considered group of strata are represented mainly by medium- and fine-grained sandstone and siltstone. The UV_1 horizon layers were formed under various facies conditions, both shallow marine and continental due to fluvial processes (including transient ones). Transitions between shallow-water and fluvial facies lead to sharp changes in thicknesses and reservoir properties.

The noted lithological and petrophysical features of the formation determined, on the whole, the low poroperm properties of these strata. Reservoir properties vary over fairly wide ranges. Intercommunicating porosity varies from 10 to 20.7% (average of 15.8%). Permeability of strata rarely exceeds 10 mD (average of 6 mD), and the reservoirs with a permeability of more than 20 mD is only 2%.

Disjunctive faults in Jurassic deposits is another factor complicating development of the field. The disjunctive faults were formed in two stages. The first stage took place during the Jurassic period - the beginning of the Early Cretaceous era. A system of faults of the southwestern-northeastern strike was hypothetically formed at this time. In this case, consistent upward decrease in the horizontal displacements

along them has been observed. The second stage falls into the time interval covering the Cretaceous period and the Cenozoic era. As a result, there is a system of disjunctive faults oriented in the southeast-northwest direction. Notably, unlike the first system, the intensity of their formation increases up the section. Apparently, their formation was not due to horizontal tension and compression movement of crustal blocks, which determined formation of the structure of this field as well.

The complex structure of the field determines a number of negative problems during its development, the main of which is low well production that results into the unprofitable field development.

Despite the constant scientific support of the field development, the optimal technology for development of reserves has not been found. Traditional methods and approaches, widely tested in classical fields and proposed by project engineers in the early 90s, were inadequate in such difficult geological conditions.

The analysis of the UV_1 development showed that the potentially achievable oil recovery factor (ORF) in the drilled zone is low, about 92% of recoverable reserves, under the existing development system, will remain undeveloped. The constructed characteristic of displacement before Industrial Experiment Works (Fig. 1) shows the inefficiency of the existing development system.

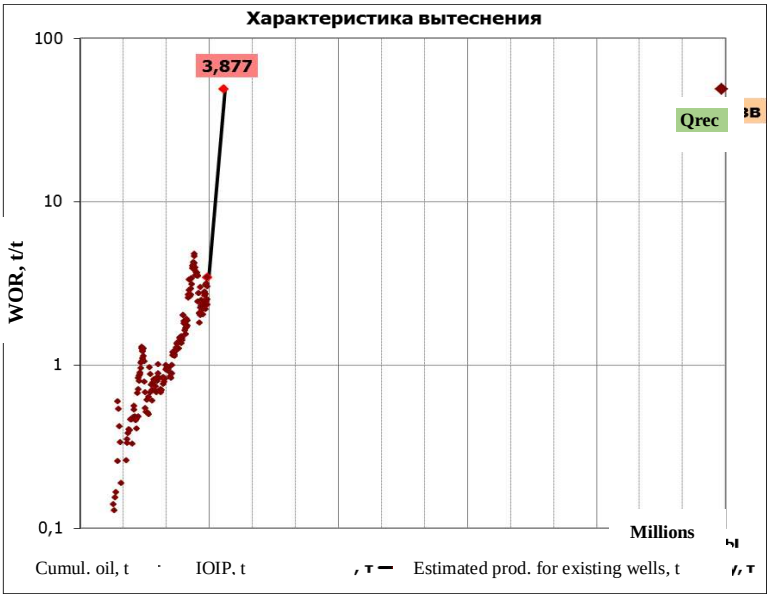

Fig. 1. Characteristic of Displacement for UV_1

The declining recovery trend observed in recent years has been mainly associated with a significant increase in watercut since 1997. The reason for the high watercut of wells was the existing development system, which is rather chaotic and obviously not optimal, both because of the large number of idle wells and because of the "immature" development system. It is also necessary to note a significant decrease in production associated with lower well delivery, which resulted from low performance of the implemented development system. The insignificant effect of the existing Reservoir Pressure Maintenance System (RPMS) led to wells periodic duty. The number of wells operating in this mode increased up to 70% by 2012.

An expert assessment of wells production capacity is required when determining HWs location and plan during design for the development of specific production targets (Aliyev & Sheremet, 1992). presents definition of statistical relationship between the HWs production rates and geological characteristics of productive formation, and technology factors. There is connection found between the initial production rate of a well and such parameters as the length of horizontal wellbore in the formation, opened-up zone thickness, and distance from the lower point of the horizontal wellbore to water-oil contact. The current HW production rate beside these parameters depends on opened-up zone percent and number of productive interlayers crossed by a horizontal wellbore. One of the factors that significantly affect feasibility of the optimal design of a horizontal wellbore is stabilization period of the production rate after the well start-up. It depends on permeability of the formation, presence and degree of pressure communication between the interlayers, thickness and sequence of occurrence of these interlayers, number of interlayers opened-up by a horizontal wellbore, location of the horizontal wellbore, pressure drawdown, etc. Based on mathematical experiments on a reservoir section, it was shown in that when substantiating the optimal length of a horizontal wellbore, it is necessary to provide for a decrease in production rate in time (Purgoyu & Shalomo, 2004). This is due to the peculiarity of oil influx to the horizontal wellbore caused by a change in the geometric shape and dimensions of the drainage zone, since a significant change in the production rate in time is associated with its size (Steklyanin & Telkov, 1962; Steel et al., 1995).

3D detailed seismic studies were performed on the central area of the main deposit to decide and implement the development system at the field in 2011-2012. Based on the results, a tectonic model of the area was built and 3D position of the faults was determined. Additionally, 3D seismic survey was conducted in the east and north in the field season 2012-2013.

Substantiation of the industrial experiment work site was carried out on a sector geological-hydrodynamic model. The options for well placement and wellbore passage were calculated for various types of section: horizontal, upward, downward, sinusoidal (Romanchev et al., 2013). A well placement system along and across tectonic stress was obtained and substantiated for testing, types of wellbore passage and tailing were determined as a result of constructing the sector geological-hydrodynamic model. The implementation of a "rigid" water flooding system (the ratio of production and injection wells is close to 1:1) without delay in organizing a RPMS, with constant monitoring of well operation modes, proved its advantage. Horizontal well bores were planned to be placed in the UV_1^{2+3} horizon where the main oil reserves are concentrated, and as a result of MSHF, the UV_1^1 layer should be additionally developed. The horizontal well portion length was planned to be 600 m, distance between the rows - 500 m, distance between the wells in a row - 200 m. The MSHF consists of four stages, distance between the ports is 200 m, estimated volume of propping agent per Hydraulic Fracturing is 80...100 tons.

In 2012, Industrial Experiment Works for drilling HWs with MSHF were started at the field. As of 01.01.2015, 15 new Horizontal Wells were drilled at the field (Fig. 2). The start-up production rates confirmed the starting advantages of the HW with MSHF technology for low production formations compared to standard technologies. The average input fluid rate of HW is 180 tons/day, oil - 89 tons/day, average input watercut is about 44%.

Over the entire period of their operation, HWs withdrew a total of 210.3 thousand tons of oil (Table 1). On average, one Horizontal Well accounts for 14.0 thousand tons of oil produced. To date, wells with horizontal tailing-in operate with an average oil rate of 46.2 tons/day, fluid of 84.1 tons/day. Current and accumulated indicators of drilled wells correspond to design, with the exception of the 9G well. The

reason for this was the watercut above the planned one, due to primary development of the water-saturated part of the UV_1^3 layer against the following geological factors: improved properties of the UV_1^3 layer relative to UV_1^2, no UV_1^2 - UV_1^3 shale break.

Efficiency of the reserves development by Horizontal Wells is confirmed not only by higher initial oil production rates, but also by accumulated indicators. Indicators for Horizontal Wells in comparison to Directional Wells are presented in Table 2.

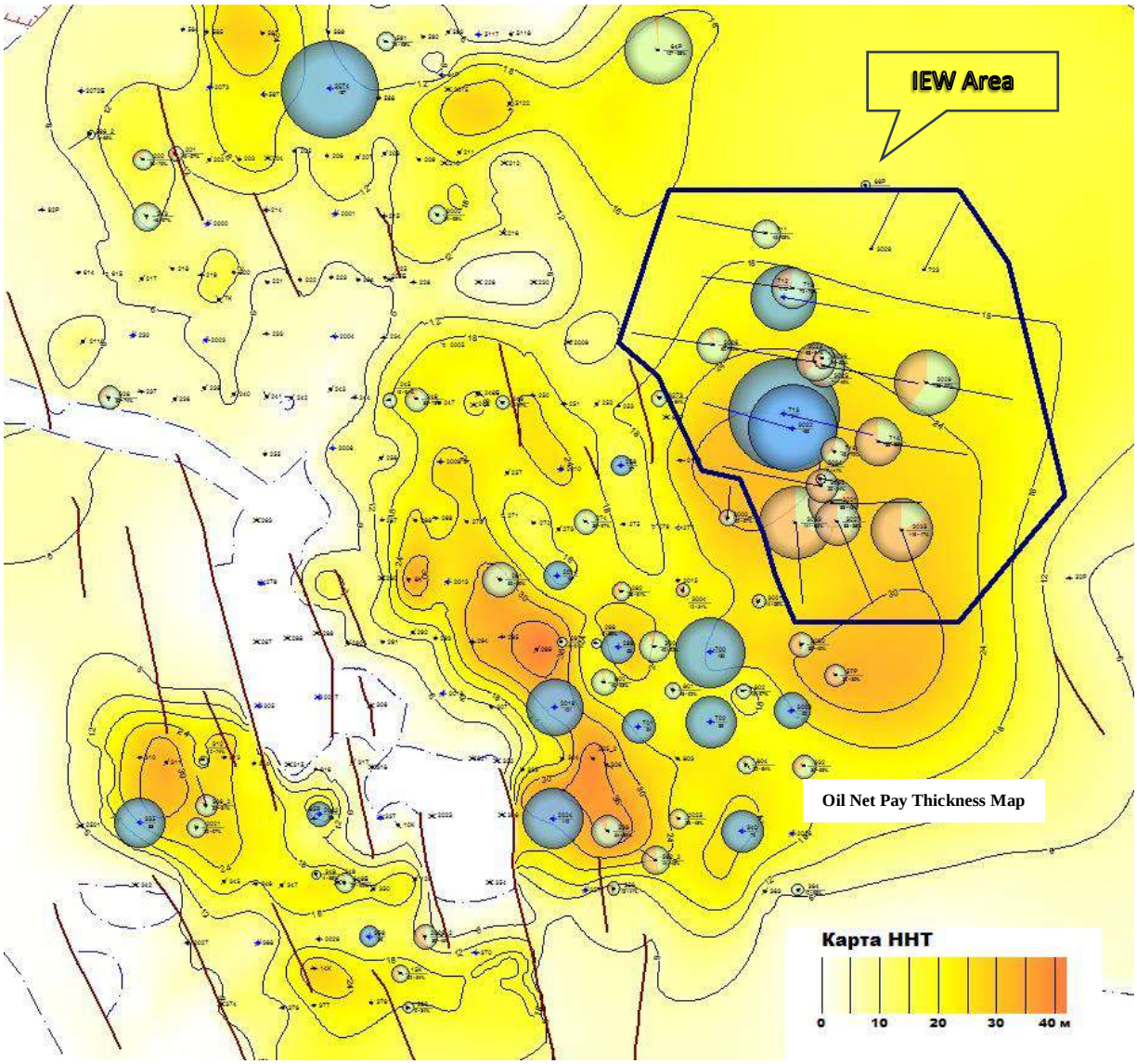

Fig. 2. UV_1 Bubble Map

Table 1. Main Process Parameters of WC with MSHF

Well	Com. Oper. Date	Production Condition of Well	Lift Method	HW Usefull Length	Qty of HF Stages	Start-up mode		
						Qo, t/day	Qf, t/day	WC, %
1G	06.13	switched to RPM	ESP	601	4	103	159	35
2G	07.13	producing	ESP	738	4	107	148	28
3G	08.13	switched to RPM	ESP	671	4	57	127	55
4G	09.13	producing	ESP	716	4	81	107	24
5G	10.13	producing	ESP	734	4	124	181	31
6G	11.13	producing	Nat. flow	656	4	154	217	29
7G	02.14	producing	ESP	714	4	80.1	165	40
8G	04.14	producing	Nat. flow	674	4	148.1	218	16
9G	05.14	producing	ESP	705	4	13.3	206	92
10G	06.14	producing	ESP	693	4	101.8	242	48
11G	07.14	producing	Nat. flow	689	4	60	140	47
12G	08.14	producing	ESP	652	4	14	154	91
13G	09.14	producing	ESP	720	5	132.9	265	38
14G	10.14	producing	ESP	550	4	80.2	168	41
15G	11.14	producing	ESP	674	5	80.1	198	50

Table 2. Horizontal Wells Comparing to Directional Wells

Bore Type	**Qty of Wells**	**Start-up date**	**Accumulated indicators**					**Current indicators**					
			oil, th.t	oil, per 1 well, th.t	fluid, th.t	fluid, per 1 well th.t	WOR	Qty of wells	oil, th.t	oil, per 1 well, th.t	fluid, th.t.	Fluid per 1 well th.t	WC %
DW	191	May 1988	3746	19,6	7591	39,7	1,0	58	84	0,4	290	0,3	71,1
HW	21	June 2013	380	18,1	649	30,9	0,7	17	170	8,1	305	0,3	44,4

Side-tracking	118	September 2013	72	4,0	141	7,8	1,0	18	46	2,6	96	0,1	51,8
Total	230		4197	18,2	8380	36,4	1,0	93	300	1,3	691	0,7	56,6

Microseismic mapping of Hydraulic Fracturing was carried out in No. 1G HW to analyze the effectiveness of MSHF in the HW. A microseismic study of the treated well No. 1G was carried out using well No. 11. Based on the results of the obtained material, the areas of micro-fractures (areas of the fracture) were visualized (Figs. 3 and 4).

Stage 1 DFIT
Stage 1 Main HF+ Stage 2 DFIT
Stage 2 Main HF + Stage 3
DFIT
Stage 3 Main HF + Stage 4
DFIT
Stage 4 Main HF

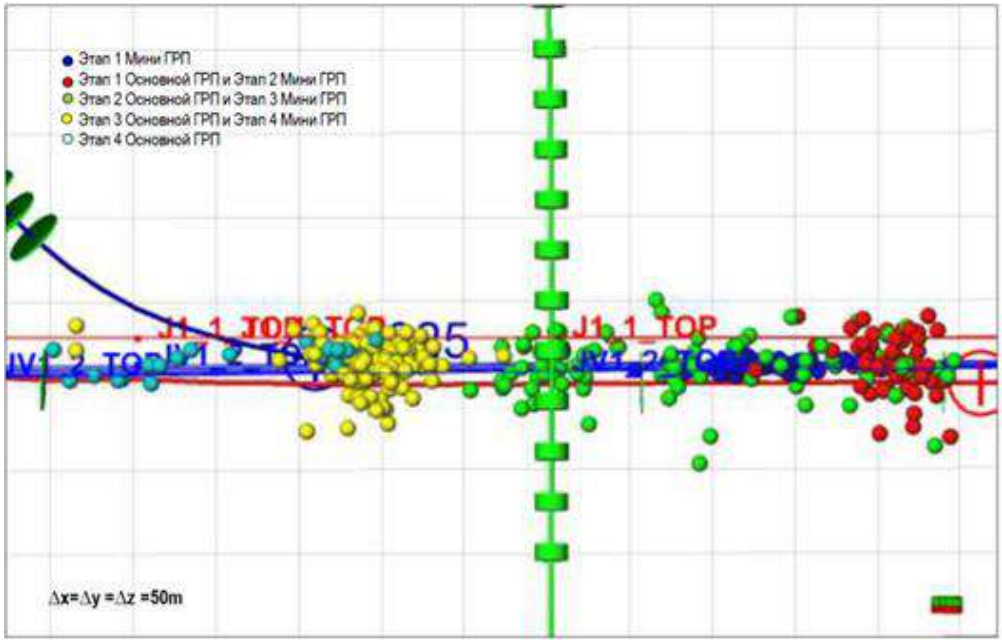

Fig. 3. Vertical Projection (W-E distance)

Stage 1 DFIT
Stage 1 Main HF+ Stage 2 DFIT
Stage 2 Main HF + Stage 3 DFIT
Stage 3 Main HF + Stage 4 DFIT
Stage 4 Main HF

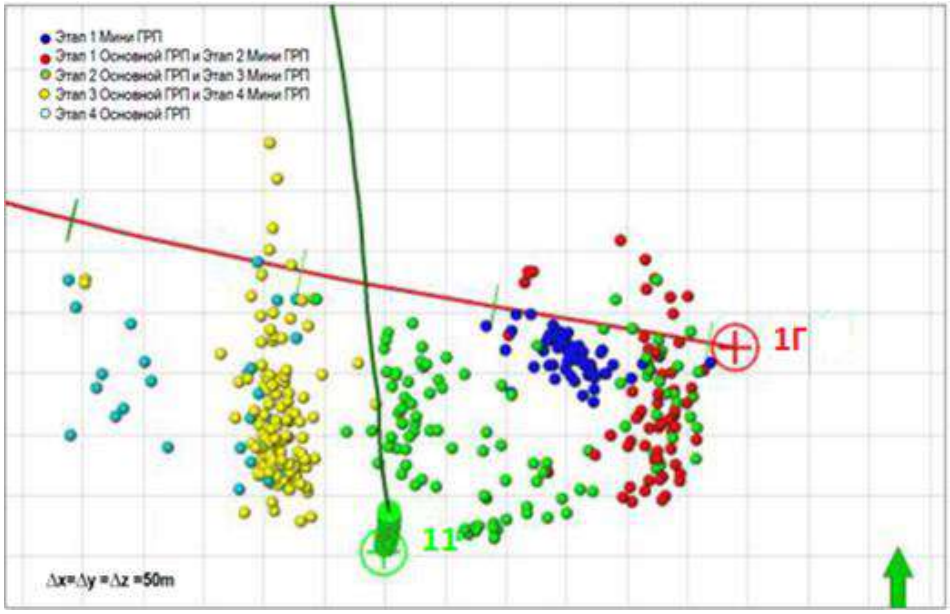

Fig. 4. Horizontal Projection (W-E distance)

When mapping MSHF in the Horizontal Well No. 1G, the following data were obtained:

- average half-length of the microseismic volume of the main stages of HF is about 154 m;
- average height of the microseismic volume of the main stages of HF is about 53 m;
- average number of microseismic events per stage one stage 97;
- average microseismic volume at the stage of 444000 m^3.

As the Figures show, events of the main stages are located opposite the layout ports. All stages of HF (except Stage 1 DFIT), spread orthogonally to the wellbore. Hydraulic Fractures cover the entire stratigraphic thickness of the UV1 layer, which was confirmed by research data. The use of this technology makes it possible to

selectively intensify the sections of the horizontal wellbore, which will allow involving 2 UV_1^1 and UV_1^{2+3} layer with different properties into the development.

As a result of Industrial Experiment Works on drilling of Horizontal Wells with MSHF, it was possible to increase production, the percent of reserves involved in development and the oil recovery coefficient, which allowed changing the multiplicity of reserves several times. Fig. 5 shows the actual and design development indicators for the UV_1.

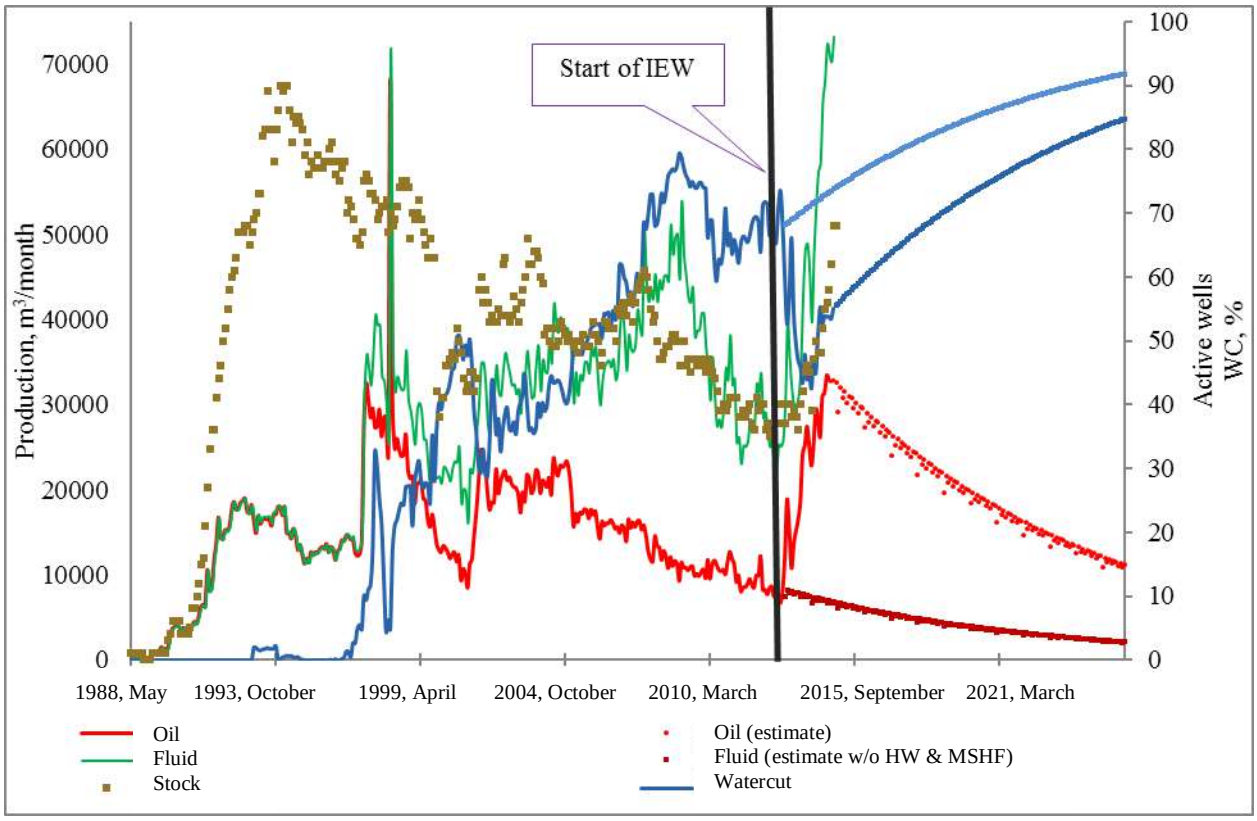

Fig. 5. UV_1 Production Diagram with Arp's Estimate

Conclusion

The introduction of Multi-Stage Hydraulic Fracturing in Horizontal Wells allows for an increase in recoverable reserves, and also allows to recover reserves at the highest possible speed today.

Drilling Horizontal Wells with MSHF shows a higher technological efficiency of putting low-permeability formations into development, in terms of well delivery,

which allows recommending this technology for the development of complex fields in Western Siberia.

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Detection of raveling layers of water well by electrical resistivity method and evaluation of the causes of sand making of deep well and it's confronting approach

Sayed Abdalreza Mostafavi *

ABSTRACT

The collapse and destruction of the wall of drilled wells is one of the challenges of drilling water wells, leading to a shortening and reduction of well irrigation over time. This research has been carried out in an area where most of the drilled wells have faced the problem of sand generation in various dimensions. Many drill holes in Bardaskan City, Khorasan Province, their layers at depths of more than 90 meters, face the challenge of drilling, due to the presence of loam and silty sand, which first requires the drilling of wells at low distances and, secondly, the average life of the wells in these areas is generally less than 8 years and in most cases between 6 and 8 years of age. Furthermore, the problem of cutting or collapsing the tube, especially in the highest part of the first network, is also indirectly correlated with the generation of sand in the wells. The appearance of sand in a well is due to a variety of reasons, although the abundance of very fine-grained loamy and sandy materials is one of the main factors in the aqueous layers of the area. Using the geoelectric and specific resistance method, it is possible to identify layers that have silt and sand with the probability of collapse and determine the point of the layer with less fraying and determine the appropriate strategy to prevent the pipe wall shell from tilt or fill, affecting the well. In this investigation, six wells from the village of Hassan Abad in Bardaskan County, and two wells from the village of Hatiteh have been evaluated, as most of their wells face the problem of wall collapse. Using the geophysical method, the resistance of its canyoning layers has been identified and, by providing engineering solutions, a large amount of damage to the wells has been avoided.

KEY WORDS: Sand, silt, specific electrical resistance, Schlumberger, screen pipe, well collapse, tilt, well damage.

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Detección del desmoronamiento de capas de pozos de agua mediante el método de resistividad eléctrica y evaluación de las causas de la formación de arena en pozos profundos y su enfoque de confrontación

RESUMEN

El colapso y la destrucción de la pared de los pozos perforados es uno de los desafíos de la perforación de pozos de agua, lo que conduce a un acortamiento y reducción del riego del pozo con el tiempo. Esta investigación se ha llevado a cabo en un área donde la mayoría de los pozos perforados se han enfrentado al problema de la generación de arena en varias dimensiones. Muchos pozos de perforación en la ciudad de Bardaskan, provincia de Khorasan, sus capas a profundidades de más de 90 metros, enfrentan el desafío de la perforación, debido a la presencia de marga y arena limosa, que primero requiere la excavación de pozos a bajas distancias y, en segundo lugar, la vida promedio de los pozos en estas áreas generalmente tiene menos de 8 años y en la mayoría de los casos entre 6 y 8 años de edad. Además, el problema de cortar o colapsar el tubo, especialmente en la parte más alta de la primera red, también se correlaciona indirectamente con la generación de arena en los pozos. La aparición de arena en un pozo se debe a una variedad de razones, aunque la abundancia de materiales limosos y arenosos de grano muy fino es uno de los principales factores en las capas acuosas del área. Mediante el método de resistencia específica y geoeléctrica, es posible identificar capas que tengan limo y arena con la probabilidad de colapso y determinar el punto de la capa con menos deshilachado y determinar la estrategia adecuada para evitar que la carcasa de la pared de la tubería se incline o se llene, afectando el pozo. En esta investigación, se han evaluado seis pozos de la aldea de Hassan Abad, en el condado de Bardaskan, y dos pozos de la aldea de Hatiteh, que la mayoría de sus pozos enfrentan el problema del colapso de la pared. Mediante el método geofísico, se ha identificado la resistencia de sus capas de barranquismo y, al proporcionar soluciones de ingeniería, se ha evitado una gran cantidad de daños en los pozos.

PALABRAS CLAVE: Arena, limo, resistencia eléctrica específica, Schlumberger, tubería de pantalla, colapso de pozo, inclinación, daño de pozo.

Introduction

-The geographical location of Bardaskan city

The Bardaskan city with an approximate area of 7100 square kilometers on the northern margin of salt desert extends between 56 degrees and 14 minutes to 58 degrees and 15 minutes of eastern longitude and 34 degrees and 42 minutes of northern latitudes. The geographic location of the study area has been shown in Figure 1-1. This city has been limited from the north with Sabzevar city, from west with Khalilabad city, from north east with Kashmar and from south with Tabas in South Khorasan province and from west with Shahrood in Semnan province. Its center, Bardaskan city, is located in 57 degrees and 57 minutes of eastern longitude and 35 degrees and 15 minutes of northern latitudes and in 265 kilometers of southwest of Mashhad.

The height of the city is 985 meters above sea level, and according to the latest decisions, it has 3 sections including central, Anabad and Shahr Abad with 393 inhabited and inhabited villages. Shahrabad is a city in the area of Shahr Abad, the city of Bardaskan in Razavi Khorasan Province of Iran. Based on the general census of population and housing in 2016, the population of this city has been 2, 083 people (in 644 households).

The location of the city relative to the surrounding towns: North: Bardaskan, Northeast: Khalilabad and Kashmar, south east: Bajestan (Ahmadipour, Shaibani, & Mostafavi, 2019; Youli Li, 1999). This city as hydrologic is located in large-scale in Kalshoor basin - Salt Desert and in the small-scale in hydrologic unit of Darooneh. Height from sea level: 880 meters. Distance to city center: 14 kilometers (figure 1).

-Weather features

The northern areas of Bardaskan are mountainous and the southern and central parts is plain and its air is dry due to its proximity to the desert (Vearncombe. JR, 1989). The average annual precipitation is 150 millimeter. The air temperature of the city of Bardaskan is about 45 degrees in the warmest summer days and falls below zero at 5 ° Centigrade on the coldest nights of the winter.

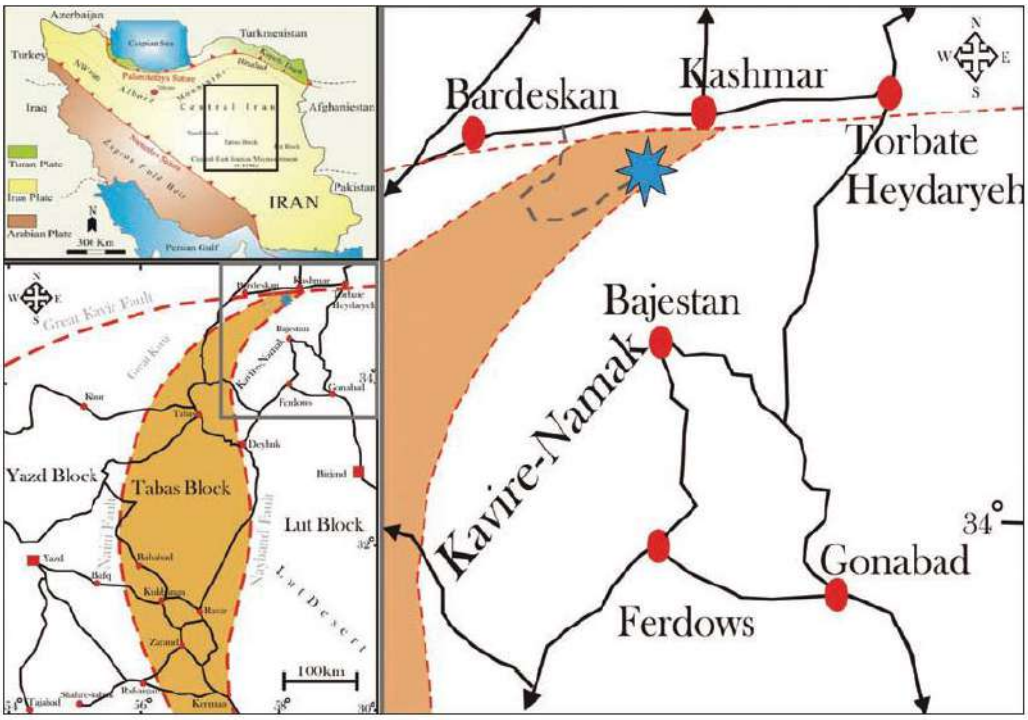


Figure 1. Geographic location of the study area (adapted from the maps of Khorasan Razavi Governorate, and Geological Survey).

Because of this, the temperature difference is high in different parts of the city. Its northern and eastern sides are relatively cold, but its western and southwest winds due to its proximity to deserts are hot and burning with dust. (Climatology.ir Comprehensive Iranian Meteorological and Climatic Site) (Teod, 2016).

-Climate

This city has been formed from two mountainous regions of the north and southern plains, including deserts, salt woods and salt deserts.

The Bardaskan area has been located in the northwest of central Iran and is part of the central Iranian sedimentary and structural zone. The position of the studied area relative to Iran's structural divisive units have been shown in Figure 1-2. In this range, different outcrops of Precambrian rock units up to the present day are observed (Jagat & Mahesh, 2018). The most extensive lithology of this region are formed of igneous rocks and metamorphoses. The precambrian stones of this region are located in a

wedge-shaped massif between the main faults of Taknar and Darooneh (pierpaolo Guarnieri, 2008).

The 1:100000 map of the Geology of Bardaskan city has been shown in Figure 1-3. One of the most influential masses of this area is the Precambrian penetrative mass that is made of granite, granifiers and granitoid, and is the equivalent of era granite. Another important intrusive mass is the granite area, whose time of influence has been determined as Eocene-Oligocene. According to the recent research on the age measurement of the zircon Uranium-galena in the Sarhangi Mountain located in the Tectonic zone of Kashmar-Kerman, the age of the intrusive bedrock (high silica) of Precambrian or Cambrian has been determined (535-575 million years) (Martin Stokes 2007; Samiei & Mobaraki, 2019).

The Soltanieh formations, Shirghast, Nior, Padeh, Sibazar, Bahram, Sardar, Jamal (Paleozoic units), Shemshak, red walnut layers, conglomerate-sandstone units, former Cretaceous unit, Ophiolite blend, Superphilic rocks, Diabase and Diabase tuffs , volcanic and pyrogenic rocks, Plagic limestones (Mesozoic units), Kerman Formation, Eocene Flicchi basin deposits, Eocene-Oligocene conglomerates and Neogene conglomera, red ganes and Pliocene-Ploshtoceen conglomers (tertiary units), and lateral ancient alluvium terraces, sandy hills and sandy lagoons, clay roofs, old alluviums, mud muddy- salty areas and young alluvials and cones (quaternary units) are within the scope of the study. One of the most important faults in this area is the Darooneh, Taknar, Maro andKalshoor faults, which Darooneh fault is the largest and most active fault in this area (Boomeri, 1998).

From a morphological perspective, the Bardaskan area can be studied in two separate parts. A part of the area located above the Darooneh fault is a mountainous region with a variety of deposits, while the southern part of the fault, with the exception of the southeast rough country which continue the outcrops of the Uzbek mountain is fallen area with an average elevation of 850 meters above sea level, which formed at a vast surface of quaternary deposits, such as alluvial tributaries, floating cones, clay and salt slabs (figure 2).

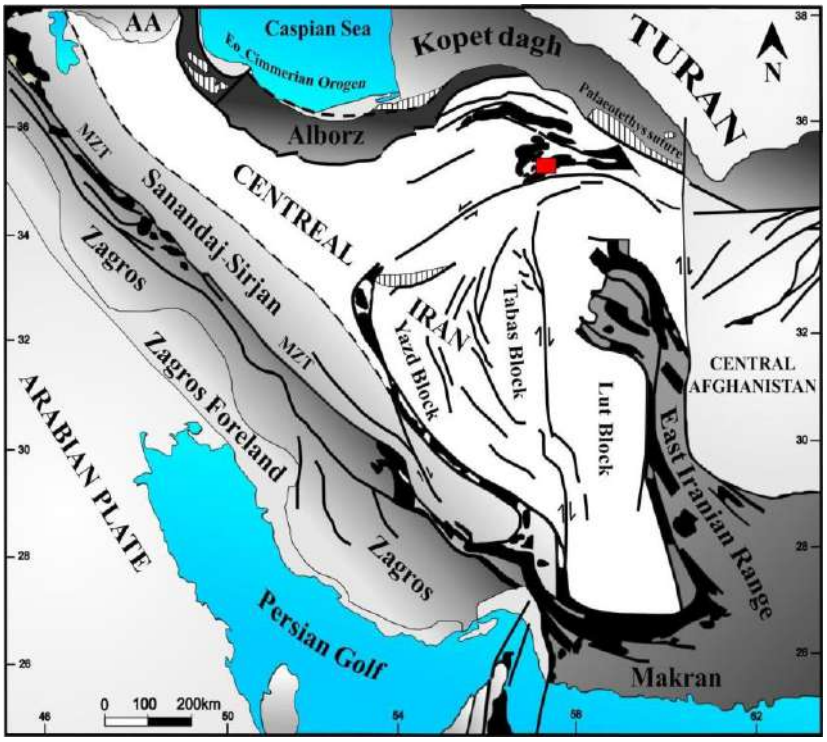
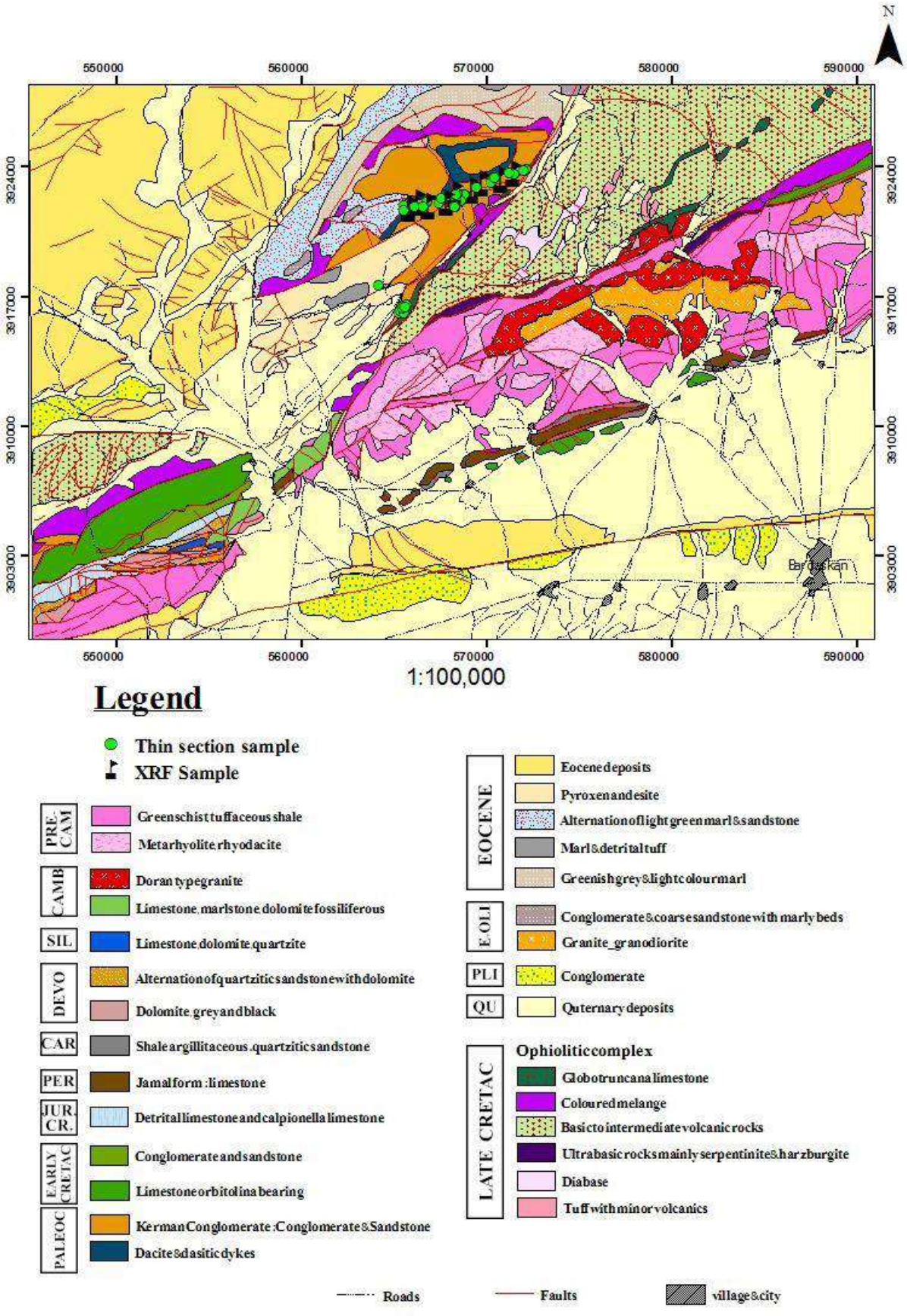


Figure 2. Division of structural units of Iran map, representing neighboring countries, (Berberian and King 1981; Angiolini 2007) (Red quadrangle represents the studied area).

The prominent geotechnical face of this area is the Darooneh fault with the east-west trend, which is the separation factor of two logistical sections. There are no permanent rivers in Bardaskan, but several seasonal rivers such as Dahan Qaleh, Anabod (Kal Asyab), Ebrahim Abad and the Bardaskan (Kaal) River Noahar are in the stream where the recent river flow from the slopes of Bijjord Mountain, 21 km north Bardskan originates from north to south (figure 3). This river after passing through the Bardaskan city crosses the Sir River and creating Shoor River that feeds the groundwater table of the Bardaskan plain (Harris, 1987).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XRF Sample
PRE-CAM
Greenschist tuffaceous shale
Metarhyolite,rhyodacite
CAMB
Doran type granite
Limestone,marlstone dolomite fossiliferous
SIL
Limestone dolomite quartzite
DEVO
Alternation of quartzitic sandstone with dolomite
Dolomite,grey and black
CAR
Shale argillitaceous,quartzitic sandstone
PER
Jamal form :limestone
JUR. CR.
Detrital limestone and calpionella limestone
EARLY CRETAC
Conglomerate and sandstone
Limestone orbitolina bearing
PALEOC
Kerman Conglomerate :Conglomerate&Sandstone
Dacite&dasitic dykes
EOCENE
Eocene deposits
Pyroxen andesite
Alternation of light green marl&sandstone
Marl&detrital tuff
Greenish grey&light colour marl
E.OLI
Conglomerate&coarse sandstone with marly beds
Granite_granodiorite
PLI
Conglomerate
QU
Quternary deposits
LATE CRETAC
Ophiolitic complex
Globotruncana limestone
Coloured melange
Basic to intermediate volcanic rocks
Ultrabasic rocks mainly serpentinite&harzburgite
Diabase
Tuff with minor volcanics
Roads
Faults
village&city

Figure 3. Geological map 1:100000 in Bardaskan city (Hajat, 2011).

1. Materials and Methods: Geophysical Studies Method

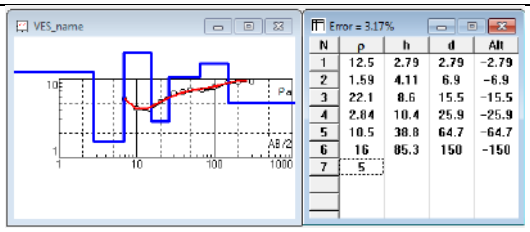
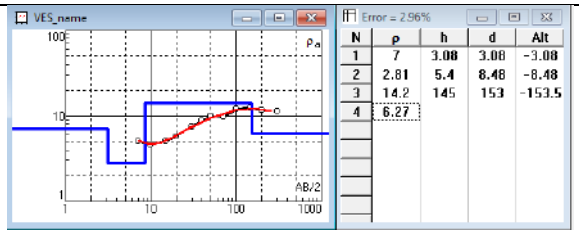
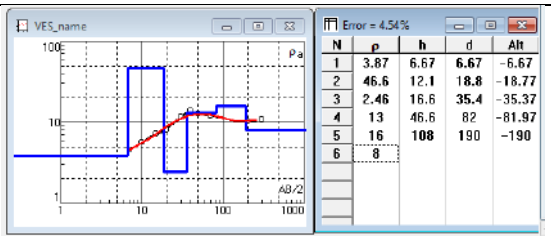
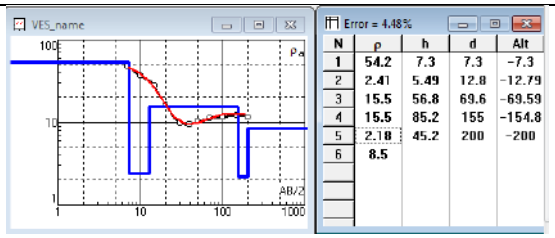
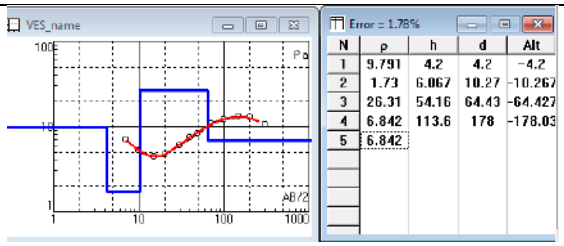
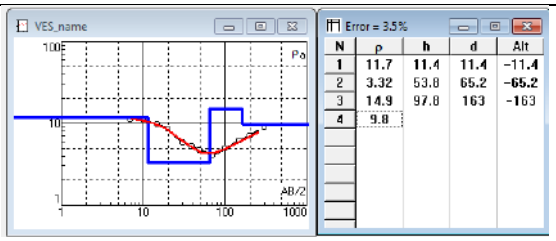
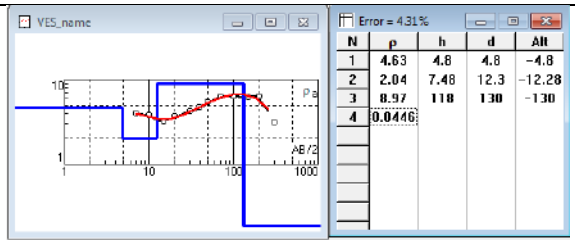
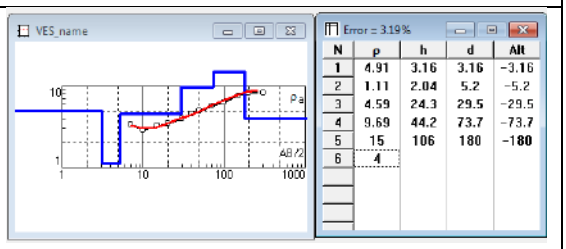
The method used in this research is the schlumberger method, which is based on the transferring electrical current to the ground and measuring the potential difference created between two points to obtain the specific resistance of different depths of the earth (Craig Hardgrove 2009). The device used is a geoelectric device with power of 1000 watts and resolution of 0.00001 mW and mA. The distance between points A and B from each other had been 600 to 800 meters, and the Electric erect sondage method has been used (table 1).

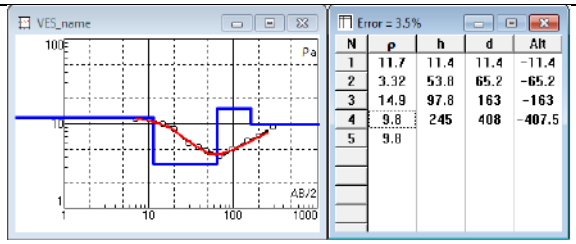
Table 1. GPS positioning of the soundages.

Position of sondages	latitude	Longitude	Sondage name
Point 1 Allameh Well 3	3889736	0579428	S_1
Point 2 Allameh well 3	3889645	0579320	S_2
Point 3 Zarein Well 2	3888919	0579741	S_3
Point 4 Shahid Oftadeh well	3889540	0578285	S_4
Point 5 Bagher Khaan well 1	3889120	0580324	S_5
Point 6 Bagher Khaan well 1	3889209	0580314	S_6
Point 7 Shahid Ali Nejad well	3891370	0577482	S_7
Point 8 Allameh Mashhadi Well (Sultan)	3885683	0564003	S_8
Point 9 Shahid Norouzi Hatitieh Well	3890927	0578696	S_9
Point 10 Hatitieh well 2	3894324+	0579415	S_{10}

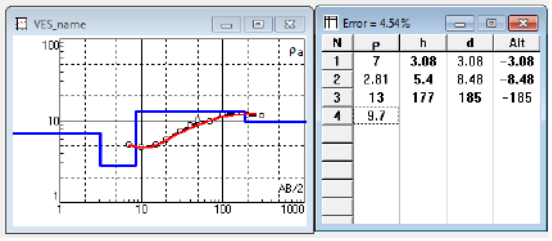
In this study, due to specific resistance measurements in a relatively large number of measured points, to find out how to extend the zones with ravelling layers and silt wind stones, specific resistance data with exploratory wells and drilled wells

in the drilling area have been Integrated, the work what the researcher followed and used in this research (Bauer, 1995). And the layering characteristics of the wells are characterized by the separation of ravelling layers, which are usually at a depth of more than 130 meters, and the following results are obtained from the ground layer scan (figure 4):

<table>
<tr><td> 
</td><td> 
</td></tr>
<tr><td>Allameh 3 well
(e.sounding 1)</td><td>Allameh 3 Well Secondary takeover
(e.sounding 2)</td></tr>
<tr><td> 
</td><td> 
</td></tr>
<tr><td>Zarein well 2 ((e.sounding 3)</td><td>Shahid Oftadeh well ((e.sounding 4)</td></tr>
<tr><td> 
</td><td> 
</td></tr>
<tr><td>well 1 Bagher Khaan first impression
(e.sounding 5)</td><td>well 1 Bagher Khaan first impression
(e.sounding 6)</td></tr>
<tr><td> 
</td><td> 
</td></tr>
<tr><td>Shaheed Ali Nejad's Well
(e.sounding 7)</td><td>Allameh Mashhadi Well (Sultan)
(e.sounding 8)</td></tr>
</table>



Shahid Norouzi Hatitieh Well ((e.sounding 9)



Hatitieh well 2 ((e.sounding 10)

Figure 4. Specific resistance of performed soundings tables

By studying 8 done sondages near the Hassanabad wells, it was found that the aqueous layer starts at an average of 80 meters and extends to a depth of about 150 meters to 170 meters, and then with a drop of layer resistance to less than 10 we see that is located between the resistance of 4-10 and the experience of the excavations and the samples obtained from the well represents the wind and silt sand, which caused the state of the ravination of the well, although this layer also has some water that exceeds collapse, only in one well with a specific resistance drop of less than 1 gane soil sample was present with a very low percentage of silt.

Since the gane mud is also very unstable and along with a percentage of silt and wind sanding form a faint layer, where any drilling in it leads to destruction and shortening of useful life and a sharp decrease in well flow.

In the Hatitieh wells of the cemeter No. 9 and No. 10, which have a depth of about 170 meters from the ravelling layer with a resistance of 8-10, with a fine sand content plus sand and silt, its aggregation has been taller than that of Hasanabad and the phenomenon of collapse of the well in these two wells is slower and its shelf life has been about 6 years.

In a mixture of clay and other minerals with a calcium carbonate content of between 35% and 65% is said gane , If the hardening or melting occurs in them, the word Marleston or Marlit refers to them (Akiko Hashimoto 2008), In ganes, minerals of calcite and clay are the main mineral with other minerals such as quatz, albite, etheringite and tomazite and etc. The size of the particles and minerals in the ganes is

in size of clay, silt, sand, and sometimes even in grain size. Thus, ganes, based on the type of mineral, texture and the percentage of particles, form different gane groups that have different chemical, physical, mechanical and erosion features. Ganey rocks have been considered as one of the most problematic sedimentary rocks due to the formation conditions and behavior that they show during exploitation (figure 5).

Divergence is a phenomenon of physics and chemistry, in which the particles of the clay adjacent to their adhesion water are lost and repel each other, so that the particles are suspended in water and easily and with very little energy is washed out of environment. The potential for divergence and erosion in a given soil depends on several factors, including mineralogy, soil chemistry, and soluble salts in the pore water of the soil and adjacent water. Such soils, even in comparison with non-adherent soft soils such as soft sand, are rapidly eroded by the flow of water at a slow pace. Divergent clay soils particles react in the water also and soil particles are suspended in water (A. Gomez-Villar 2000).

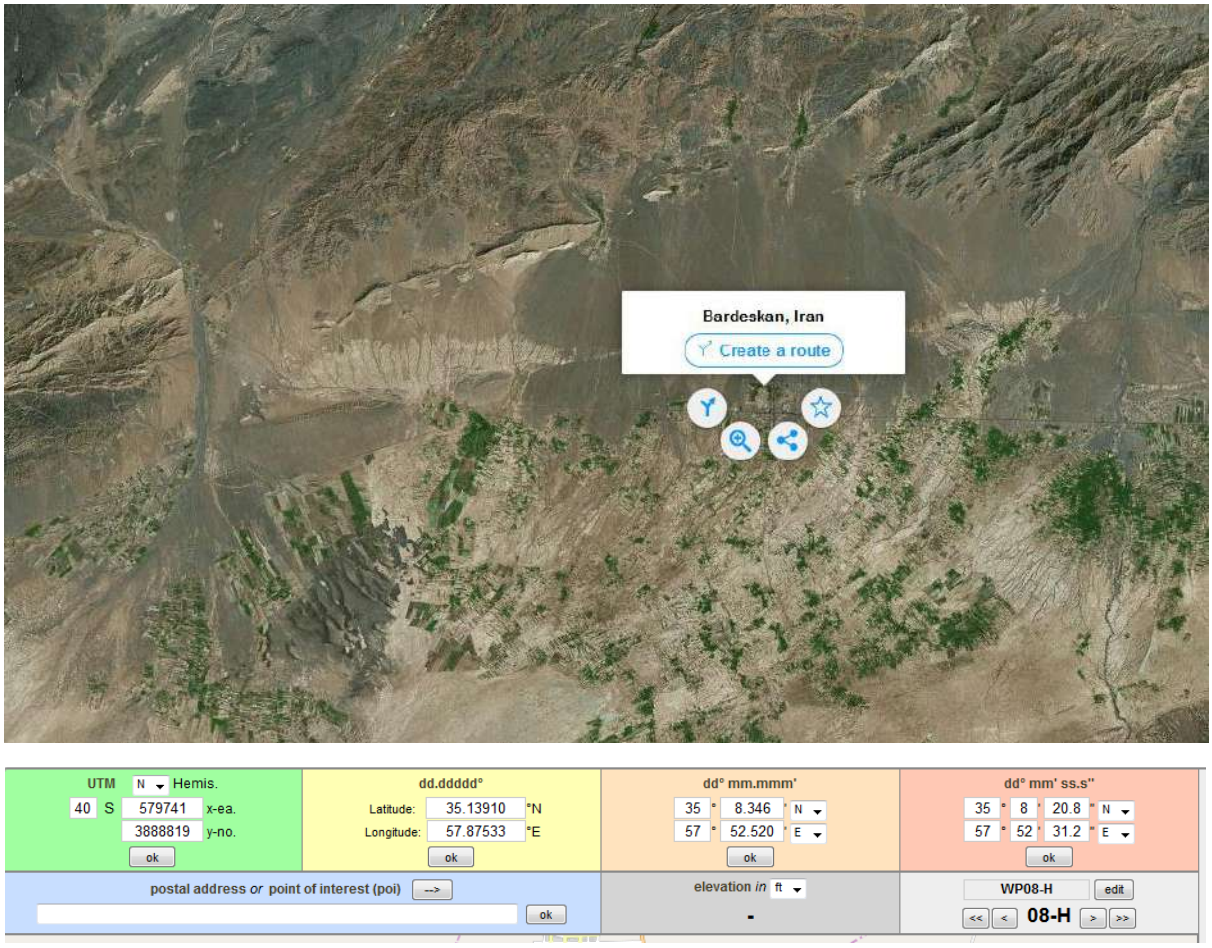


Figure 5. Aerial map of Exploratory well and location of electrical sondages and conversion of GPS units.

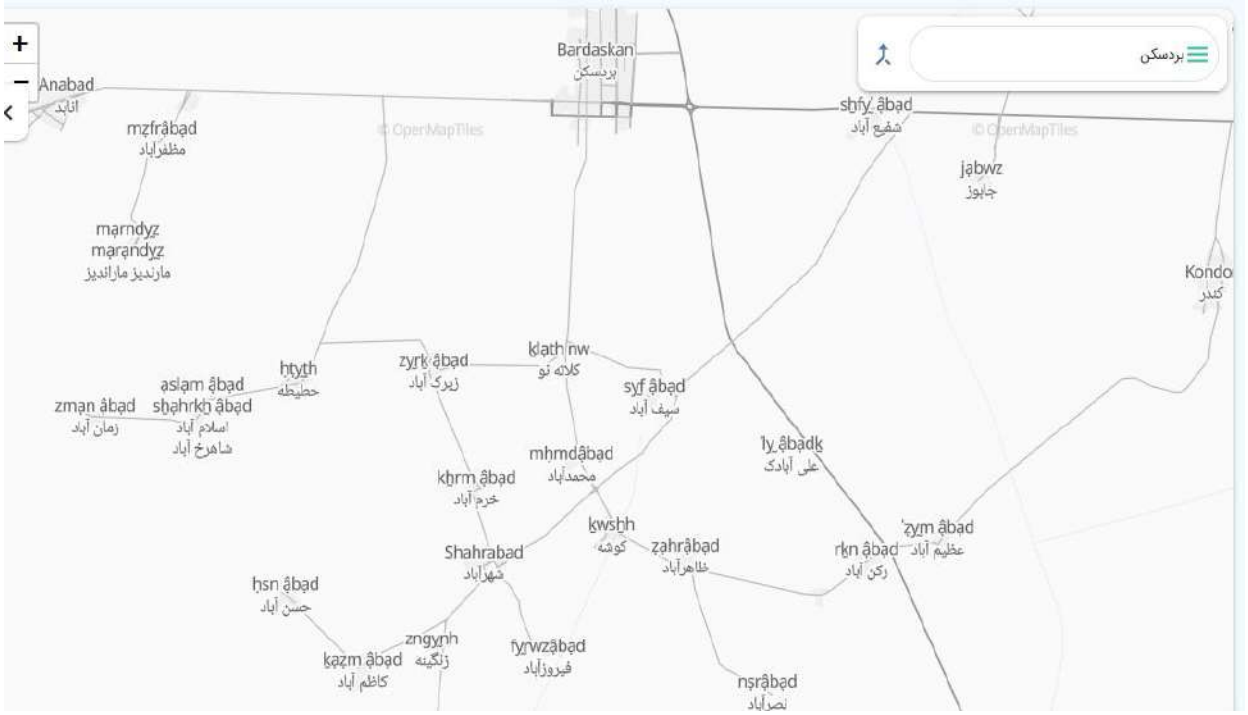


Figure 6. The ways accessing to location of studies map.

In order to detect the ravelling layer and with windy sand and silt and providing water extraction strategies, it has been found that, with surveys and geophysical field studies, it has been found that there is only one main aqueous layer in the vicinity of the well, which is buried in the middle depths of 70 to 160 meters, where the ravelling layer is located below this aqueous layer (figure 6) (Amanlou & Mostafavi, 2017; Banaei, 2019; Bassey & Edoamodu, 2018; Obidoa & Ugueche, 2017).

Which is located at a depth of 150 meters, with more silt and a percentage of clay and wind sands, and a small amount of drainage water that has made the collapse of the layer intense.

Drilling in this raveting layer is usually difficult for drilling machines and usually causes tilt of the wellbore or drilling time, and the life of most of these drilling sites in the raveting layer is less than 6 years, because wind sands and silt penetrate into the tube and causes the well to fill up and or by pulling this wind and silt sand into the tubing and pumping with water into the bubble, the space around the pipe wall is

depleted and suddenly collapse the massive mass of soils around the pipework and the wellbore.

The collapse phenomenon is also found in wells with gane mud layers, and in wells with sandstone and silt layers, but in the case of silt sand pits this phenomenon has been reported more. However, the following factors, individually or in combination of several factors, can cause the well to sand up:

1-Select an inadequate location to install a grid pipe or install a pump.

2 - Very low cross-section for water entry in rectangular tubes or saw blades.

3- The width of the grooves is usually between 3 and 8 millimeters, which is between 2 and 3 times the maximum diameter of the particles in the majority of the region's aqueous layers.

4-Use a sandblast against the grid by closing the bridge.

5-Failure to reach the "sand filter" against the grid by bridging.

6- Failure to develop adequate or proper well

7-Over-well discharge, especially if the well is not fully developed.

Among the above factors, the maximum effect on the sanding of wells is 2, 3, and 4. However, in spite of the lack of proper sandblasting, the well can be expanded naturally and the amount of sand gravity is very low, if the water cross-section and the width of the slots are appropriate. (Grizni, 2019; Heidary & Riahi, 2018; Rashid & Al-Marzoqi, 2019)

Providing a solution to prevent collapse of the well wall and counteracting the excavation of wells is as follows:

1- The best point for drilling a well with a aqueous layer containing gravel and coarse sand should be determined by geophysical operations and the clay layer of silt or silty sandy, raveling from the aqueous layer be separated to avoid additional excavation in this layer.

2- Preferably, instead of Lattice tubes, use a screen pipe in wells with a depth of less than 150 meters.

3- If you use the lattice walls, you should surely to use of two lattice tubes that between fiiled with gravel and coarse sand, that in which case the space between the wall pipe is sufficient and the wall grooves are appropriate to the soil texture (table 2). Table of reconstruction of wells according to sediment type and its extension (Yazd Regional Water Company) (Ahmadipour et al., 2019; Mostafavi, 2015; Mostafavi, Eissazadeh, & Piryaei, 2019; Rahman & Vaheed, 2018; Samira Eissazadeh & Taskhiri, 2019; Shamsipur et al., 2012).

Table 2. Comparison of different wells and recovery methods.

Recovery method	The well wall has deposits of iron deposits	The well wall is deposited with carbonate deposits	The well wall has no precipitate but has sand making and silt making	New wells
ultrasonic		***		
Explosive		***		
Air injection (jet)	***		***	***
Water injection (jet)	***		***	***
Jet sonar		***		
Nitrogen shock		***		***
Eco-fide-co2		***		
brushing	***	***		
pistoning	***	***	***	***
Acid washing	***	***		

Drilling mud solvent				***
Chlorination	***	***	***	***

Experience has shown that if the water velocity in the well does not exceed 3 centimeters / second, the minimum particle displacement is carried out, and thus the amount of wells' sandwiching is greatly reduced. This value has been selected and implemented as standard for many years in America, Europe, Australia, Japan, and so on (Barbosa, 2018; Kumar & Gapta, 2017; Márquez & Gunzalez, 2017; Modaresi & Kazemi, 2019; Salimian & Mirzaei, 2018).

In the table 3, the cross-section of the grid section of gas or saw blade has been presented in a common 12-inch tube. Additionally, the maximum water that can be fitted to each meter of the latched tube according to the International Standard for Mineralization has been also mentioned.

Table 3. The extracted water from the well based on Screen pipe.

Maximum allowed discharge	Cross section at 1 meter	Number of grooves	Cross section of each groove	Groove width	Groove length	Row number
(Liters per second)	Lattice (Square centimeters)	Per meter	(Square centimeters)	(Millimeter)	(centimeter)	grooves
0.12-0.18	40-60	10	4-6	2-3	20	4
0.18-0.27	60-90	15	4-6	2-3	20	6
0.24-0.36	80-120	20	4-6	2-3	20	8
0.30-0.45	100-150	25	4-6	2-3	20	10

The solution to the cross-sectional entry of water with low entry rates has been solved over the years in Europe and the US by using screen tubes. For example, the

strongest screen tube with a minimum cross-sectional area of 594 centimeters and a 0.5 millimeter groove has a cross-sectional area of 1122 centimeters per square meter of screen (Al-Khalifah, 2018; Eslami & Ahmadi, 2019; Gujirat & Kumar, 2018; Kimasi, Shojaei, & Boroumand, 2019; Timakhov & Kasparov, 2018). Thus, for example, the above-mentioned example, for taking 36 liters per second at a speed of 3 centimeter per second, requires only a 22-meter screen tube with a 0.25 millimeter groove or just 12 meters with a 0.5 millimeter groove. (Discharge allowed for each screen meter with a 0.25 millimeter groove is 1.78 and a 0.5 millimeter is 3.36 liters per second) (figure 7).

Figure 7. Advantages of using screen pipe instead of lattice tubes.

1. Severe reduction or removal of sand.

2. Reduced cost of operation due to the decrease in water loss due to the reduction in network losses, each 15 liters per second water drained from a depth of 5 meters, approximately 1 kilowatts of electricity (with good efficiency of 75% of the system), or the equivalent of gasoline is consumed in an hour. Thus, with the decrease in water level due to the use of a screen pipe, the cost of exploitation during the life of the well dramatically decreases.

3. The lack of a need for a large sedimentation tube due to the introduction of much less sediment into the well.

4. Screen tube gravity is much slower than lattice tubing because the total volume of water containing salts in the lattice tube enters a low cross-sectional area, and as a result, the density of sediments in the front and around the grooves is much larger than the screen pipe, which cross-sectional area of entrance is between about 5 to 12 times

the lattice tubes, and as a result, the speed and thickness of the mass fraction also decrease (Nakhaee & Arab Nasrabadi, 2019; Timakhov & Kasparov, 2018; Upikang, 2017).

5. One of the problems with latching wells is to cut or assemble the tube, especially at the top of the first grid. In general, in common lattice or screen pipes, with the same groove density across the grid or screen, the water velocity at the top of the lattice or screen is maximum and reaches zero to the bottom. In lattice tubes, due to the very high flow rate and (turbulent floe), the ratio of the poisson ratio of the earth's layers has increased of normal mood (about 0.25 for sand and 0.5 for clay) and as a result, a greater proportion of the soil weight above the layer is applied horizontally to the tube, and when the force exceeds the resistance of the tube, it bends or tear into the pipe.

This is especially true in the upper part of the highest lattice tube or the sheathed pipe in front of the most permeable layers. In addition to the aforementioned, which is gradual, in well-sanded wells due to rapid sand discharge, cavities are generated especially on the back of the tube and in the upper part of the layers, which can also lead to excessive collapse of collapse, and finally, cut the tube. This problem is commonly used in rotary drilling wells with sand filters (Rasouli, Mohammadali, & Houshmandan, 2019).

However, in the screen tube, due to the laminar flow state (not the turbulence mode), a change in the natural poisson number of layers has not been deposited or the magnitude of its increase is negligible and, as a result, this risk does not exist or its amount is significantly reduced and also, the problem of creating cavities behind the tube is also excluded due to the low input speed .

6- Since the two above mentioned 4 and 5 are in fact the main factors determining the useful life of a well, the useful life of the wells using the screen pipe is much greater than the wells with the lattice tube.

Conclusion

Due to specific resistance data, layers obtained from the wells of Hassan Abad and Bardaskan villages show a resistance range of 4-10 in the deep layers after the

aqueous semi-deep and deep layer, as well as evaluation of soil samples drilled from new wells excavated to a depth of more than 180 meters indicate this:

1. A windy sand and silt layer with a specific resistance of 4-10 can be identified, that this resistance range can be used to determine the ravelling layer in the wells of the surrounding villages in geophysical operations, due to the fact that the resistance of the sweet aqueous layer of this region begins from the resistance range 12, it can be interpreted that a drop in resistance of less than 10 is very likely to occur in this region of silt or clay soil or silt gane or sand silt and with collapse of well (Farah & Kalsoum, 2018; Jafari & Mostafavi, 2019; Kaltas & Javidoglu, 2019; Riahi, 2018; Samiei & Mobaraki, 2019; Tasnim & Farasat, 2018)

2. The gane mud layer that has a very low percentage of silt (less than 10%) exists only in a well sample in the Bardaskan of Hatiteh village , whose true resistance to this layer was less than 1 and due to the presence of calcium carbonate and other calcareous compounds faced with water dissolved in it and causes cavities in gane to form, which also causes the instability of the soil around the pipe, and because of the lime dissolution of this layer and the formation of large water cavities on the turbine, it does not accumulate until it is pumping and so the water rushes into these cavities and causes decreasing of watering of the well.

3. The lowering of the wells watering mentioned above was due to the high drilling in the ravining layer, which was lower than the main aqueous layer, and the lack of use of the screen pipe or the double glazing of the well tubes and the absence of injections of the gravel pack between the two walls.

4. The cause of tilt of the well during or after the drilling and tilt of the pipe wall and the overall destruction of the well, has been too much drilling in the ravining layer, which by removing the wind sand and silt along with water from the well and emptying around the tube wall, the massive masses of the soil around the well has fallen suddenly and causes tilt of the pipes wall.

5. Another important reason for the sand making of the wells in these two villages is the existence of a large number of grooves per square meter and the size of the pipe wall groove that is between 3 and 8 millimeter and usually between 2 and 3 times the standard size.

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Análisis de viabilidad técnica del suministro de energía eléctrica en Mantecal, estado Apure, mediante un sistema solar

José Ramón Aguilera Nieves *

RESUMEN

Esta investigación muestra los resultados de un análisis sobre la viabilidad técnica y ambiental de un sistema solar en Mantecal – Apure, basado en una ruta teórico global sobre las energías alternativas, la disponibilidad del recurso solar en el escenario de estudio específico y las características tecnológicas del sistema de energía solar fotovoltaica. Se realizó un análisis donde se evaluaron los beneficios ambientales de reemplazar o acompañar el suministro de energía actual por energía solar. Se concluye que la instalación del sistema solar fotovoltaico es viable para las condiciones climáticas diagnosticadas tales como: radiación solar y brillo solar del escenario de estudio; así como las condiciones técnicas requeridas. De acuerdo con los resultados de todo el enfoque teórico y de investigación, así como el alcance de este proyecto, se deja el camino para continuar con los estudios correspondientes al dimensionamiento técnico del sistema propuesto y al diagnóstico de la demanda energética de la zona, que son necesarios para una posible ejecución de esta investigación.

PALABRAS CLAVE: análisis, energías alternativas, sistema solar, ambiente, Mantecal.

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Technical feasibility analysis of the electricity supply in Mantecal, Apure state, using a solar system

ABSTRACT

This research shows the results of an analysis on the technical and environmental viability of a solar system in Mantecal - Apure, based on a global theoretical route on alternative energies, the availability of the solar resource in the specific study scenario and the technological characteristics of the photovoltaic solar energy system. An analysis was performed where the environmental benefits of replacing or accompanying the current energy supply by solar energy were evaluated. It is concluded that the installation of the photovoltaic solar system is viable for the diagnosed climatic conditions such as: solar radiation and solar brightness of the study scenario; as well as the technical conditions required. According to the results of the entire theoretical and research approach, as well as the scope of this project; the way is left open to continue with the study corresponding to the technical sizing of the proposed system and the diagnosis of the energy demand of the area, which are necessary for a possible execution of this research.

KEY WORDS: analysis, alternative energy, solar system, environment, Mantecal.

Introducción

El ambiente es necesario para todos y se debe conservar para no arriesgar su futuro. Estudios demuestran que las costumbres del hombre de hoy nos llevarían a un problema de difícil solución. Nos enfrentamos a una crisis ambiental, donde los seres humanos comenzamos a darnos cuenta que el desarrollo impacta en el deterioro ambiental (Apud, 2019; Ferrer et al., 2011). Por otro lado, la energía es imprescindible para mantener la calidad de vida. Hoy día existe gran tensión entre la demanda de más energía, en particular de electricidad, y las exigencias de que se proteja la vida, la salud y el ambiente. Aunque se ha pretendido analizar ambas problemáticas por separado, ya es bien aceptado que estas guardan estrecha relación, en otras palabras, ambas son variables de una misma ecuación político - estratégica cuya solución es en extremo compleja.

Pese a esto, se sabe por ejemplo, que para generar más electricidad, en algunas zonas posiblemente haya que construir represas e inundar grandes extensiones de tierra, también que sería preciso construir centrales nucleares o quemar combustibles fósiles cuando ya el 25% del CO_2 que se encuentra en la atmósfera

proviene de la generación de electricidad en centrales alimentadas con este tipo de combustible. Otras opciones vanguardistas sugieren la implementación de los llamados biocombustibles, una fuente potencial de energía renovable. Sin embargo, sólo algunos de los actuales programas de biocombustibles son viables, y la mayoría implican altos costos sociales e irónicamente ambientales.

La electricidad desde hace mucho tiempo ya se ha instaurado en nuestra civilización como una necesidad de la cual no podemos prescindir y que va en aumento, ya que cada vez existen más dispositivos y/o aparatos que funcionan a partir de esta forma de energía, la cual dicho sea de paso es una de las más limpias. Sin embargo es importante aclarar que la energía eléctrica es una energía limpia pero solo en lo que respecta a su utilización, en cambio en su producción y transporte puede acarrear importantes consecuencias negativas sobre el medio, como lo son: ocupación de espacio para las instalaciones, utilización y consumo de recursos, generación de residuos materiales o energéticos, y quizás la consecuencia más relevante sea la modificación física, socioeconómica y hasta cultural de la zona de implantación o influencia.

La generación de electricidad depende principalmente de combustibles fósiles. Para finales del siglo pasado, más del 60% de la electricidad se produjo en centrales térmicas. Uno de los inconvenientes del uso de combustibles fósiles son las emisiones contaminantes locales y de gases de efecto invernadero. Por otro lado, las perspectivas del incremento del consumo de electricidad y los consecuentes problemas ambientales por la combustión parecen favorecer a la energía nuclear. Sin embargo, los problemas de seguridad originados por desechos radiactivos de alto nivel así como las características de la estructura actual del sector eléctrico, desfavorecen el uso de esta tecnología en el corto plazo.

En Venezuela por su parte la energía mayormente es hidroeléctrica, cuyo principio es transformar en electricidad la energía potencial de una masa de agua mantenida a desnivel entre un embalse y la central situada aguas abajo, en la cual la turbina acoplada a un alternador convierte en electricidad la energía mecánica del salto de agua. Esto implica la creación de un obstáculo (presa) en el cauce fluvial, que lleva asociado un cambio del régimen natural del río. Aunque el

funcionamiento de la central hidroeléctrica trae cierto impacto ambiental, los principales efectos están en la construcción de la presa y el régimen de operación del embalse. Las alteraciones fundamentales afectan el agua y el suelo, siendo escasa la incidencia sobre el cambio climático. Estas alteraciones dependen más del tamaño y localización del aprovechamiento hidráulico.

Es por todo esto que no es casual que desde hace algunos años la energía y el ambiente han comenzado a ocupar un lugar preponderante en la opinión pública. Esta creciente preocupación resulta consecuencia lógica de la toma de conciencia de que las alternativas energéticas deben ir asociadas a una mejor calidad de vida, objetivo el cual es de un más amplio alcance e importancia que el del mero consumo de energía. Luego se deben buscar los mecanismos para generar y transportar electricidad de una forma sostenible y respetuosa con el ambiente, por lo que surge la necesidad de desarrollar y difundir investigaciones sobre la energía eléctrica y su relación con el ambiente, de modo de fomentar conciencia a cada individuo frente al desarrollo sostenible a través de formas más eficientes de obtener energía y que respeten al medio.

En este orden de ideas, se han venido desarrollando alternativas a este escenario como la energía solar que, "es un recurso renovable, es decir, está siempre disponible, no se agota y se puede aprovechar en cualquier momento gracias a que es posible almacenarla" (Salamanca-Ávila, 2017). Desde tiempos remotos de la civilización, el hombre ha sido consciente del poder de la energía solar, y ha hecho uso de ella de diversas formas (Ladrón, 2018). En cuanto al desarrollo de la energía solar, este está delimitado por la intensidad y los ciclos de radiación solar captada por la superficie terrestre, las condiciones meteorológicas existentes y la posibilidad de convertir esta radiación en calor o electricidad.

Luego, en esta investigación, se plantea en primer lugar la hipótesis de que el uso de las energías alternativas o emergentes dan solución al problema del impacto ambiental de la generación de electricidad; para corroborar la misma, se debe interpretar la incidencia que a través del tiempo han tenido las energías convencionales en el medio y a la vez instruirse respecto a las fuentes alternativas, con lo cual se puede hacer una valoración del impacto de las energías tradicionales

y simultáneamente permite hacer un contraste con las fuentes renovables. Además, se aborda el estudio enmarcándolo en un radio de acción más específico, el cual es la parroquia Mantecal, municipio Muñoz del Estado Apure; planteándose así una propuesta de la fuente alternativa más viable para las condiciones geográficas y climatológicas de dicho escenario.

Siendo Mantecal una población ubicada en la región de los llanos venezolanos, posee un clima tropical en el cual se tienen básicamente dos periodos o temporadas: sequía y lluvia. Vale aclarar que en los últimos años con la agudización del cambio climático en el mundo, estas temporadas se han visto seriamente afectadas, cambiando los ciclos en que estas ocurrían, teniéndose ahora y cada vez más meses de sequía que sin duda han afectado los ciclos de siembra en la región. De igual manera esta situación ha trastocado seriamente el sistema eléctrico venezolano, el cual como ya se dijo es mayormente hidroeléctrico. Sin embargo, en esta nueva realidad se podría hallar una cierta ventaja en términos de fuentes alternativas de energía.

Las elevadas temperaturas que hoy día se hayan en la región llanera claramente se deben a la mayor incidencia que hoy tienen los rayos del sol sobre la misma, con lo cual se tiene allí una fuente primaria de energía, la solar. Entonces corresponde analizar la posibilidad de usar un sistema de generación eléctrica que se base en este tipo de fuente. La viabilidad del suministro de energía mediante implementación de un sistema solar fotovoltaico requiere la evaluación de varios aspectos entre los que se encuentran meteorológicos, energéticos, técnicos, financieros y de beneficio ambiental para justificar la "transición energética".

1. Metodología

En primera instancia el enfoque de esta investigación es cualitativa, aunque presenta algunos datos estadísticos, estos simplemente se tomaron de una fuente para luego interpretarlos o analizarlos. En cuanto al nivel de investigación, esta se enmarca en una de tipo descriptiva, ya que se lleva a cabo todo un abordaje teórico para caracterizar el fenómeno de la generación de la energía eléctrica en general, estableciendo su estructura y su comportamiento; así como de las energías

alternativas y en particular el sistema solar. Así mismo, se tiene que el diseño de investigación es documental, puesto que se requirió de una exhaustiva revisión bibliográfica para obtener información detallada del fenómeno objeto de estudio.

En este mismo orden, la técnica para la recolección de información fue la búsqueda de fuentes bibliográficas de primera y segunda mano. Luego las técnicas de procesamiento de la información están referidas al conjunto de pasos a realizar con el objeto de poner de manifiesto y sistematizar dichos aportes. El propósito es el de descubrir, analizar, interpretar y reflexionar sobre el estudio planteado. Para ello en primer lugar se lleva a cabo una revisión exhaustiva de la literatura disponible, estableciendo estrategias de búsqueda y criterios de selección, lo cual permitió una eficiente documentación del tema a fin de contextualizar el fenómeno y explorar los referentes teóricos que existen. Finalmente se procedió a organizar la información a partir de la elaboración de gráficos de datos otorgados por las fuentes y un posterior análisis de los mismos.

2. Análisis

Comúnmente se denomina energía alternativa a aquella fuente planteada como opción a las tradicionales o clásicas (combustibles fósiles). Sin embargo, vale aclarar que no existe consenso respecto a qué tecnologías están englobadas en este concepto, y la definición de "energía alternativa" difiere según los distintos autores, en las definiciones más restrictivas, energía alternativa sería equivalente al concepto de energía renovable o energía verde, mientras que las definiciones más amplias consideran energías alternativas a todas las fuentes de energía que no implican la quema de combustibles fósiles (carbón, gas y petróleo); en estas definiciones, además de las renovables, están incluidas la energía nuclear o incluso la energía hidroeléctrica.

Una definición más precisa sobre energías renovables puede ser planteada así: "son aquellas que en un período determinado natural vuelven a disponerse en una cantidad similar a la que se ha gastado, dicho lapso de tiempo sería relativamente breve en un orden de magnitud a escala humana" (Peña, 2012). Entonces las energías renovables, como lo indica el término, se renuevan naturalmente, he allí

la razón por la que se suelen llamar energías verdes. De acuerdo a este enfoque, toda fuente renovable entraría en el orden de las energías alternativas. Otro hecho que corrobora esta última teoría es que además a lo largo de la historia el uso de estas fuentes ha sido mucho menor en comparación con las provenientes de combustibles fósiles.

Por otro lado, tenemos como ha sido la evolución de la energía a través de la historia, ya que desde siempre el hombre ha utilizado las energías renovables como fuentes; y no es hasta después de la revolución industrial cuando se inicia la utilización generalizada de los combustibles fósiles. Este último periodo de unos 200 años, se ha caracterizado por un consumo creciente e intensivo de energía que prácticamente ha acabado con esta fuente de energía no renovable. Con lo cual se tiene un primer problema, y es que es cada vez más costosa implementar instalaciones basadas en este tipo de energías, además del impacto ambiental que producen.

Al respecto, el Programa de las Naciones Unidas para el Medio Ambiente ha sido muy crítico, tal y como expresa Cabello (2006), existe un abuso de los recursos del ambiente "por una imposición de criterios y tecnologías desde la óptica de los países industrializados que son los que tienen los mayores requerimientos energéticos". Luego la misma historia nos ha traído de vuelta la necesidad de retomar el uso de energías alternativas, así como también los últimos datos científicos sobre el cada vez más acentuado deterioro del planeta por la contaminación, que no tiene otro origen sino un uso desproporcionado de fuentes de energía basadas en combustibles fósiles. Respecto a esto Nina y Valencia (2007) comentan:

> Mejorar la calidad de vida de las personas no radica solamente en proporcionarle mayor comodidad para el uso de nuevos objetos, sino de generar un mundo sin contaminación, para esto se requiere fomentar el uso de aparatos de energía renovable, así el usuario transmitirá conciencia en cadena.

Con lo cual se tienen dos grandes vertientes bien definidas que nos inclinan cada vez con mayor fuerza al uso de energías alternativas: Por un lado, la escasez de combustibles fósiles y por ende su elevado costo de producción; y por otro la

necesidad imperiosa de disminuir los niveles de contaminación en el planeta, como ya se había hecho énfasis.

Luego, profundizando sobre la contaminación generada a raíz del uso de combustibles fósiles, tenemos, por ejemplo, que las emisiones de gases por efecto invernadero (GEI) causadas por este tipo de energía, han aumentado las concentraciones de esos gases en la atmosfera.

> En el Cuarto Informe de Evaluación (CIE) del IPCC se concluyó que la mayor parte del aumento observado en el promedio de las temperaturas desde mediados del siglo XX se debe muy probablemente al aumento observado en las concentraciones de GEI antropogénicas. (Edenhofer et al. 2011)

Entendiéndose por GEI antropogénicas a emisiones de gases no naturales, es decir causadas por la acción del hombre. Lo que indica con claridad la responsabilidad directa del ser humano en el aumento promedio de la temperatura global, causante a su vez de los cambios climáticos observados desde mediados del siglo pasado.

Es por estas razones que en los últimos tiempos desde diversas partes del mundo que organizaciones gubernamentales y no gubernamentales, se han puesto en marcha en la búsqueda de soluciones que logren mitigar el impacto ambiental producido por las energías convencionales. Gomez, Murcia y Cabeza (2017) argumentan al respecto que sin embargo esto no ha sido suficiente para que personas naturales y jurídicas se motiven a destinar recursos en tales actividades por el costo inicial y por la falta de conocimiento de esta fuente de generación.

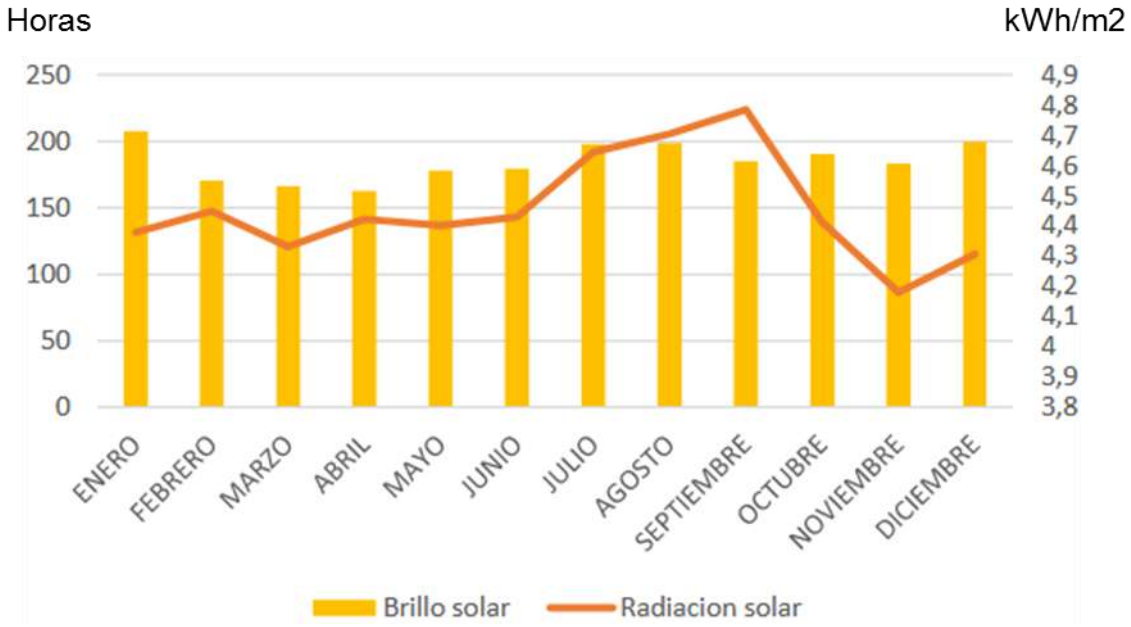
Entonces se deben dar los pasos en todos los niveles para contrarrestar el daño ambiental que ya se ha dejado claro está bastante avanzado. Ya se instauró líneas atrás el hecho de que las energías alternativas son sin lugar a dudas la opción ideal para generar electricidad de forma sustentable. Extrapolando el análisis a la población de Mantecal, se debe en primer lugar estudiar las condiciones climatológicas de esta región, con lo cual se podría proponer el modelo de fuente alternativa que mejor se adapte a dichas condiciones. Dicha energía renovable podría basarse en un sistema fotovoltaico, que técnicamente es un conjunto de equipos eléctricos y electrónicos que producen energía eléctrica a partir de la radiación solar (Perpiñan, 2018).

En este sentido, siendo el estado Apure una zona de características tropicales, cuyas elevadas temperaturas persisten durante prácticamente todo el año por tratarse de grandes extensiones de sabana; se propone como fuente de energía alternativa un sistema solar fotovoltaico, que básicamente "son sistemas que producen electricidad a partir de la luz solar" (Uzquiano et al., 2015). Para lo cual se requiere contar con información base del recurso solar disponible en la zona de estudio, medida correspondiente a radiación solar global sobre superficie horizontal en unidades de kWh/m^2. Existen datos de radiación solar global de muchos lugares del mundo recogidos en tablas y bases de datos, pero lo más recomendable es recurrir a la estación meteorológica más próxima al lugar de la instalación

Adicionalmente, se utilizan los datos de brillo solar y radiación con propósito de comparar estos parámetros que están relacionados directamente entre sí. También se requiere conocer la temperatura del lugar pues de esta depende la temperatura de trabajo de los módulos, lo que a su vez determina la eficiencia de operación de todo el sistema. Los datos se obtuvieron en la estación meteorológica ubicada en la sede del INEA de Mantecal. Vale destacar que aunque no se disponen, los datos de precipitación fueron requeridos de cara a la limpieza de la superficie de captación de los módulos fotovoltaicos. Esta parte constituye un aspecto importante como línea base del proyecto debido a que el funcionamiento de los paneles solares está directamente relacionado con el comportamiento climático del lugar de instalación.

Según los datos obtenidos y mostrados en la gráfica 1, es posible correlacionar estos parámetros para analizar el comportamiento del recurso solar en la zona de estudio. La relación planteada es radiación solar - brillo solar y las unidades de medida son el número de horas por cada mes y los kWh/m^2. Se puede observar en la gráfica que la tendencia para ambos parámetros es similar durante los meses del año. Para el mes del peor escenario de radiación solar global multianual se registra también uno de los peores valores de brillo solar dando correspondencia a las mediciones realizadas en la estación. Como ya se citó, el parámetro correspondiente a las precipitaciones no se encuentra disponible, pero no debe

obviarse en estudios de este tipo teniendo en cuenta que este último representa transversalmente el comportamiento de la nubosidad.



Gráfica 1. *Radiación solar global vs Brillo solar*

Por otro lado, el dimensionado del sistema fotovoltaico tiene que ver con la elección de los materiales de la instalación y las consideraciones previas a su cálculo (López, 2015). Dicho dimensionamiento no está dentro del alcance de esta investigación. Sin embargo, se pueden hacer algunas consideraciones a modo de propuesta. Existen diversos métodos que requieren un número elevado de datos correspondientes a radiación solar para su aplicación, estos datos no se encuentran disponibles. Por esta razón se propone el "método del peor mes", por el cual el sistema se dimensiona con el propósito de que pueda trabajar en el mes en el que el recurso solar sea más desfavorable, de modo que en los meses restantes su funcionamiento está asegurado. Este método tiene validez general y proporciona resultados satisfactorios.

Entre los cálculos y consideraciones necesarias para obtener el dimensionado del sistema se encuentra la orientación e inclinación de los módulos, las horas solares pico, el factor de pérdidas del sistema, el número de módulos necesarios, la conexión de la instalación y el área necesaria que se debe destinar. La selección de

los módulos fotovoltaicos que mejor se adaptan a las condiciones requeridas es de acuerdo a la potencia nominal (kW) o máxima a partir de la cual puede calcularse el número de módulos o paneles necesarios para cubrir el consumo energético. La energía eléctrica que se produce en cada uno de los módulos fotovoltaicos que componen la instalación es almacenada en baterías (Sánchez, 2017). La cantidad de paneles que tenga el sistema es una variable limitante del área que se tenga dispuesta para la instalación.

Conclusiones

En primera instancia, se tiene que es de vital importancia el hecho que se estén desarrollando diferentes estudios sobre la situación energética, los cuales han arrojado que el uso indiscriminado de las fuentes no renovables son la principal causa de la crisis energética, la cual en la actualidad es realmente compleja. Luego, es precisamente esta realidad la que nos insta al estudio de las energías alternativas, ya que se hace necesario en un mundo responsable y consciente, apoyar un desarrollo tecnológico alternativo, sustentable y futurista. Entonces el uso de energías alternativas en lugar de las convencionales en los próximos años, pasa en primer lugar por la aceptación del hombre de su responsabilidad total en el caos que se encuentra inmerso el mundo.

En este mismo orden de ideas, se tiene que a partir de este estudio surgen interrogantes que abren la posibilidad de nuevas investigaciones, como pueden ser: ¿cuáles son las fuentes de energías alternativas que mejor se adaptan a las condiciones geográficas y climáticas de una determinada región?, así como también ¿hasta qué punto estas energías alternativas son sustentables? Es decir, develar la mejor opción en cuanto a energías emergentes en un territorio, para luego evaluar el impacto de la implementación de dichas fuentes en los tres factores en que se basa la sustentabilidad, estos son: ecológico, social y económico. Este impacto debe determinarse para corto, mediano y largo plazo; y de este modo se tiene una visión precisa de la sustentabilidad de las energías propuestas para combatir la problemática ambiental en la zona establecida.

Además, con esta investigación se concluye que la incidencia de las energías convencionales en el ambiente es innegable y muy negativa, esto es fundamentalmente a consecuencia del consumo incontrolado por mucho tiempo de combustibles que afectan directamente a una zona de la atmosfera que es vital para el mundo, la capa de ozono, razón que explica el por qué se ha incrementado el calentamiento en el planeta, con sus consecuencias en la salud del hombre, la extinción de especies vegetales y animales, entre otras. Así mismo, esta indagación ha revelado que se debe proyectar una migración progresiva hacia las energías alternativas, ya que las fuentes tradicionales lejos de reducir su producción, se espera que en los próximos años tengan un repunte considerable, esto para abastecer un incremento pronosticado en la demanda de electricidad.

La energía solar fotovoltaica ha sido motivo de algunos mitos y prejuicios que sin voluntad son los que dan mayor peso a sus impactos ambientales identificados. El impacto visual es generado por las personas que realizan la instalación sin integrarla adecuadamente al paisaje como ocurre con muchos elementos tales como cultivos intensivos en invernaderos. Este impacto puede desaparecer fácilmente logrando que las instalaciones se incorporen apropiadamente en el entorno. La disposición de los materiales peligrosos que componen el panel solar hoy en día es tema de investigación y desarrollo con el fin de mitigar esa etapa de su ciclo de vida a través de reciclarlo en un alto porcentaje, lo que posiciona este tipo de energía como una tecnología estratégica que en el corto plazo seguirá creciendo para ser más competitiva.

Como método para evaluar los beneficios ambientales de implementar un sistema solar fotovoltaico se utilizó una exhaustiva revisión bibliográfica la cual implicó acoplar información sobre los impactos típicos de los proyectos de interés. Para el caso de este estudio se tuvo en cuenta que en Venezuela las centrales hidroeléctricas tienen el porcentaje más alto de participación dentro del Sistema Interconectado Nacional como fuente de generación de energía, esto con el propósito de realizar una comparación basada en las ventajas que posee la energía solar fotovoltaica que la hacen idónea para ser competencia y/o complemento del uso de energía hidráulica.

Al diagnosticar el recurso de radiación solar se encontró que el rango oscila entre 4,1 y 4,7 kWh/m^2 en la zona de estudio. Se observa un comportamiento uniforme a lo largo del año que beneficia el uso de la energía solar como fuente de generación del recurso energético que demanda la población para el desarrollo de sus actividades. Las proyecciones correspondientes a costos de kWh por lo general muestran una tendencia al alza en el futuro, lo que representa un mayor valor de ahorro por el uso de energía solar fotovoltaica. Es importante recomendar la extensión de este análisis en cuanto al cálculo de todos los parámetros del dimensionamiento del sistema solar, así como del diagnóstico de la demanda energética actual de la población de Mantecal, de modo que pueda contarse con un proyecto con todas sus especificaciones técnicas.

Desarrollar el dimensionamiento bajo el peor escenario de radiación solar permite que la instalación funcione correctamente durante todos los meses del año debido a que las condiciones reales serán más favorables para el sistema y sus componentes, por lo cual se dice que la instalación es técnicamente viable. De igual manera esto permite dimensionar el sistema con los datos que se disponen, de modo que no hay excusa para que este proyecto no se continúe y luego se evalúe un posible escenario de ejecución del mismo, lográndose así el fin último de esta iniciativa, el cual no es otro sino el de disponer de una fuente de energía alternativa que ofrezca mayores bondades al medio y que este en una mejor armonía con los recursos naturales disponibles.

La precipitación en forma de lluvia no se considera un efecto negativo para la integridad del sistema sino por el contrario un factor beneficioso debido a que puede limpiar polvo e impurezas que lleguen a acumularse sobre la superficie de los módulos, sobre todo porque por su ubicación, el sistema con toda probabilidad quedaría expuesto a este tipo de suciedad. Esto además permite mejor incidencia de la radiación solar y por lo tanto mayor eficiencia del sistema. La presencia de la precipitación en los días que registran valores altos de temperatura, sería de gran ayuda para refrescar el sistema con el fin de que trabaje con mayor rendimiento. Lo ideal entonces es contar con este recurso y más aun con un registro en tiempo real del mismo.

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Assessment of the main reasons for the stagnation of territorial development in Russia

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ABSTRACT

Globalization, accompanied by a continuous increase in competition, complicates the conditions for the development of market relations in the Russian Federation. The priority development territories should have functioned as a tool for industrial and productive reform. These territories and their special economic zones should have become territorial centers of innovative and industrial development. However, it does not happened. The article analyzes some of the main reasons for this situation in Russia.

KEY WORDS: Special economic zones, priority development territories, strategic management model.

Evaluación de los principales motivos de estancamiento del desarrollo territorial en Rusia

RESUMEN

La globalización, acompañada de un aumento continuo de la competencia, complica las condiciones para el desarrollo de las relaciones de mercado en la Federación de Rusia. Los territorios de desarrollo prioritario debieron funcionar como una herramienta de reforma industrial y productiva. Dichos territorios y sus zonas económicas especiales, debieron convertirese en focos territoriales de desarrollo innovador e industrial. Sin embargo, esto no sucedió. El artículo analiza algunas de las principales razones de esta situación en Rusia.

PALABRAS CLAVE: Zonas económicas especiales, territorios de desarrollo prioritario, modelo de gestión estratégica.

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Introduction

In September 2016, the Government of the Russian Federation terminated ahead the operation of eight Russian special economic zones (SEZs), due to the absence of any specific work for the previous three years. We have to admit that the TAD and the SEZ have not become yet national innovation and economic spaces, the areas of consciously organized entrepreneurship built on the production of competitive high-tech products.

During the activities of special economic zones, the territories of priority development and diverse clusters in the Russian Federation, it became clear that there is no systematization of the structure key elements for the methodological support of strategic management in these entities, there is no model for strategic management of new economic zone development, which would make it possible to create an effective mechanism for interaction between management companies of the ECO with regional authorities of the Russian Federation constituent entities, with numerous residents, investors, and also with the business community.

A special economic zone has a special legal status; the territory of such a zone is subject to preferential economic conditions for the implementation of innovative industrial and other activities.

Enterprises operating in special economic zones are called the residents of the SEZ.

When they create the SEZ in the Russian Federation, the state assumed many complex obligations, including the attraction of private (both domestic and foreign) capital in breakthrough technologies, infrastructure, the development of conditions for job creation, especially for qualified personnel (which helps to keep the intellectual potential in the country), the stimulation of the state import substitution policy implementation.

1. Research Methodology

The theoretical and methodological basis of the article was the fundamental and applied works of Russian and foreign scientists in the field of strategic management of the SEZ, economic growth, etc.

Reasonable conclusions and results of this study were obtained based on the application of general scientific methods of management and the organization of the economic territorial complex, the methods of expert assessments, the methods of organizational and structural modeling and comparative analysis.

2. Research Results

The basis for the creation of territorial innovation systems is the idea of building up competitive advantages, which characterizes their purpose as the "locomotive" for the development of the regional economic system.

The activities of such systems, for example, in the United States, are controlled by the interagency Council. The EU has developed a set of legislative standards that provide for the regulation of special economic zone activities. In the Asia-Pacific countries they are guided by the legislative acts of the parliaments from the corresponding Chinese provinces.

Moreover, while private capital of the country acts as the main financial resource in the USA, they are focused mainly on engaging non-state structures in the management process within the EU.

In this regard, Asia-Pacific countries are more focused on customs and tax incentive provision for foreign investors.

This fact is also interesting - the basis for the development of SEZs in the USA is the particularities and needs of the state, and in Europe, this is the need to stimulate entrepreneurial activity, and the development of a flexible investment regime and in China (Baklanov, 2014; Myakisheva, 2015).

For comparison, in Russia - for example, in the North Caucasus Federal District, in particular, in the Kabardino-Balkarian Republic, the basis for the opening of the SEZ was the depressed state of the regional economy. So, there was no social infrastructure in the republic corresponding to modern standards.

The production and transport infrastructure were almost in the same situation, the unemployment rate in the mountainous regions of the republic exceeded 70%, an extremely low level of wages, insufficient quality or the absence of a number of socially

significant services (Aloeva & Misakov, 2013; Afashagova et al., 2014; Kushbokova et al., 2009). All this led to the depopulation of the republic.

To eliminate all these negative factors and bring the depressed republic out of this state, it was planned to create conditions for accelerated balanced development in the republic.

Unfortunately, although the SEZ was opened in the Kabardino-Balkarian Republic, nothing came of it - not a single new job was created, it was not possible to attract foreign and also Russian investors, and the climate of investment attractiveness was not developed. Under these conditions, one can't think foreign technologies, expert attraction, etc.

To be fair, we must mention the events of 2005, when an armed attack was carried out on Nalchik by militants on October 13. There were more than 300 militants, which fundamentally undermined investor confidence in the republic.

Besides, the republic had a rather strong bureaucratic mechanism, which made a serious problem, for example, for opening a business or an enterprise connection to gas, electricity, water, etc. All this led to the collapse of the SEZ in the region.

In the Kabardino-Balkarian Republic and other similar regions where the SEZ did not take place, the leadership of these territories could not (or did not want) to understand that the SEZ must be positioned as possible growth points for economic stability in a separate geographical point, which allows the development of an economic framework at the macroregion level. It is appropriate to recall that F. Perroux during the substantiation of “growth poles” theory came to the conclusion that there is a dominant unit within which the processes of nature change and competition maintaining take place. Indeed, the basis of competition is not only the motivation to maintain the maximum individual profit for an organization, but also the maximum profit for the macro unit as a whole (Perroux, 1968).

The dominant macrounit can be considered as a “growth pole”, creating an effect for agglomeration, when complementary activities are combined into a single whole (Under the "pole of growth" we consider an enterprise, and an industry, and the totality of industries). It has the ability to create a powerful effect of "enthusiasm" for itself, and

then transform into the zones of sustainable development and the axis of sustainable development in the macroregion.

In accordance with the provisions by F. Perroux, the key task of state economic policy is the creation of such "growth poles" and the conscious management of the achieved effect distribution environment (Perroux, 1968).

H. Bos argued that the mobilization of a group of business entities in a kind of localized centers is the best option for placement with significant transport costs for the transportation of specialized industry products (Bos, 1970).

As can be seen from the foregoing, the preconditions for a long-term cooperative cluster tie development are formed through localization, which helps to reduce transaction and transportation costs.

However, in order to analyze and diagnose the potential impact of the SEZ on the socio-ecological and economic environment of the region, it is necessary to consider a complete set of spatial and production factors, which will allow us to give a reasonable forecast of the regional economy growth efficiency (Bos, 1970; Enright, 1993).

Creating the economic framework of the macro-region, SEZs are forced to enter into economic ties with other localized points (business entities) in related industries, which inevitably contributes to the development of cooperative value-added chains. Moreover, such economic frameworks can later be transformed into territorial or cross-border clusters (Krutikov, 2017).

It is also appropriate to recall M. Enright, who substantiated that competitive advantages are formed exclusively at the regional level, and not at the national or even international level in the theory of regional economic cluster development (Perroux, 1968).

The analysis of special literature allows us to argue that it is unacceptable to create a SEZ from scratch. Apparently, for this reason, the green-field principle, which is popular in international practice, is not used in the Russian Federation. The consequence of this situation is that when you choose the definition of SEZ, all work was reduced to the struggle of individual constituent entities of the Russian Federation, municipalities and for "their" interests, while the interests of the state were discarded.

In our opinion, this is natural, because the state strategy for the SEZ creation and development was not a systemic, but "mosaic". During its development, they ignored certain aspects of strategic management fundamental foundations.

As can be seen from the foregoing, special economic zones and territories were not able to act as its drivers in the national economy, as was expected at the time of their creation.

And this is a natural (albeit negative) result, because contrary to the ideology of their development, special economic zones, instead of establishing "special" products competitive in international markets, mainly began to produce typical products, which, incidentally, are produced in neighboring regions or even in the same city. This led to the fact that the SEZ, in fact, performed unfair competition with other Russian producers, producing the same products and working according to general rules. It seems to us that businessmen did not realize (or do not want to realize) that it is unacceptable to place all emphasis in their work only on the preferences received "from above" in the form of tax cuts in comparison with average Russian entrepreneurs.

According to the Accounts Chamber of the Russian Federation, more than 80% of the products created in the SEZ go exclusively to the domestic Russian market, although it was supposed to be exported as planned (Grinevich, 2019).

International experience of the SEZ shows that this approach discredits the very idea of creating a SEZ and is doomed to failure.

During the audit by the Accounts Chamber of the Russian Federation they found out that 566 residents were registered in all SEZs of the Russian Federation, moreover, more than 350 residents (53%) were placed in four SEZs. However, only 25% (76 residents) are covered by foreign economic activity.

Over the years of SEZ activity, the agreements were terminated and 166 residents were liquidated as inappropriate to their functional purpose.

What is characteristic is that any SEZ is a priori designed for the sustainable development of high-tech sectors of the national economy and for the development of the latest products.

However, judging by the audit results of the Accounts Chamber of the Russian Federation, the industrial products imported into Russia by the residents of special

economic zones, in general, were intended for more ordinary purposes - for the production of standard products, in particular, tires, building materials, etc., which is extremely contrary to their main tasks. Apparently, for this reason, the creation of one workplace in the SEZ had the treasury cost of 10 million rubles (Grinevich, 2019).

It can be clearly stated that the residents of the SEZ are focused not so much on the socio-economic development of the territory as on their own tax minimization. The residents tried to justify such serious omissions, for example, by the fact that projects actually began to be funded only the year after their opening (SEZ "Ulyanovsk"), etc.

To be fair, it should be noted that among the residents of the SEZ there are mainly the enterprises that produce high-tech products or the products of a high degree of processing - they have increased the volume of customs payments and taxes by several times.

In our opinion, it is necessary to attract other diverse enterprises for the successful development of the SEZ. The creation of integrated structures within the framework of the SEZ may become a major factor in national industry modernization.

It is no secret that in most cases the enterprises established in Russia within the SEZ, were interested only in the opportunity to reduce the tax burden.

This is the reason by which we explain the fact that, although a number of preferential conditions, such as preferential export, infrastructure development, etc., was provided to establish production in special zones with a special regime, these competitive advantages remained unclaimed (Andreev, 2016; Bodrunov, 2018; Misakov et al., 2016). Although, of course, the human factor cannot be discarded when such temptations are announced.

But we do not call for an end to the format of special economic zones under consideration due to their inefficiency. Indeed, the world practice of such territory organization has shown the advantages of such projects convincingly for several decades.

It is necessary to return to the beginning of this process and to allow only those enterprises into the zone that, due to their innovativeness, are required to appear as SEZ residents. For this, a special council should be created, consisting of public experts and members. Although this is not a panacea, for an enterprise that met the

requirements of a special council can may produce the products not corresponding to the application very easily. We believe that in such cases it is necessary to remove such enterprises immediately from the list of residents of the SEZ with all the ensuing circumstances without any warning.

A number of examples can be cited when an enterprise that does not fully comply with the rules of the SEZ nevertheless it received "go-ahead" in the form of an "exception". All this destroys the competitive environment and discredits the very idea of the SEZ.

Because of this situation, 24 billion rubles allocated for the development of thirty-three SEZs have not been disbursed over the past 11 years, and with the total cost of 186 billion rubles, the return in the form of tax revenues amounted to 40 billion rubles only (Grinevich, 2019).

Apparently, this can explain the introduction of curators by the Government of the Russian Federation for 10 lagging, depressed regions. They were selected in the ranking as the regions with the worst positions on the most important estimated indicators, such as the average per capita income for the regional population, the share of the population with the incomes below the subsistence level, the unemployment rate, the investment in fixed assets, etc. Note that the government allocates substantial funds from the federal budget for all these regions annually.

At that, federal ministers act as curators. So, the RF MA D. Patrushev was appointed curator in the depressed republic of Adygea that we mentioned, where the SEZ were not developed.

It is difficult for us to talk about the validity of this approach, since it is impossible to imagine the way, for example, the Ministry of Agriculture of the Russian Federation should and the way he will develop a strategy for the socio-economic development of the Republic of Adygea. It is difficult to imagine how the experts from the Ministry of Agriculture of the Russian Federation will synchronize the work of all various ministries of the republic and determine the priority areas for the development of the territorial economic complex. And this is not the end of the matter - all regional programs developed by the new curators should be protected in the Government of the Russian Federation.

Obviously, with this approach, the effect for the economy is not obvious if we put it mildly. After all, the main problem of the Russian Federation subjects is an unevenly distributed tax base (without taking into account corruption - this is a separate issue). It is difficult for us to agree that some minister (even a federal one) will be able, in addition to his daily, laborious and voluminous work, to understand in more detail all the problems of a single republic, in all its vicissitudes. In particular, with the same corruption, which is usually "covered" quite often by the same law enforcement agencies, etc.

The new work of 10 ministers for depressed region restoration just begins. But it seems to us that such an institution of supervision is doomed. Here we see another thing - an extraordinary increase of the federal center intervention in the regional economy.

In our opinion, such centralization of socio-economic and budgetary decisions will only reduce the incentives and motivation of the regions for regional economy development and show fake "growth".

Conclusions and Offers

- Due to the circumstances considered in the article the RF SEZs were not able to provide "accelerated socio-economic development". It seems to us that when the SEZ was opened, a formal approach was allowed and there was no objective control over the compliance of the RF subject territories and the residents with the requirements imposed in such cases.

- In Russia, when the SEZ was opened, the gree-fild principle, well-established in international practice, is ignored. The consequence of this assumption is that when you choose the location of SEZ, all work was reduced to the struggle of individual subjects of the Russian Federation, municipalities, etc. for "their" interests, while the interests of the state were discarded.

- In our opinion, this is natural, because the state strategy for the creation and development of the SEZ was not a systemic, but "mosaic". During its development, certain aspects of the fundamental foundations of strategic management and planning were ignored.

- In a generalized form, it is advisable to consider the strategic management of the SEZ from two aspects:

- In the form of structural management as a process;

- In the form of a way to ensure desired results.

In this case, the organizational and economic model of SEZ strategic management can be represented in the following aspects:

- in the form of a process organizational and economic model of SEZ strategic management in the regional socio-ecological-economic system;

- in the form of a mechanism for the interaction between the SEZ management company and the authorities of the constituent entity of the Russian Federation and municipalities, with the SEZ residents, investors and other interested partners.

Conflict of Interest

The authors confirm the absence of a conflict of interest.

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Cluster Technology as a basis for the competitive development of industries in Russia

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ABSTRACT

In the context of globalization (Acuña, 2011) and the pressure of sanction on the national economy of the Russian Federation, the problem of the provision of competitiveness of industrial companies stands out. Economic policy in the national economy, oriented more towards the raw material component, has ceased to correspond to the modern requirements of society. In relation to this provision, new state priorities appeared, focused on improving scientific and technological development, innovation and modernization of the industrial complex, etc., which, in turn, requires the development of new mechanisms and appropriate instruments for the regulation of economic relations in the industrial sector, and the implementation of government support for the industry. However, it must be recognized that federal and regional sustainable development programs and industrial management mechanisms used in modern realities are not effective enough because they generally aim at the isolated solution of local problems. It is indisputable and obvious to all that it is impossible to reach the level of global competition without the progressive and competitive development of the main industries. One of the most constructive solutions to this problem is the cluster approach. Our country has some experience and achievements. So in 2012, employees of the Ministry of Economic Development of the Russian Federation developed a group-oriented program, the implementation of which involves twenty-five industrial groups. Cluster technologies allow the creation of synergistic and multiplier effects, which, in the end, is a boost for the development of economic growth. But despite all the preferences of the cluster approach, national cluster technologies were unable to implement their advantages, indicating the continued stagnation of industrial production. In this way, the purpose of this research is to study the possibilities of effective use of cluster technologies in the Russian industrial field.

KEYWORDS: Economic crises, sanctions, global competition, industrial complex, strategy, cluster technologies.

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Tecnología de Clúster como base para el desarrollo competitivo de las industrias en Rusia

RESUMEN

En el contexto de la globalización (Acuña, 2011) y la presión de sanción sobre la economía nacional de la Federación de Rusia, destaca el problema de la provisión de competitividad de las empresas industriales. La política económica en la economía nacional, orientada más hacia el componente de materia prima, ha dejado de corresponder a los requisitos modernos de la sociedad. En relación con esta disposición, aparecieron nuevas prioridades estatales, centradas en la mejora del desarrollo científico y tecnológico, la innovación y modernización del complejo industrial, etc., lo que, a su vez, requiere el desarrollo de nuevos mecanismos e instrumentos apropiados para la regulación de las relaciones económicas en el sector industrial, y la implementación del apoyo gubernamental para la industria. Sin embargo, debe reconocerse que los programas federales y regionales de desarrollo sostenible y los mecanismos de gestión industrial utilizados en las realidades modernas no son lo suficientemente efectivos porque, por lo general, tienen como objetivo la solución aislada de problemas locales. Es indiscutible y obvio para todos que es imposible alcanzar el nivel de competencia global sin el desarrollo progresivo y competitivo de las principales industrias. Una de las soluciones más constructivas para este problema es el enfoque de clúster. Nuestro país tiene cierta experiencia y logros. Entonces, en 2012, los empleados del Ministerio de Desarrollo Económico de la Federación de Rusia desarrollaron un programa orientado a grupos, en cuya implementación participan veinticinco grupos industriales. Las tecnologías de clúster permiten crear efectos sinérgicos y multiplicadores, que, al final, es un impulso para el desarrollo del crecimiento económico. Pero a pesar de todas las preferencias del enfoque de clúster, las tecnologías nacionales de clúster no pudieron implementar sus ventajas, lo que indica el estancamiento continuo de la producción industrial. De esta manera, el propósito de esta investigación consiste en estudiar las posibilidades de uso efectivo de las tecnologías de clúster en el ámbito industrial de Rusia.

PALABRAS CLAVE: Crisis económicas, sanciones, competencia global, complejo industrial, estrategia, tecnologías de clúster.

Introduction

There are many scientific works in the specialized literature on competitive advantages of business entity development in the industrial sphere and industrial cluster creation on their basis. However, we did not find any works that provide a

systematic idea of cluster strategy use to form the competitive development of the industrial complex as a whole and its individual industries and enterprises. As a rule, researchers pay more attention to certain aspects of industrial cluster production and financial activities, ignoring the complex problems of a strategy development for business entity competitiveness increase within the framework of the created cluster formations.

Based on this situation, the goal was set during writing the article, - to propose and justify a conceptual scheme for analysis and diagnosing of economic entity competitiveness at different stages of their development; to develop the contours of the organizational and economic mechanism for the formation of an industrial cluster to increase the competitive advantages of specialized enterprises, taking into account internal and external system-forming factors formed by two structural elements, providing:

- The modeling of an optimal organizational and economic structure of cluster formation and the degree of development of its production and technological infrastructure;

- the development of an adaptive algorithm mediating the technical and economic dynamics of the cluster development and the competitiveness of all its participants based on effective tools (road quotas for cluster development), the sources of financing activities (PPPs, private investments, outsourcing, etc.)

In our study, we proceed from the fact that the tasks of industrial enterprise competitiveness growth provision are directly associated (methodically) with the search for effective mechanisms of their growth, as well as with the diagnosis of their competitiveness level.

We believe that nowadays the cluster approach acts as the optimal approach to increase the competitiveness of domestic diversified enterprises of the industrial complex, because it synthesizes the provisions of other concepts of new sources of competitive advantage development with most priority from the positions of previously identified competitive dominants.

All this allows us to consider the cluster strategy as the most promising organizational and managerial mechanism for the development of competitive advantages of the industrial complex regional enterprises.

1. Research Methodology

The theoretical and methodological basis of the study was the conceptual provisions of competitive development theory of Russian and foreign scientists, a number of the latest theoretical and applied studies on the problems of industrial enterprise competitiveness increase in the framework of industrial cluster development and territorial cluster formations.

In the process of establishing, analyzing and diagnosing of factors that have a multidirectional effect on the growth of industrial enterprise competitiveness, they used the methods of comparison, expert assessment and classification.

The empirical base of this scientific article was the statistical materials of the Federal State Statistics Service of the Russian Federation, as well as the industrial statistics on production and financial activity of economic entities of the depressed republics in the North Caucasus.

2. Research Results

Within the conditions of constantly increasing competition, state support for cluster technologies and the initiatives for the participation in cluster technologies should act as the priority area of state industrial policy. In our opinion, only such an approach will create incentives for the required structural changes, increase the competitiveness of diversified enterprises in the industrial complex and act as an effective tool for innovative long-term development.

It is recognized that mechanical engineering in any country is regarded as a strategically significant branch of industrial production, since the further growth and the quality of manufactured industrial products, as a rule, depend on the level of its development. It is clear that engineering is a key industry sector and only it is able to

set the main tone in the implementation of the innovation scenario within the national economy.

Indeed, only this industry can provide all the necessary equipment to industrial enterprises in the field of raw material processing and industrial production, which will increase the country production potential. It should also be noted that the creation of new (high-quality) types of industrial equipment makes it possible to reduce the material and energy intensity of industrial product significantly, which will effectively affect the economy of the respective industries (Ansov, 1989; Azoev, 2012; Misakov et al., 2016).

The illiterate privatization affected the state of manufacturing industry quite negatively, especially in mechanical engineering. The industry transition to market relations was also accompanied by the excess of production capacity, a high share of technological equipment with moral and physical depreciation (more than 70% are 20 years old or more), high production costs due to unacceptably low productivity of equipment, the lack of modern production infrastructure, an acute deficit of credit and investment funds, low level of cooperation between enterprises in the engineering industry.

All this required the development of urgent measures to increase the competitiveness of industrial enterprises intended to produce high-tech equipment.

It should be noted that in recent years they created several fairly large-scale industrial clusters, within the framework of which there is a significant consolidation of assets of industrial enterprises engaged in mechanical engineering. There has also been the tendency to increase financial support for the transport sector, power engineering, aircraft manufacturing and other high-tech sectors of the engineering industry, and stable budget subsidies have been established for production infrastructure.

Under these conditions, there is no longer any need to prove the advantages and importance of clustering for the successful solution of the main problems in the areas of innovative and technological development of the national economy. The cluster approach allows to compensate for the insufficiency of the main types of resources,

including such as raw materials, energy, innovation, etc. (Aloeva & Misakov, 2013; Korchagina, 2003; Basyuk et al., 2016).

In order to make engineering become the driver of the industry and the source of renewal and modernization of the industrial sector and be able to transfer the entire industry to an innovative development path, it is necessary to develop a set of targeted government support measures for a radical restructuring of the industry. Under these conditions, it is advisable to form 6-8 large-scale engineering clusters in the country. The rational use of a combination of external and internal system-forming factors allows us to generate a cluster effect, which contributes to the creation of new and activation of existing competitive advantages, the formation of modern infrastructure and even active interaction in the cluster formation of enterprises that are direct competitors (Afashagova et al., 2014; Artamonova, 2013; Prokhorova et al., 2018).

It should be noted that within the framework of the cluster, the process of constant modernization of technologies and products is inevitable, the life cycle of industrial products, etc. is shortened, which, ultimately, has a positive effect on the final results.

All varieties of industrial clusters can be reduced to two main types:

- The clusters formed on the basis of large industrial production structures;
- The clusters formed in new sectors of the economy (Lagodyuk, 2010).

As a rule, the clusters included in the first group, implement process innovations in the form of new production technologies, and the modern methods of industrial production.

The clusters of new branches of the industrial complex are engaged in product innovation and in the development of new industrial product exclusively.

The financial and investment basis of the cluster is the consolidated activities of various investment funds, banks and other specialized financial structures.

There are sufficient conditions for cluster strategy application in the republics of the North Caucasus. There are several large enterprises of the engineering industry, in particular, mining, metallurgical, petrochemical, energy, building materials ...

The analysis of industrial development economic indicators in the depressed republics of the North Caucasus allows us to note that, although the volume of regional

production has been constantly growing since 2010 in absolute terms, at the same time the annual growth rate falls. It is also appropriate to say that the annual growth of industrial volumes with a constant (annual) reduction of workers allows us to talk about some labor productivity growth (Kushbokova et al., 2009; Rzhevskaya, 2012; Zakharova et al., 2015).

But substantial investment is very necessary for the full revitalization of industry.

Foresight analysis made it possible to verify once again that the region has no prospects for competitive advantage development, because there is no developed production and innovation infrastructure, industrial and scientific potential are not involved, which raises concerns about the possibility of investor attraction to implement the necessary technical and technological modernization.

Depending on the characteristics of the present integration ties, the entire set of industrial clusters is divided into three groups: aggregated, mixed and specialized clusters.

The first group of cluster development based on the principles of outsourcing is engaged in the production of industrial products that meet the needs of the target market for a number of parameters, including such as price, quality and the number of technical specifications.

The second group of cluster structure is built on the principle of horizontal integration. It is more effective than the aggregated structure of clusters, because the competitive environment formed inside such cluster formations has a much stronger positive effect on the development of the overall industrial cluster competitiveness.

The development of the industrial cluster in a depressed and labor-intensive region is impossible without an innovative production infrastructure. This requires large-scale investments, which are absent in the depressed region. They can be found only on the principles of partnership between the public and private sectors.

This approach forces the mobilization of all financial, economic, technical and other resources of the public and private sectors within a single industrial cluster. At that, if necessary, it helps to maintain the state ownership of the most significant

production and social infrastructure objects (Bryazgina, 2016; Vinokurova, Yudanov, 2012).

The development of competitive advantages and their implementation allows the most effective implementation of the import substitution policy.

In our opinion, the strategy of building up the competitive advantages of the industrial cluster is, ultimately, the system of effective measures for the sustainable development of cluster institution.

An approximate algorithm for competitiveness increase strategy in respect of industrial cluster formation is given below.

1. The analysis of the external and internal environment factors of the industrial cluster is performed at the first stage.

2. The second stage is the refinement of goal formulation for competitiveness growth.

3. They develop and select the strategic alternatives for the formation and development of the cluster industrial enterprise competitive advantages during the third stage.

4. They determine the target indicators to assess the provision of specified parameters at the fourth stage.

5. The priority intracluster areas (projects) are selected during the fifth stage, in particular, the modernization of production, the development of a modern production infrastructure, etc.

6. They perform the optimization of cluster institution, develop optimal diversified product programs of multidirectional cluster enterprises during the sixth stage.

7. During the seventh stage, they develop the system of mutual coordination within the cluster institution in order to increase the effectiveness of all its participants.

8. The monitoring and control of the strategy involvement is performed during the final (the eighth) stage to increase the competitiveness of the industrial cluster.

This algorithm is not final. Actually, it can be of 5 stages, and of 10 stages. This is not fundamental - the main thing is to cover all procedures, from the formulation and goal setting, to the development and implementation of cluster projects.

Conclusions

Thus, it can be noted that the tasks of an industrial cluster competitiveness increase are methodologically associated with an effective mechanism development for its formation, as well as with cluster member competitiveness diagnosis. The clustering of diversified industrial enterprises of various industries makes it possible to influence both the determinants of the competitive position of all its participants and the cluster as a whole, as well as the determinants of competitive forces, because these institutions also include government agencies that can create institutions that affect the business environment of industrial cluster effectively.

Under the conditions of Russian reality, state support for cluster initiatives should be considered as a priority for the implementation of regional industrial policy, because it can mobilize the necessary structural changes, increase the competitiveness of diversified enterprises in various industries and act as an effective tool for the innovative development of depressed republics.

We have proposed a modified algorithm to optimize diversified business entities by their incorporation into large cluster industrial groups that can be successfully (and easily) used in the development and implementation of targeted cluster development programs within various sectors of the national economy.

The formulated developments, whose effectiveness was tested during optimization within the industrial cluster of one of the depressed republics of the North Caucasus (Adygea), can be successfully applied in the process of competitive strategy development for the industrial complex and other similar republics of the region.

Conflict of Interest

The authors confirm the absence of a conflict of interest.

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Illegal economic phenomena in the Russian agricultural sector

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ABSTRACT

The current unstable market situation in Russia forces undesirable measures to be taken, mainly in the field of tax legislation for economic entities in the agricultural sector. This becomes a prior factor for the development of economic crime and the development of illegal phenomena. In recent years, there has been an increase in these crimes in the country. The agricultural sector of the Russian economy, as well as other countries, requires the availability of state financial support. However, during almost the entire post-Soviet period, a partial theft of state funds allocated to support and develop agricultural sectors can be observed under free market conditions. Such a problem exists everywhere in Russia. Existing methods of supervision and control over the use of budget allocations do not give the expected effect. In the context of such a negative situation, there is a need to develop effective methodological tools to assess the effectiveness and integrity of the use of budget funds for the agricultural sector, the algorithm of which is quite accessible and involves the use of scientific and practical methods, experience and knowledge of experts in the field of agriculture. This article aims to identify patterns of economic crime in agricultural and livestock production, and to propose methods for the evaluation and monitoring of public funds to Russian agricultural entities.

KEY WORDS: economy, agricultural sector, illegal phenomena, state support.

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Fenómenos económicos ilegales en el sector agrícola de Rusia

RESUMEN

La inestable situación actual del mercado en Rusia obliga a tomar medidas indeseables, principalmente en el campo de la legislación fiscal para las entidades económicas del sector agrícola. Esto se convierte en un factor previo para el desarrollo del delito económico y el desarrollo de fenómenos ilegales. En los últimos años, se observa un crecimiento de estos delitos en el país. El sector agrario de la economía rusa, así como otros países, requiere la disponibilidad de apoyo financiero estatal. Sin embargo, durante casi todo el período postsoviético, se puede observar un robo parcial de fondos estatales asignados para apoyar y desarrollar sectores agrícolas en las condiciones del libre mercado. Tal problema existe en todas partes en Rusia. Los métodos existentes de supervisión y control sobre el uso de las asignaciones presupuestarias no dan el efecto esperado. En el contexto de una situación tan negativa, existe la necesidad de desarrollar herramientas metodológicas efectivas para evaluar la efectividad y la integridad del uso de fondos presupuestarios para el sector agrícola, cuyo algoritmo es bastante accesible e implica el uso de métodos científicos y prácticos, experiencia y conocimiento de expertos en el campo de la agricultura. Este artículo tiene como propósito identificar patrones de delitos económicos en la producción agrícola y ganadera, y proponer métodos para la evaluación y seguimiento de fondos públicos a entidades agrícolas rusas.

PALABRAS CLAVE: economía, sector agrícola, fenómenos ilegales, apoyo estatal.

Introduccion

A well-known fact and problem is the presence of illegal phenomena in the agrarian sphere, whose origin is associated primarily with the availability of large material and financial flows. Such flows are the result of state (federal, regional and municipal) support, without which it is simply impossible to ensure the solution of extremely important socio-economic problems.

In this regard, particularly close attention should be paid to the reproduction processes between the entities of the agro-industrial complex of the region, which are based on the use of natural resources and capital, the movement of material and financial flows. They are of real mercenary interest for a person or a whole group of

people. Therefore, one should not underestimate the detrimental influence of the illegal economy:

- Direct impact on the economic development of agricultural business in the region;

- Indirect influence on the social development of rural residents and rural areas themselves (Panin, 2012).

At a first glance, the question arises: "what interest can a priori unprofitable agricultural sector of the economy cause?" The answer to it is quite obvious and lies in the fact that government investment in this sector of the economy is growing annually, while monitoring their use is not effective enough. Along with this, it should be added that it is attractive to put into the shade a number of natural resources used in agriculture and forestry, for example, land, forest, water bodies, etc.

In this article we have set ourselves two objectives: a) identify patterns of economic crime in agricultural and livestock production; b) propose methods for the evaluation and monitoring of public funds to Russian agricultural entities. To achieve these objectives, we rely on consulting specialized literature on the subject of economic crime control.

1. Analysis

The statement is absolutely true that there is a direct and close relationship between the level of economic development of the region and the level of the illegal economy. This is due to an elementary pattern: the more financial resources are involved in a particular sector of the economy, the greater is the interest of “illegal” structures in transferring part of the capital from the official economy of this sphere to the illegal one.

The modern economy is subject to the influence of multiple factors and conditions, which in the agricultural sector, in part, can act as prerequisites for the development of economic crimes (fig. 1).

In the view of many people, the illegal economy is associated with tax evasion through falsification of financial statements. However, in fact, its scope is much wider and can be represented by: illegal entrepreneurship; legalization of proceeds of crime;

offenses in the field of financing business entities; illegal monopolization of sales markets, and so on.

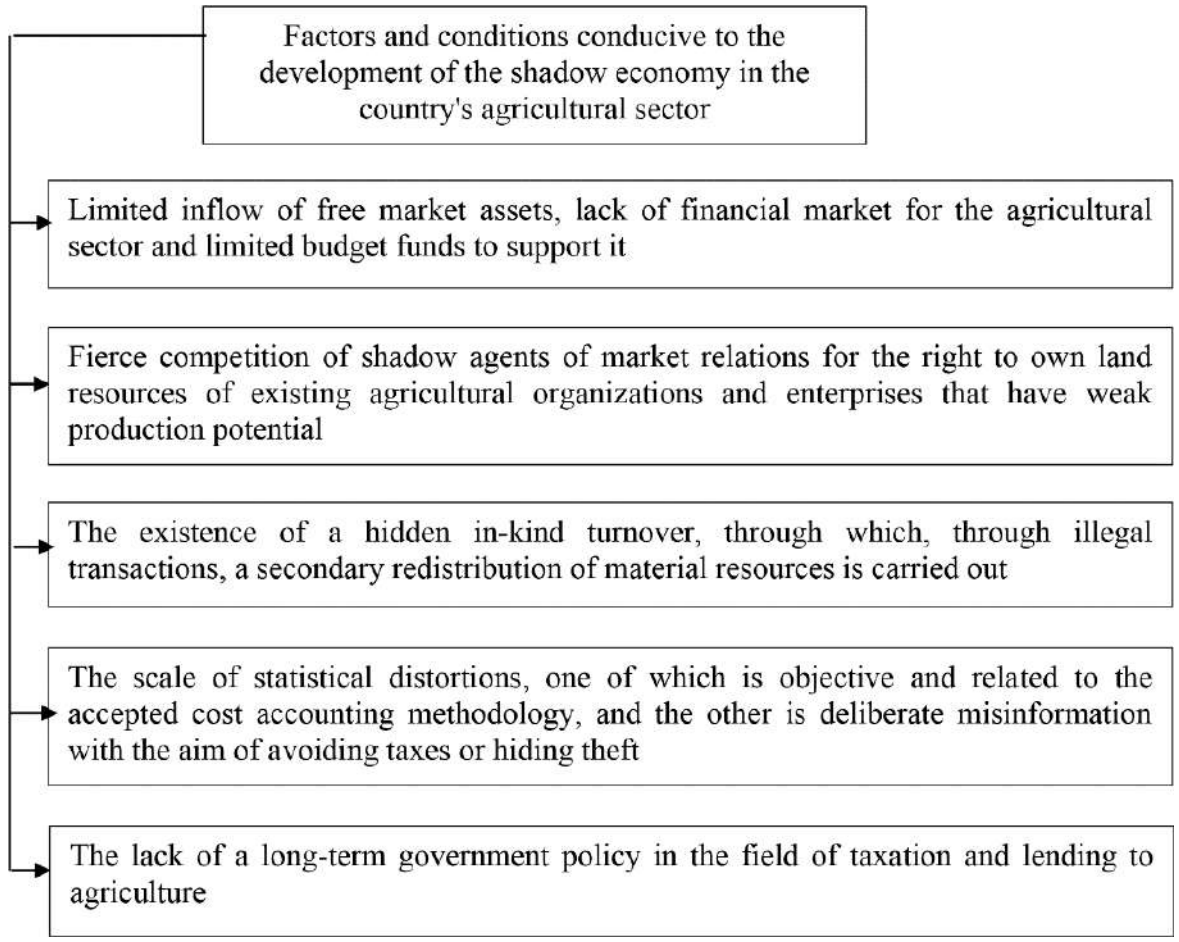

Figure 1. Factors and conditions for the development of illegal phenomena in the Russian agricultural sector (Trotsenko, 2019)

The instability of modern tax legislation in Russia gives rise to the tendency of a business executive to seek tax evasion and other obligatory payments to state extra-budgetary funds. Especially in recent years, individual entrepreneurs have suffered, who are forced to minimize their financial losses through double-entry bookkeeping. Such tax law violations in Russia are gaining momentum. There is an outflow of enterprises from legal business to the illegal one, and the illegal sector as a whole is also growing (Dadalko, 2010; Repin, 2015).

It is known that agricultural organizations are almost entirely grant-aided and subsidized. Due to this "status", farmers not only compensate for losses in agricultural production, but also compensate for part of the cost of production, for example, milk,

meat, etc. from the budget. Existing software tools for the development of agriculture and food markets in Russia also involve the development and updating of production and economic capacities. In recent years, the construction of dairy farms has become widespread. The need for their construction arose against the background of insufficient production of raw milk for the uninterrupted and sustainable functioning of the domestic market. This direction required significant state financial investments and showed interest among unscrupulous representatives of agribusiness. As a result, the following economic unlawful actions were identified in many Russian regions:

- Theft of state funds, construction materials, as well as abuse of authority by heads of agricultural organizations and representatives of regional Ministries and departments responsible for the targeted use of allocated funds (Gafurov, 2018);

- Abuse of authority and taking bribes by officials. For example, "purchases" of the possibility of concluding an agreement for construction and contracting has become widespread;

- Overstatement according to the estimated documentation of the cost of purchased equipment, building materials, as well as their unreasonably high volumes.

Such crimes characterize many types of capital construction in agriculture and in rural areas in general.

As a result of the increase in the illegal sector, the budgets of particular regions and the country as a whole are being damaged. Amounts that were not received into the budget create the risk of the region and the state not fulfilling their powers to the population. In particular, in 2019 the damage to the budget from tax crimes amounted to 95 billion rubles. One average economic crime can be estimated at about 13 million rubles. At the same time, the share of such tax economic crimes amounts to a little more than 70%, which in some cases can be classified as grave and especially grave and are considered, depending on the damage, by the Code of Criminal Procedure of the Russian Federation (Melnikov, 2012).

The result of such illegal phenomena in the economy is expressed, first of all, in the deformation of the overall market structure, because there is a reduction in the chain in the market mechanism and unfair competition is formed.

Under the current state support, the following unlawful tools that underlie economic crimes and the illegal economy of the agricultural sector as a whole were widely used (fig. 2).

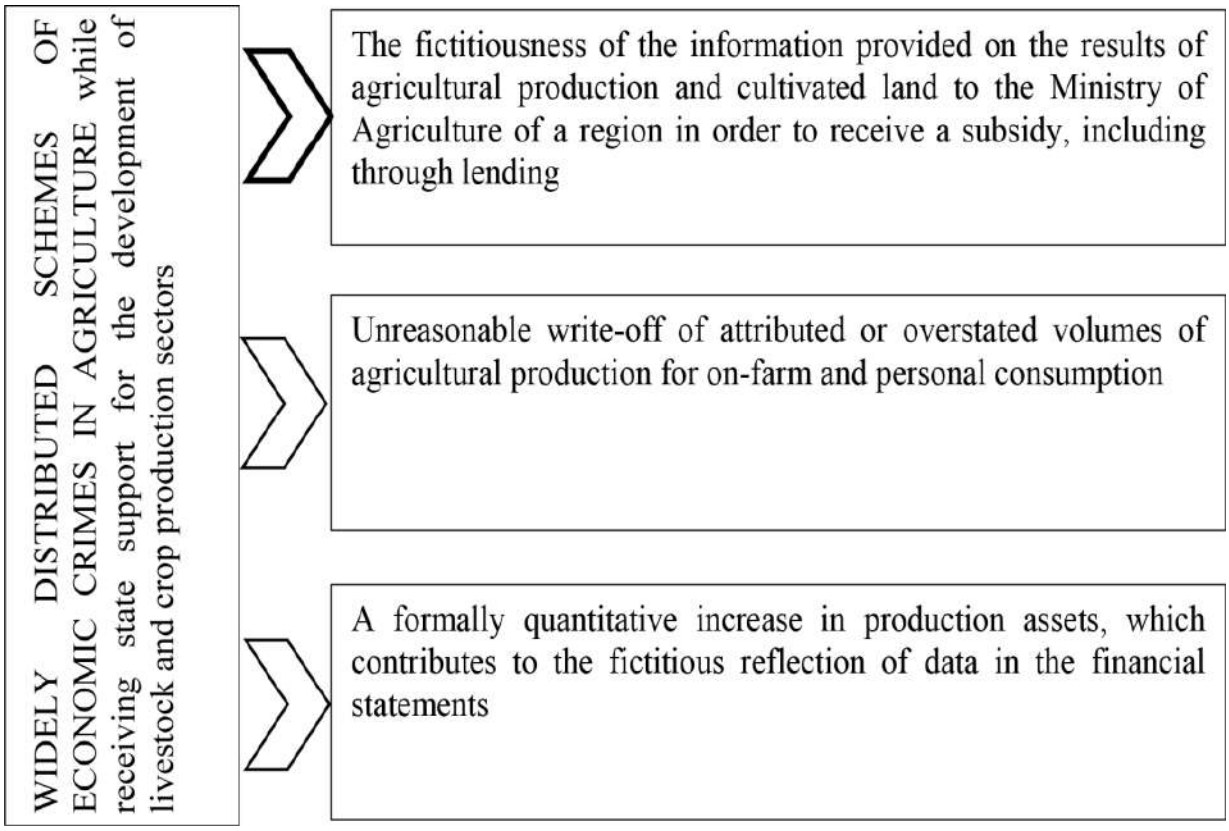

Figure 2. Widely distributed patterns of economic offenses in crop and livestock production.

The schemes that underlie economic crimes in the crop and livestock sectors also contribute to the receipt of completely distorted current, operational and statistical information in the authorities, which subsequently forms the basis for wrong decisions to support and regulate these industries.

In relation to organizations conducting agricultural business, it should be noted that illegal economy expansion gives them additional, but hidden income, which agricultural business entities that conduct their business completely transparently cannot have. However, the illegal economy should not be the motive and encourage the crimes. Consequently, a comfortable state policy with partly loyal tax exposure should be built in relation to agricultural organizations. Such an approach cannot be universal and should be shown in relation to competitive types of economic activity from the

agricultural sector or may have its own projection on individual agricultural associations and entire territories (Yarkova, 2018; Khairullina and Yarkova, 2018; Khairullina and Yarkova, 2019).

Our decisions are based on the fact that grounds for many economic crimes are state funds which are either not received by the state under the tax regime, or they are wasted inappropriately through crime in whole or in part.

The first step in the fight against illegal processes and phenomena in the agricultural sector should be assessing and monitoring the effectiveness of implementation of state financial investments in this sector of the economy. The evaluation technique is comprehensive and can be implemented in practice in the following algorithm (fig. 3).

Along with the presented assessment methodology for monitoring the effectiveness of the use of budgetary funds, we also propose to use an instrument which provides the monitoring of the legalization of agricultural business.

A direction among many others in the fight against economic crimes in the agro-industrial complex may be a gradual transition to the conditions of widespread cashless payments and multivariate digitalization and automation systems for accounting and control, and in the case of entities with a full production cycle, to an automated cash-control system.

The capacity of such areas can be ensured only through the implementation of the universality principle. That is, the business entities themselves, government agencies represented by ministries, departments, agricultural departments, tax services, private farms, farmers, consumers and other participants in the agricultural and food markets should be directly involved in the project.

Conclusion

The directions recommended for use in practical activities will contribute to the fight against illegal phenomena in the economy of the agricultural sector of the Russian Federation and other countries, as they have a completely universal nature of their impact.

The effectiveness of such measures is global, lasting and will affect the most important components of the socio-economic development of the modern state.

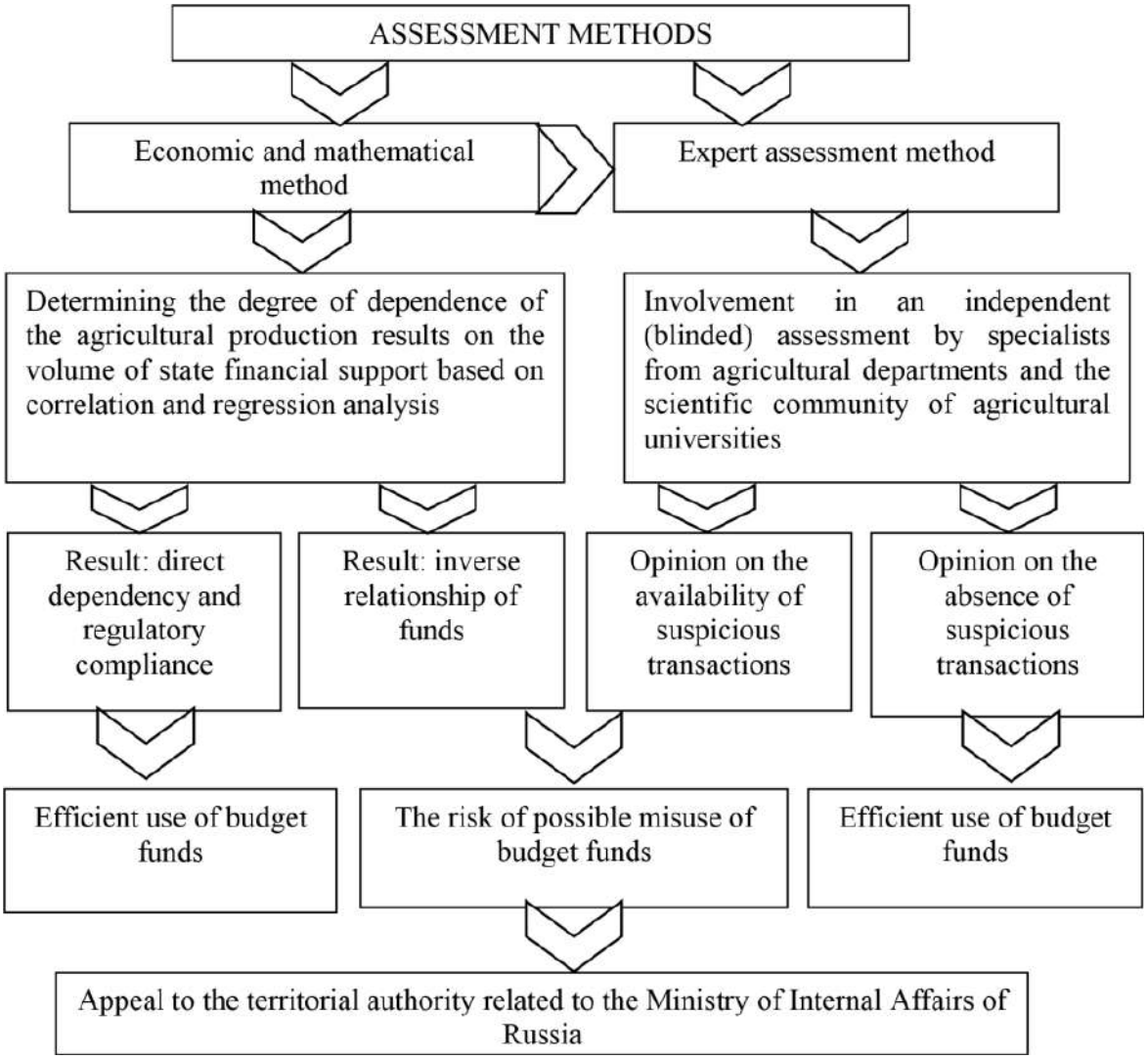

Figure 3. Evaluation methods for the effectiveness of the development of public funds in the form of subsidies and grants by agricultural entities

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Visión y revisión de artículos científicos sobre temática agrícola en la Revista Amazonía Investiga

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Magda Julissa Rojas-Bahamón **

RESUMEN

En las economías globalizadas el desarrollo del agro constituye una pieza clave dentro de las estrategias para superar la pobreza, minimizar el latifundio y reducir la conflictividad social, en un marco de política públicas que fomentan el uso y explotación racional de los recursos naturales. Por estas razones, la producción de artículos arbitrados en una perspectiva multidisciplinaria en el ámbito temático de la agricultura, ocupa un sitial destacado en las revistas científicas de alto impacto de mayor difusión internacional. El objetivo de esta investigación es revisar una muestra de la producción científica sobre agricultura publicada en la revista Amazonia Investiga en el periodo 2019-2020. Para procesar la información recabada se optó por la metodología documental y por la técnica del balance bibliográfico, como condición de posibilidad para develar lo que se ha escrito y como se ha escrito sobre la materia. A modo de conclusión, se evidencia que se producen saberes sobre el agro desde disciplinas tan diversas como: el derecho, la economía, la ciencia política y la agronomía, entre otras, lo que demuestra que se trata de un tema multidimensional que no puede ser abordado en todo su alcance desde una única perspectiva disciplinar, teórica o metodológica.

PALABRAS CLAVE: agricultura; balance bibliográfico; revistas científicas de alto impacto; Amazonia Investiga; producción científica.

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Vision and review of scientific articles on agricultural issues in the Journal Amazonía Investiga

ABSTRACT

In the globalized economies, the development of agriculture constitutes a key part of the strategies to overcome poverty, minimize large estates and reduce social conflict, in a public policy framework that promotes the use and rational exploitation of land resources. For these reasons, the production of arbitrated articles in a multidisciplinary perspective in the field of agriculture occupies a prominent place in the scientific journals of high impact of greater international diffusion. The objective of this research is to review a sample of the scientific production on agriculture published in the Amazonia Investiga magazine in the year 2019. To process the information collected, the documentary methodology and the bibliographic balance technique were chosen, as a condition of possibility for unveil what has been written and how it has been written about the killing. As a conclusion, it is evident that knowledge about agriculture is produced from disciplines as diverse as: law, economics, political science and agronomy, among others, which shows that it is a multidimensional issue that cannot be addressed in all its scope from a single disciplinary, theoretical and methodological perspective.

KEYWORDS: agriculture; bibliographic balance; high impact scientific journals; Amazonia Investigates; scientific production.

Introducción

En las economías globalizadas el desarrollo del agro constituye una pieza clave dentro de las estrategias para superar la pobreza, minimizar el latifundio y reducir la conflictividad social, en un marco de política públicas que fomentan el uso y explotación racional de los recursos de la tierra. Por estas razones y por otras, la producción de artículos arbitrados en una perspectiva multidisciplinaria en el ámbito temático de la agricultura, ocupa un sitial destacado en las revistas científicas de alto impacto de mayor difusión internacional. Así lo indican los trabajos de (Gabaldón, 2006) y, muy particularmente, de la (FAO, 2012) quien ademas situa el desarrollo agricola como una herramienta particularmente eficaz para reducir el hambre y la malnutrición en el sur global en el que se ircentan los pises en vias de desarrollo (Acuña, 2011).

El objetivo de esta investigación es revisar una muestra de la producción científica sobre agricultura publicada en la revista Amazonia Investiga en el periodo 2019-2020. Para lo cual se seleccionaron más de 20 artículos científicos producidos

desde distintas ópticas y disciplinas. El procesamiento de la información se hizo mediante los parámetros de la metodología documental y de la técnica del balance bibliográfico, como condición de posibilidad para develar lo que se ha escrito y como se ha escrito, directa o indirectamente sobre la materia, en este importante órgano de divulgación científica de Colombia. Por lo demás, el objetivo que nos ocupa se formula o traduce en la pregunta: ¿Qué aportes y contribuciones científicas se visualizan en la producción sobre agricultura publicada en la revista Amazonia Investiga en el periodo 2019-2020?

De igual modo, se definieron 4 criterios de análisis como insumo hermenéutico para la lectura minuciosa de las fuentes seleccionadas, a saber: a) tema; b) metodología; c) fuentes empleadas y perspectiva teórica; d) aportes para el desarrollo del tema y; e) observaciones (opcional), similares a lo que ya se hizo en una investigación anterior de (Arbeláez-Campillo, 2019) pero con un objetivo diferente. Nuevamente este enfoque permitió observar las tendencias generales y particulares presentes en el tratamiento del tema por parte de autores de distintas nacionalidades que, sin embargo, comparten un interés temático y científico de gran valor para el logro del desarrollo sostenible.

Con el ánimo de resolver el objetivo enunciado, el trabajo transcurre en 5 secciones particulares: en la primera, se muestran al lector cuales son los fundamentos teóricos que hicieron posible el desarrollo de este trabajo; en la segunda, se da cuenta de la metodología empleada para procesar la muestra documental seleccionada, en estricta concordancia con la naturaleza del tema; en la tercera, se efectúa un balance bibliográfico y un estado del arte de las fuentes analizadas, haciendo uso de los 4 criterios que se explicitaron anteriormente. Por último y como es común, se arribó a la etapa de análisis y discusión de resultados y a las conclusiones del caso, con un efecto que sabrán valorar nuestros afables lectores.

1. Aspectos teóricos

Los trabajos de metodología documental que tienen como propósito el desarrollo de un balance biblio-hemerográfico sobre un tema de interés científico, responden a los parámetros de lo que (Sánchez, 2011) define como artículos de revisión teórica y, sin

lugar a dudas, significan un género textual dentro del discurso académico por derecho propio. De modo que:

> Las revisiones son investigaciones en las que los autores responden un interrogante, y en función de éste, analizan y sintetizan la información para llegar a una conclusión. Este tipo de artículos tienen como propósitos:
> - Sintetizar conocimientos fragmentados.
> - Actualizar e informar sobre el estado de un tema (recopilar la información más relevante sobre el tema de investigación mediante fichas de lectura y resumen).
> - Comunicar nuevos conocimientos.
> - Informar y evaluar la literatura publicada.
> - Comparar la información de diferentes fuentes.
> - Sustituir los documentos primarios.
> - Establecer tendencias investigativas.
> - Identificar las especialidades que surgen en un determinado campo.
> - Detectar nuevas líneas de investigación.
> - Sugerir ideas sobre trabajos futuros.
> - Contribuir a la docencia... (Sánchez, 2011, p. 177)

Aplicando estas ideas a la especificidad de nuestra investigación, todo indica que la revisión realizada se enfocó en proporcionar –al lector especializado– una panorámica general sobre una pequeña muestra de artículos sobre el agro, capaz de sintetizar conocimientos fragmentados sobre el tema y, al mismo tiempo, evaluar la literatura publicada desde un aparato analítico crítico, útil cuando se trata de indicar las tendencias de investigación o evaluar el modo como diferentes disciplinas aportan saberes, desde sus lógicas y métodos específicos, para el desarrollo de un determinado campo epistémico que, por su complejidad, no puede reducirse a los dominios de una sola ciencia o disciplina.

En este sentido (Merino-Trujillo, 2011) agrega que los artículos de revisión se constituyen en un tipo de estudio selectivo, detallado y crítico que se enfoca en una muestra de la bibliografía publicada sobre una problemática en específico, al tiempo que la sitúa en cierta perspectiva. Aunque se trata de exploraciones de base documental que no tienen por finalidad figurar como un contenido original, sus aportes son fundamentales cuando se trata de entender el alcance y significación científica de un tema desde una visión abarcante que propicia el diálogo interdisciplinario. Por lo demás, los balances bibliográficos funcionan muy bien como técnica de recolección de datos en

el marco de metodologías como: el análisis del discurso, el análisis de contenido o los estudios bibliométricos, entre otras.

Por su parte, (Garcés Cano & Duque Oliva, 2007) destacan el hecho de que toda revisión demanda de la existencia previa por parte del investigador o del equipo de investigación de un aparato crítico o "nivel crítico adecuado" que no lo garantiza ninguna metodología, sino que es el resultado del conocimiento y la experiencia en un área del saber que se solo se logra con constancia y lectura sistemática de abundante bibliografía especializada. Desde nuestra perspectiva, los trabajos de revisión bibliográficas se sitúan además dentro de una visión holística del conocimiento científico, a pesar de que muchos autores no tengan plena conciencia al respecto, ni formación solida en epistemología, toda vez que:

> La holística se refiere a la manera de ver las cosas enteras, en su totalidad, en su conjunto, en su complejidad, pues de esta forma se pueden apreciar interacciones, particularidades y procesos que por lo regular no se perciben si se estudian los aspectos que conforman el todo, por separado. (Barrera Morales, 2006: 13)

En consecuencia, el género artículo de revisión que cada vez gana más espacio en las revistas multidisciplinarias de alto impacto, porque propicia el diálogo intertextual como estrategia para abordar una muestra textual específica, desde una lectura holística y hermenéutica que trata de entender los textos --en su lugar de enunciación-- para dar cuenta de su trascendía, si es que tienen alguna, para lo cual se pueden asimismo conjugar o contrastar planteamientos similares y diferentes que coinciden en el tratamiento de un tema y quizá en nada más, circunstancia que impulsa procesos de transdisciplinariedad y, llegado el caso, la síntesis de conocimientos contrapuestos o complementarios sobre un tema: real o teórico.

1. Metodología

El caso concreto de esta investigación, nos ceñimos al diseño documental de investigación científica desde la perspectiva de (Arias, 2006), para quien este sistema se caracterizar por desplegar un proceso de búsqueda, recuperación, estudio y análisis de fuentes secundarias escritas o audiovisuales, electrónicas o impresas, que conducen al

aporte de nuevos o renovados saberes sobre un tema. En el mismo orden de ideas, (Gómez, 2011) explica que esta metodología se vincula muy bien con el paradigma cualitativo, aunque ciertamente no todos los estudios documentales son necesariamente cualitativos en el sentido profundo del concepto. No obstante, el abordaje documental intenta comprender e interpretar una temática sin recurrir a técnicas de medición o a escalas de cuantificación, de ahí que este tipo de estudios terminan propiciando el desarrollo de aproximaciones hermenéuticas de la documentación recabada en el arqueo de fuentes primarios o secundarias.

En cuanto a la hermenéutica que se perfila como una tradición filosófica que pretende interpretar adecuadamente el sentido y significado de un texto, escudriñando para ello las coordenadas espacio-temporales donde fue producido, como condición de posibilidad para entender las ideas y representaciones del mundo que condicionó a su autor, (Martínez, 2004) siguiendo a Dilthey, agrega que:

> (...) la hermenéutica tendría como misión descubrir los significados de las cosas, interpretar lo mejor posible las palabras, los escritos, los textos, los gestos y, en general, el comportamiento humano, así como cualquier acto u obra suya, pero conservando su singularidad en el contexto de que forma parte. (Martínez, 2004: 102)

En resumen, la presente investigación se sirvió de la metodología documental próxima a la hermenéutica para el logro del objetivo planteado; en ningún momento, debe suponerse que se hizo uso de una metodología hermenéutica en sentido riguroso, porque no es el caso. A modo de técnica de recolección de información se empleó el balance bibliográfico y, como ya se dijo en la introducción, se definieron y aplicaron 4 criterios para la lectura pormenorizada de todos y cada uno de los 25 artículos procesado en la muestra textual. Específicamente, el proceso indagativo transcurrió por cuatro etapas o momento diferenciales, a saber:

- Definición y delimitación del tema.
- Enunciación del objetivo de la investigación.
- Arqueo y selección de la muestra documental
- Elaboración del articulo con base a la normativa para autores de la Revista de la Universidad del Zulia.

El trabajo que hoy se presenta responde al interés de revisar la producción científica que figura en determinadas revistas de alto impacto, sobre ciertos ámbitos

temáticos en específico, actividad pertinente para investigadores y editores ganados a conocer las tendencias actuales que marcan pauta en el escenario académico internacional en el desarrollo de líneas de investigación y edición.

2. Balance bibliográfico y estado del arte

En este apartado se procede a la lectura o interpretación de las fuentes recabadas con base a los reiterados criterios de: a) tema; b) metodología; c) fuentes empleadas y perspectiva teórica; d) aportes para el desarrollo del tema y; e) observaciones (opcional). Aclarado el punto, en el artículo de (Nóvoa Souza Lara, Cortinhas dos Santos, Nunes Pereira Costa, & Almeida Vieira, 2019), que versa sobre el tema de la Agricultura Urbana en Brasil en el Período (2008-2017), se analiza esta novedosa forma de agricultura mediante una metodología descriptiva que recopiló sistemáticamente información de fuentes secundarias sobre el tema, disponible en la base de datos: *Journal Portal*, que funciona como biblioteca virtual de la producción científica que emerge de los postgrados de Brasil; por tal motivo, en lo teórico, esta investigación se inscribe en las coordenadas de los artículos de revisión bibliográfica. En cuanto a sus aportes, destacan el hecho de que bien entrado el siglo XXI son escasos todavía la producción científica sobre agricultura urbana en Brasil, ello a pesar de la relevancia social, económica y ambiental del tema y del apoyo del estado a ciertas investigaciones en el área.

El artículo de (Maksimovich, Vladimirovich, Vladimirovich, Petrovna, & Leonidovich, 2019) aborda el tema Cambio en agroquímicos, propiedades y distribución vertical del compuesto Cs en suelo aluvial, tratado con medidas de rehabilitación, con ocasión de los suelos de Chernóbil afectados por el catastrófico accidente de la central nuclear en 1986. El objetivo del trabajo fue precisamente estudiar la transformación de la fertilidad del suelo bajo la influencia de medidas de rehabilitación y el comportamiento de 137Cs en el perfil del suelo de los prados de llanuras aluviales. Para obtener los resultados, se hizo uso de variados métodos de medición de indicadores de agroquímicos y radiación del suelo en diferentes periodos de tiempo, antes y después del proceso de rehabilitación de los suelos de la zona. Como resultado de la investigación se demuestra como el radical de la capa vegetal mejoró significativamente

con la introducción de minerales, al tiempo que los fertilizantes utilizados aumentaron el contenido nutriente de la tierra.

Por su parte, (Dudnikova, Sukhanova, Lyavina, Bulgakov, & Kalinichenko, 2019) abordan desde la perspectiva económica las características y consecuencias de la sustitución de importaciones de alimentos en Rusia. Con el objetivo general de analizar las peculiaridades de la política de sustitución de importaciones e identificar sus consecuencias: positivas y negativas, para la autosuficiencia alimentaria de la población rusa durante el período de las sanciones. A nivel teórico la investigación se inserta en el arduo debate politológico y económico sobre la efectividad de las políticas de sustitución de importación como estrategia de desarrollo endógeno. Para el procesamiento de la información se empleó el método de presupuestos económicos, el método estadístico, el método de alineación analítica junto a las evaluaciones de expertos. Entre los aportes de la investigación destacan, por un lado, la descripción del proceso mediante el cual las personas han retomado el consumo de alimentos domésticos y, por el otro, como ciertos alimentos que no pueden producirse internamente han desaparecido de la dieta diaria por el efecto perjudicial de las sanciones impuestas por occidente, todo lo cual empuja al desarrollo de las capacidades internas de Rusia con el ánimo de potenciar su soberanía alimentaria.

El trabajo de (Afonasyevna Kazak et al, 2020) da cuenta de los cultivos de trigo de primavera media-temprana según su nivel de nutrición mineral en la estepa del bosque del norte de la región de Tyumen, ubicada en Siberia occidental sobre el rio Turá. Su objetivo general fue analizar la calidad de los cultivos por rendimiento de granos de trigo en las cosechas de primavera que dependen, a su vez, del rendimiento de nutrición mineral, en consecuencia, se trata de una investigación típica de las ciencias del agro. Metodológicamente estamos ante una investigación experimental que se centró en explicar las características de los suelos de la región, como condición para evaluar la calidad de los cultivos que se dan en la zona. A modo de resultados, se muestra cómo según cálculos económicos los cultivos de primera son los mejores, siempre y cuando se acompañen el proceso de siembra con fertilización mineral.

En otro ámbito temático, el trabajo de (Kolesnikov, Moshchenko, Kuzina, Kazeev, & Akimenko, 2019) sobre el desarrollo de concentraciones máximas de plomo,

cromo, níquel y cobre permitidas en el petróleo, afectan los suelos negros de Ciscaucasia Central. Se infiere que la investigación tuvo por objetivo, aunque no se precisa claramente en la redacción, estudiar la toxicidad de ciertos metales pesados presentes en los suelos negro de Ciscaucasia. Metodológicamente se emplearon procesos de simulación en laboratorio que dieron cuenta de cómo algunos productos químicos contentivos de minerales pesados alteran la composición natural de los suelos de la zona. A modo de conclusión se indica que, la contaminación de estos suelos como resultado de la explotación petrolera a dañado su estructura biológica normal con consecuencias imprevisibles para la biodiversidad de la región.

(Panyshev & Katlishin, 2020) presentan una investigación sobre la eficiencia de la regulación estatal y la eliminación de la industria del ganado lechero en el Federación Rusa, desde el punto de vista de la planificación de la industria agrícola, con el objetivo de identificar las direcciones principales de esta política y, el tamaño del apoyo del presupuesto estatal para la lechería en Rusia y, del mismo modo, analizar la dinámica de la industria láctea, sus indicadores de desarrollo y su economía de eficiencia. En lo metodológico, se trata de una investigación documental que sintetizó distintas fuentes científicas sobre el tema, en la que además se empleó el procedimiento de análisis de correlación para medir ciertos indicadores de la industria lechera. Entre los resultados del trabajo destaca el hecho de que el presupuesto estatal para el desarrollo de esta industria es insuficiente, lo que *de contera* impide la implementación de importantes programas para el desarrollo del agro en el país en general.

(Kovalenko, Sarkisova, Kolomiitseva, Marchenko, & Siuiva, 2020) presentan un sugestivo trabajo sobre las perspectivas y problemáticas de la regulación legal de las tierras agrícolas en Ucrania, investigación que tuvo por objetivo el análisis del marco legal del régimen de tierra en este país. Metodológicamente la investigación es documental y se sirvió de la recopilación de un conjunto de fuentes legales, nacionales e internacionales. También se empleó el método comparativo que sirvió, entre otras cosas, para contrastar las decisiones sobre la materia en distintos tribunales de Europa. Los autores concluyen que, la política de rotación de tierras agrícolas, en tanto mecanismo de mercado, es muy efectivo para asegurar un futuro digno para las personas

y empresas dedicadas a la producción agrícola, siempre y cuando se cumplan las leyes que protegen el medio ambiente.

En otro orden de ideas, (Ravilovich Rakhmatullin, Anvarovich Suleimanov, Kamilevich Valeev, & Askarovich Daukaev, 2019) trabajan el tema de la evaluación higiénica de la cubierta del suelo y productos de vegetación en zonas adjuntas a refinerías de aceite y complejos petroquímicos de la república de Baskortostán, con el propósito de estudiar los residuos polimetálicos en la composición de los suelos en las zonas circundantes de las petroquímicas. Metodológicamente se procesaron un conjunto de datos de estudios ecológicos e higiénicos en las áreas afectadas. A modo de aportes, se alerta que los principales elementos contaminantes se extienden a cultivos y vegetales en un radio de hasta 25 kilómetros, poniendo en riesgo el bienestar y la salud de varias comunidades de la región.

En la perspectiva del derecho, el artículo de (Sydorov, Drobush, & Hulievska, 2020) aborda el tema de las empresas agrarias y los derechos humanos a nivel internacional, con el objetivo de revisar el estado de los derechos humanos en el contexto del negocio agrícola o, más concretamente, la relación asimétrica derechos humanos y agricultura. Los autores procesan un conjunto de fuentes documentales en la modalidad de artículos científicos y cuerpos normativos. Entra las conclusiones más importantes se describe lo que ellos denominan como antropologización, ecologización y socialización del derecho internacional y nacional, como respuesta lógica a las contradicciones que emergen continuamente de las economías globalizadas, que tienden a entorpecer el goce y disfrute de los derechos fundamentales en beneficio de la lógica empresarial, para la cual la tierra es una mercancía que hay que explotar sin la interferencia del estado.

En la perspectiva de las matemáticas y la economía, (Siptits, Ganieva, Romanenko, & Evdokimova, 2019) abordan el tema de los Algoritmo de planificación para una producción de cultivos eficiente y sostenible, con el objetivo de proponer un modelo económico-matemático capaz de optimizar la estructura productiva del agronegocio, mediante el procesamiento de diversos indicadores de carácter: climático, tecnológico, biológico y socioeconómico, entre otros, que le permitan al generante la toma de decisiones inteligentes así como planificar con visión integral. Para efectuar su

propuesta, los autores plantean distintos métodos algorítmicos capaces de resolver problemas reales. Entre los aportes más destacados de la investigación se muestra una vía científica basada en modelos algorítmicos que se ajusta a las necesidades de la industria agroalimentaria, capaz de generar decisiones eficientes al tiempo que podría minimizar las perdidas.

Por su parte, (Khairullina & Yarkova, 2019) presentan un artículo que se traduce como: *Instrumentos objetivo del programa del mecanismo de apoyo estatal para la agricultura*, con el propósito de reflexionar sobre el funcionamiento del mecanismo económico de apoyo a la agricultura en Rusia, como parte de un enfoque orientado a programas para la regulación de la economía. En lo metodológico, se empleó la técnica de análisis retrospectivo para valorar el efecto concreto de este programa de apoyo. A modo de aporte, los autores cimentan las bases para una clasificación de las políticas públicas de apoyo a la agricultura en Rusia que se concentra en factores como: las fuentes de financiamientos, los niveles y modalidades de regulación estatal, la duración del periodo de acción de las medidas implementadas y las etapas de producción.

También enfocado en Rusia, el trabajo de (Olegovich, 2019) aborda el tema de la experiencia internacional de protección judicial de los derechos territoriales y tribunales de tierras en Rusia, con el objetivo de examinar la usanza internacional en el campo de la protección judicial de los derechos que regulan la materia agraria, con especial énfasis en la solución de controversias vinculadas a la tierra y sus múltiples implicaciones. Para recabar y procesar la información se empleó el diseño documental de investigación. El énfasis estuvo en el análisis de una muestra de sentencias de tribunales con competencia en materia del agro de países como: Australia, Estados Unidos, Escocia, Sucia y República Dominicana. Entre las principales conclusiones de la investigación resaltan varias ideas, por un lado, la asignatura pendiente del desarrollo de un órgano judicial, eficiente y eficaz, con materia de protección del medio ambiente y el uso de recursos naturales en la federación rusa y, por otro, se efectúa una propuesta encaminada a este propósito que sintetiza lo mejor de las doctrinas y experiencias judiciales de los países estudiados y se adapta a las particularidades del caso ruso.

Haciendo hincapié en la temática sobre radiación (Nikolaevich, Fedorovich, Petrovna, Vladimirovich, & Leonidovich, 2019) nos traen un trabajo especializado sobre

la efectividad de los químicos en el cultivo de centeno de invierno en suelos contaminados por radiación, el cual tuvo como propósito, aunque no se hace visible a lo largo del texto, pero se puede sobreentender, aumentar el rendimiento en el cultivo de centeno de invierno en suelos contaminados por radiación. Haciendo uso de un método experimental que sirvió para procesar evidencias empíricas concretas. La práctica se estudió en 4 sesiones distintas en el mismo territorio (cultivo de centeno de invierno). Su aporte principalmente se inserta en la demostración de que el uso de fertilizantes, tanto por separado como en combinación con productos químicos, favorecieron a un acrecentamiento significativo en los indicadores físicos y de cocción de la calidad del grano en relación con el estándar de control.

(Fedoseev, Mariskin, & Bogatyrev, 2019) investigaron sobre la crisis de la propiedad de la tierra noble en la segunda mitad del XIX y principios del siglo XX en la región del Volga Medio. Para su trabajo se empleó una diversidad herramientas de análisis de diferentes ciencias como: el histórico, económico y estadístico. Los métodos escogidos fueron el comparativo histórico, sistémico, cuantitativo y el cronológico. Por lo demás, las fuentes que se utilizaron son: cifras de bancos de la época y documentos de periódicos. Su aporte radica en reconstruir el proceso histórico que dé cuenta de las principales causas negativas que dieron paso a la crisis del latifundio de la nobleza y su respectivo desbalance en el contexto de la economía de la época en Ucrania

Hacen lo propio (Zyukin, Svyatova, Zolotareva, Bystritskaya, & Alyokhina, 2020) con un artículo que se traduce como *La mejora del modelo para desarrollar la infraestructura del grano subcomplejo como atributo esencial para aumentar la eficiencia y aumento de la exportación de granos rusos*, por tanto, su propósito es mejorar el desarrollo de la producción de granos en el presente. Se basaron metodológicamente en el modelo del desarrollo de la producción y logística e infraestructura del subcomplejo de productos de granos. Teóricamente, su valides se fundamentó en el sistema de medidas de regulación estatal y económica. Su aporte radica en mostrar las estrategias y avances que se generaran en el campo de la agricultura de granos, al tiempo que asevera que la industria en general de los granos en Rusia podrá emplear mejoras sustanciales en su modelo para obtener progresos en los resultados de producción, importación y exportación del mismo.

(Kondratyev, y otros, 2020) abordan el tema sobre mecanismos organizativos y de gestión para reformar la agricultura, con el objetivo de estudiar la introducción de metodologías progresivas y enfoques para evaluar la efectividad de transformación de las entidades económicas, en el ámbito de organizaciones basadas en la cooperación e integración de sistemas económicos. Las herramientas metodología manejadas en la investigación fueron variadas, como: el análisis económico, histórico monográfico, estadística, análisis de sistemas, abstracción estructural-funcional, computacional-constructivo y abstracto-lógico. Como fuentes, se observaron de manera detallada los resultados de la actividad económica y la experiencia de reformas en entidades económicas, sobre lo hay una abundante documentación. En cuanto al aporte de la investigación, los autores promueven la instauración y consolidación legislativa de un sistema de reforma competitivo para organizaciones agrarias insolventes que intentan reactivarse. El artículo resalta la necesidad existente de palear los efectos negativos de la metodología y experiencia de la reforma agraria para instaurar organizaciones a través de la cooperación e integración de entidades económicas, con el abastecimiento del soporte estatal en todas las dimensiones que afectan el proceso de producción agrícola.

Seguidamente, (Boykov, Startsev, Protasov, Vorotnikov, & Pavlov, 2019) trabajan sobre las formas de mejorar la eficiencia de la labranza primaria en las zonas secas de la Federación de Rusia. En consecuencia, su propósito es optimizar la eficiencia del cultivo básico del suelo sin vertedera mediante el perfeccionamiento de los parámetros operativos y tecnológicos de las unidades de arado con base a la técnica del uso de un arado no inversor. Como métodos manejaron el estudio teórico de la interrupción de materiales, en particular la capa de suelo labrado y, estudios experimentales de la unidad de arado con el sistema no inversor desarrollado. Teóricamente, se afianzaron en documentos sobre la fractura o desmoronamiento de la capa de suelo labrada de investigadores como: Goryachkin, 1965; Gureev, 1988; Dyakov, 1988; Lurie, Lyubimov, 1981; Revyakin, Prosvirin 1990. La investigación aporta luces en la resolución de este problema persistente. Se resaltan dos conclusiones: 1) Se puede reducir el consumo de energía y, al mismo tiempo, generar la mejora de la calidad del cultivo básico sin molduras a través de la forma del órgano de trabajo; 2) La usanza del

arado con el ancho óptimo acrecentara significativamente la eficiencia del cultivo básico sin vertedera en las tierras áridas de la Federación de Rusia.

Continuando con la agricultura en Rusia (Ostaev, y otros, 2019), trabajaron sobre la mejora de la contabilidad en el desarrollo de mecanismos de gestión en la agricultura, proponiéndose la creación de un criterio para evaluar el nivel de desarrollo sostenible de las empresas agrícolas. Para la recabar y procesar información se desarrolló un sistema integrado de indicadores de desarrollo sostenible de las empresas agrícolas. A nivel teórico, se conjugaron diferentes lecturas sobre problemas de contabilidad de gestión, gestión en general y análisis y eficiencia de las empresas agrícolas. En el plano de las contribuciones, sin duda, el artículo ayuda a redefinir una nueva dirección generalizada de contabilidad al tiempo que proporciona un nuevo concepto de contabilidad de gestión. Además, en lo científico el sistema propuesto de contabilidad de gestión podría utilizarse como referente para la investigación y la mejora de la contabilidad de gestión como campo de estudio teórico-práctico.

(Boykov, Startsev, & Vorotnikov, 2019) tienen como punto de enfoque la mejora de la tecnología y el arado de labranza primaria. Su intención fue aportar ideas para mejorar la tecnología del arado principal de labranza y vertedero para su implementación. Para la recoleccion de datos se manejaron los principios básicos de la mecánica clásica y agrícola, las matemáticas, de acuerdo con los GOST actuales de la Federación de Rusia, STO AIST y los métodos establecidos en la ciencia y la práctica. Teoricamente, partieron de la tecnología mejorada de cultivo del suelo, lo que sirvio de base para una nueva propuesta por parte de los autores referente a las mejoras continuas de tecnología para la labranza principal del vertedero de los campos abandonados y un tipo de arado, que garantiza la afiliación de plantas altas en la capa cultivable con bajo consumo de energía y alto rendimiento agrícola.

(Metechko, Sorokin, & Novikov, 2019) *Monitoreo aeroespacial para resolver problemas de la agricultura moderna de precisión*, así se traduce el nombre del tema escogido para la investigación de estos académicos. Ellos se dedicaron a observar el uso de sistemas de vigilancia aeroespacial que se emplean para resolver varios o muchos de los problemas de la agricultura de precisión. Teniendo en cuenta este objetivo, como método se dedicaron a ejecutar un análisis logístico para identificar los medios más

efectivos de vigilancia aeroespacial para el desarrollo de la agricultura de precisión. Como apoyo, estudiaron planteamientos anteriores sobre la agricultura de precisión y, algunas tecnologías como: tecnología de posicionamiento global (GPS) y los sistemas geográficos y de información (SIG). Concluyeron que, a su modo de ver, la agroindustria moderna complejo ya no puede existir sin monitoreo aeroespacial.

Aterrizando en Ucrania (Pyvovar, Pyvovar, Babyak, Nazar, & Ostrovskiy, 2019) trabajan sobre la cuestión del permiso para el desarrollo de un plan de gestión de tierras para la asignación de parcelas como servicio administrativo, todo esto, desde la perspectiva de un enfoque teórico para la práctica jurídica. El artículo emerge con el ánimo de fundamentar la posición, según la cual, la diligencia de una autoridad gubernamental al conceder a los ciudadanos el consentimiento para el desarrollo de un plan de manejo de tierras, para una asignación de parcelas debe reconocerse como un servicio administrativo. Del mismo modo, para lograr el punto expuesto se articularon métodos propios de las ciencias legales y sociales, como: el método formal y legal, método comparativo y legal y el método de modelado estatal. Este trabajo realiza un aporte de naturaleza empírica, pues deja como base la construcción de un algoritmo de argumentos normativos que plantea pruebas de que dicha actividad es una clase de servicios administrativos y, al mismo tiempo servirá como jurisprudencia. Se enfocaron en debatir con estudios pertenecientes al campo del derecho de la tierra, como el de Denys Kovach, quien expuso el tema de la regulación legal del surgimiento de los derechos sobre la tierra.

(Ostaev, y otros, 2019) apuntan su investigación al tema sobre Presupuesto integrado en empresas agrícolas, su funcionalidad y toma de decisiones de gestión. El propósito del estudio fue el desarrollo de métodos de presupuesto para empresas agrícolas como una herramienta de contabilidad y análisis en la gestión de sus actividades. La investigación estuvo minuciosamente producida por métodos generales científicos y especiales, tales como: análisis, síntesis, abstracción, modelado, métodos de sistematización y generalización de los resultados. Como aporte crean un modelo conceptual para evaluar el nivel de riesgo de las alternativas presupuestarias estratégicas en el campo de la agricultura, así como actividades de apoyo para las organizaciones agrícolas.

Aunque los autores (Zavalin, Sokolov, Shmyreva, & Lukin, 2019) no explican de forma clara cuales son los objetivos de la investigación y que metodología se emplea para obtener los resultados de la misma, lo que constituye una deficiencia en términos de redacción adecuada de artículos científicos, se infiere que el trabajo se inserta en el método científico propio de las investigaciones agronómicas y que tuvo por objetivo analizar la reacción de las leguminosas a la acidez del suelo.

(Osipenko, Nikonovich, Nasonova, Vekhov, & Redko, 2019) en este caso nos volvemos a encontrar con la misma situación del artículo anterior, donde los autores no desglosan con la suficiente claridad los segmentos de los objetivos y la metodología empleada. En cuanto al tema, se plantearon investigar la historia del mercado de seguros agrícolas, sus éxitos, fracasos y su establecimiento como un mecanismo separado desde 2007. En cuanto a su objetivo, se deduce que está dirigido a analiza la estructura del seguro agrícola. Su apoyo teórico se encuentra en los datos sobre el desarrollo sostenible del sector agrícola después de la introducción de la nueva campaña de seguros de 2007. El trabajo ayuda a revelar la situación actual en la que se encuentra el mercado de seguros agrícolas y resulta una fuente confiable para aquellos que deseen relacionarse con dicho mercado.

Finalmente, (Tobratov & Zheleznova, 2019) trabajaron sobre la transformación de los flujos biogeoquímicos de mercurio en los ecosistemas de tierras agrícolas abandonadas en Rusia. Encontramos que su objetivo estaba dirigido al conocimiento de las peculiaridades geográficas de los cambios en la estabilidad natural de los paisajes, con énfasis especial en aquellos contaminados por mercurio. Así mismo, para lograr su propósito, su técnica de obtener información se encauso hacia la metodología de cargas críticas. Realizan varios aportes, entre ellos, la identificación de los principales emisores industriales regionales de mercurio; también, demuestran que las tierras abandonadas con vegetación leñosa arropan solo regiones de bosque sin viento de área pequeña que ya existen en el territorio, lo que determina el deterioro general de la resistencia al suministro de Hg.

3. Análisis y discusión de resultados

De la revisión del material bibliográfico disponible en la muestra, de conformidad con el objetivo estipulado, emergen un conjunto de resultados que se describen a continuación. Esencialmente aquí el ámbito del agro se trabajó desde al menos cuatro dimensiones particulares:

a) Desde la perspectiva científica clásica, esto es, mediante investigaciones típicas de la agronomía o la ingeniería agronómica en la que se utilizan métodos químicos, biológicos, genéticos y matemáticos para, con base a evidencia empírica concreta, determinar la calidad de suelos y cultivos, evaluar los agentes tóxicos y contaminantes que los afectan o, mediar el volumen de producción de ciertos rubros como cereales, entre otros aspectos de interés académico.

b) Desde la perspectiva económica. Estos trabajos tienden a explorar las estructuras y sistemas que interactúan en el proceso de producción de tierras con el propósito de señalar las limitaciones de los modelos empresariales, financieros o, el efecto económico de las políticas públicas implementadas en la actividad agro-productiva en contextos nacionales y regionales particulares. En líneas generales, el aporte de estas investigaciones no se limita a señalar las prácticas erradas o los aspectos a mejorar por parte de los agentes económicos y sociales encargados de producir las tierras, sino además, de proponer nuevos o renovados modelos empresariales o algoritmos contables que permitirían, entre otras cosas, apalancar el desarrollo agrícola a un nivel cualitativamente superior (Clavero, 2012), lo que coloca a la ciencia al servicio del bienestar colectivo y del desarrollo sostenible que tiene en el agro un pivote fundamental.

C) desde la dimensión jurídica. Abundan investigaciones desarrolladas bajo la lógica del derecho que aportan luces sobre el alcance y significado que adquieran los múltiples cuerpos normativos que regulan, en el plano nacional e internacional, los regímenes de propiedad de la tierra, las relaciones productivas que se dan en las prácticas agrícolas y la formas como se gestionan, en los organismos jurisdiccionales de las distintas naciones con ordenamientos jurídicos específicos, las controversias que se dan entre los actores y factores de producción. En estas investigaciones, casi siempre se emplean métodos comparativos y de hermenéutica jurídica para valorar de forma general lo sucedido en el binomio derecho-agricultura en el ámbito internacional, en

una línea que se enfoca además en derechos humanos, economías globalizadas y localidades particulares como interés clave de investigación y reflexión.

d) El agro desde la perspectiva de las ciencias sociales. Con menor volumen, pero no por ello con menor relevancia, en la muestra procesada también hay artículos que, desde la perspectiva histórica, antropológica o sociológicas, abordan los fenómenos sociales (materiales y simbólicos) que surgen de la relación: comunidades humanas, agricultura y tenencia de la tierra, como bien individual y colectivo orientados a la satisfacción de necesidades y a la producción de distintos valores para beneficio de algunos grupos en detrimentos de otros. De modo que, la tierra por si misma, es un recurso de poder, recurso que genera históricamente disputas y controversias por su usufructo y posesión, susceptibles a la investigación científica en los dominios de las ciencias humanas en general, ganas a entender las prácticas, ideas y conductas que las personas construyen intersubjetivamente sobre la agricultura en este caso.

Los interesante de las cuatro perspectivas de análisis detectadas en este balance, las cuales responde a las lógicas particulares del derecho, la economía, la ciencia política y la agronomía, entre otros campos disciplinarios, es que no se excluyentes entre sí, ni configurar saberes antagónicos sobre la tierra, todo lo contrario, se trata de investigaciones multidisciplinarias que con sus aportes y resultados concretos configuran, incluso sin proponérselo, un programa de investigación internacional que conjuga en su seno diversas teorías, métodos e interés científicos que tiene en el agro y todos sus epifenómenos su principal razón de ser y que invita en consecuencia al desarrollo de investigaciones inter y transdisciplinarias.

Conclusiones

Luego de revisar una muestra de la producción científica sobre agricultura, publicada en la revista Amazonia Investiga en el periodo 2019-2020, emergen distintas conclusiones que conviene enunciar de forma concisa:

- ✓ Los que se escribe y publica en la revista Amazonia Investiga sobre el agro, al menos en el periodo delimitado por este balance, responde a los más altos estándares científicos, de conformidad con las tendencias actuales en redacción de artículos arbitrados de alto impacto. No obstante, algunos trabajos presentes en la sección

estado del arte, manifiestan algunas limitaciones formales, tales como no enunciar claramente cuál fue el objetivo o propósito de su investigación o cual es realmente la metodología que emplearon para obtener sus resultados, cosa que se indicó en las líneas que anteceden razón por la cual conviene fortalecer los procesos de arbitraje y evaluación entre pares.

- ✓ La agricultura, con todo lo que significa y representa, se constituye a todas luces en un ámbito temático de interés axial para la sociedad, las comunidades científicas y los hacedores de políticas pública en la materia; mucho más en países en vías de desarrollo que no han logrado resolver hasta el presente problemas como: el latifundio improductivo, el uso adecuado y eficiente de las tierras productivas y la reforma agraria en función de apuntalar su soberanía alimentaria como herramienta para superar la pobreza, así lo demuestra la literatura revisada.
- ✓ Por último, se evidencia que se producen saberes sobre el agro desde disciplinas tan diversas como: el derecho, la economía, la ciencia política y la agronomía, entre otras, lo que demuestra que se trata de un tema multidimensional que no puede ser abordado en todo su alcance desde una única perspectiva disciplinar, teórica o metodológica.

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Análisis de los sitios web de las Universidades Nacionales Interculturales Peruanas

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RESUMEN

El artículo se elaboró con el objetivo de realizar un análisis de los sitios web de las universidades nacionales interculturales peruanas, las cuales son cuatro y se hallan ubicadas en diversas regiones del Perú y cuentan con un sitio web activo. Los resultados indican que los sitios web de las cuatro universidades interculturales, ofrecen un canal de comunicación gratuito y rápido con la comunidad universitaria. Se concluyó que, el mayor nivel de errores (51) y advertencias (98) fue el sitio web de la Universidad Nacional Intercultural de la Amazonía (UNIA), mientras que el menor nivel de errores (5) y advertencias (1) fue el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ). El mayor puntaje y rendimiento lo tiene la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 78 puntos. El mayor nivel de posicionamiento lo obtuvo la Universidad Nacional Intercultural de Quillabamba (UNIQ), con 5,9 puntos. El mayor nivel de movilidad lo obtuvo la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4,4 puntos. El mayor nivel de experiencia de usuario lo obtuvieron la Universidad Nacional Intercultural de la Amazonía (UNIA) y la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA) con 6,4 puntos. El mejor rendimiento lo tiene el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 30 puntos. El mejor tiempo de carga lo tiene el sitio web de la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4.9 s.

PALABRAS CLAVE: Sitio web; TIC; universidad nacional intercultural; interculturalidad.

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Analysis of the websites of the Peruvian National Intercultural Universities

ABSTRACT

The article was prepared with the objective of carrying out an analysis of the websites of the Peruvian intercultural national universities, which are four and are located in various regions of Peru and have an active website. The results indicate that the websites of the four intercultural universities offer a free and fast communication channel with the university community. It was concluded that the highest level of errors (51) and warnings (98) was the website of the National Intercultural University of the Amazon (UNIA), while the lowest level of errors (5) and warnings (1) was the website of the National Intercultural University of Quillabamba (UNIQ). The highest score and performance is the National Intercultural University of Quillabamba (UNIQ) with 78 points. The highest level of positioning was obtained by the National Intercultural University of Quillabamba (UNIQ), with 5.9 points. The highest level of mobility was obtained by the National Intercultural University of the Central Jungle Juan Santos Atahualpa (UNISCJSA) with 4.4 points. The highest level of user experience was obtained by the National Intercultural University of the Amazon (UNIA) and the National Intercultural University Fabiola Salazar Leguía de Bagua (UNIBAGUA) with 6.4 points. The best performance is the website of the National Intercultural University of Quillabamba (UNIQ) with 30 points. The best loading time is the website of the National Intercultural University of the Central Jungle Juan Santos Atahualpa (UNISCJSA) with 4.9 s.

KEY WORDS: Website; TIC; national intercultural university; interculturality

Introducción

Según la UNESCO (2019), el reconocimiento de la diversidad cultural - mediante una utilización innovadora de los medios y de los TIC en particular - lleva al diálogo entre civilizaciones y culturas, al respeto y a la comprensión mutua.

En las sociedades del conocimiento, las prácticas y los valores de creatividad e innovación desempeñan un rol importante, aunque sólo sea por su capacidad de poner en tela de juicio los modelos existentes para responder mejor a las nuevas necesidades de la sociedad (Aguilar, 2019; Martínez, 2019).

El acceso a las TIC requiere de la participación de los ciudadanos, y de la sociedad en general para ayudar a generar sociedades más igualitarias, así como fortalecer los servicios de educación, salud, desarrollo económico, participación pública, disminuir la corrupción y erradicar la pobreza (Maldonado, García y Sampedro-Requena, 2019).

El uso de las TIC en la educación se ha convertido, cada vez más, en un elemento imprescindible en el entorno educativo. Este complemento, acompañado de herramientas tecnológicas ha de generar en la sociedad una realidad y presencia cada vez mayor (Hernandez, 2017).

El impacto de Internet ha sido monumental e históricamente pocos inventos en la historia de la humanidad han modificado de tal forma la vida del ser humano (Rodríguez, 2014).

Los encargados de implantar la accesibilidad en la web son los diseñadores web, que muchas veces no tienen en cuenta ni los más mínimos requisitos de accesibilidad y sus responsables y clientes tampoco son conscientes del poco esfuerzo adicional. (Fuertes & Martínez, 2017).

En el diseño de cualquier producto, y en especial en el que aquí tratamos, los sitios web, la interfaz juega un papel primordial porque es la vía por la que el usuario se comunica con el sistema (Rovira y Marcos, 2013).

Por ende, la transparencia activa resulta ser un mecanismo que puede favorecer la comunicación e interacción entre las universidades y sus grupos de interés, más aún, cuando ésta permite llegar a diferentes partes interesadas simultáneamente (Católico-Segura, Leal-Bonilla & Londoño-Jiménez, 2019).

La diversidad es un elemento definitorio de la dinámica de la historia y en la riqueza cultural sustentada en esas identidades se integran en su patrimonio cultural enlazadas en la trama de su tejido social (UNESCO, 2017).

La interculturalidad en la educación constituye uno de los principales objetivos propuestos en la Declaración Mundial sobre Educación Superior en el siglo XXI: Visión y Acción de la UNESCO (Alonso-García, Roque-Herrera & Juárez-Ramos, 2019); teniendo en cuenta que, la educación intercultural es una práctica educativa

con la que se quiere responder a la diversidad de grupos culturales para una mejor convivencia e inclusión participativa (Rueda, Paz & Avendaño, 2019).

En el Perú, se han creado cuatro universidades nacionales interculturales. La Universidad Nacional Intercultural de la Amazonía fue creada en el año 1999 por Ley Nº 27250, siendo resultado de la reivindicación de los pueblos amazónicos, liderado por la Asociación Interétnica de la Selva Peruana – AIDESEP... (UNIA, 2020). Además, Espinosa (2017), afirma que:

> Hacia finales del año 2010, luego de las protestas indígenas de los años 2008 y 2009 que terminaron con los trágicos incidentes del "Baguazo", el gobierno del presidente García decidió crear tres nuevas universidades interculturales: la Universidad Nacional Intercultural Juan Santos Atahualpa (UNSJA) en las provincias de Chanchamayo y Satipo (Junín), la Universidad Nacional Intercultural de Quillabamba (UNIQ) en la provincia de La Convención (Cusco), y la Universidad Nacional Intercultural Fabiola Salazar Leguía (UNIB) en la provincia de Bagua (Amazonas).

Es importante conocer como las universidades nacionales interculturales peruanas, gestionan su información a través de los sitios web. Por ello, el objetivo principal de esta investigación fue realizar un análisis de los sitios web de las universidades nacionales interculturales peruanas, teniendo como objetivos secundarios los siguientes: Determinar los problemas frecuentes que presentan los sitios web de las universidades nacionales interculturales peruanas, identificar si existen diferencias específicas entre los sitios web de las universidades nacionales interculturales peruanas y examinar las ventajas importantes que ofrecen los sitios web a las universidades nacionales interculturales peruanas.

1. Metodología

Las cuatro universidades nacionales interculturales peruanas, se hallan ubicadas en diversas regiones del Perú y cuentan con un sitio web activo, el cual es analizado en la presente investigación, empleando las herramientas para evaluar el sitio web. El análisis se realizó durante el mes de enero de 2020.

Tabla 1. Universidades nacionales interculturales peruanas.

Universidad	Ubicación	Url
Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA)	Provincias de Chanchamayo y Satipo (Región Junín)	http://www.uniscjsa.edu.pe
Universidad Nacional Intercultural de Quillabamba (UNIQ)	Provincia de La Convención (Región Cusco)	http://www.uniq.edu.pe
Universidad Nacional Intercultural de la Amazonía (UNIA)	Ciudad de Pucallpa (Región Ucayali)	http://unia.edu.pe
Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA)	Provincia de Bagua (Región Amazonas)	http://unibagua.edu.pe

Fuente: Elaboración propia.

Según Saquero (2019) estudiaremos qué herramientas se están ofreciendo para garantizar una buena UX y qué es lo que evalúa, ya que, al ser un campo tan grande que abarca desde los colores hasta los sentimientos.

Es común que se confundan los conceptos de interfaz de usuario y experiencia de usuario (UI y UX, respectivamente, por sus siglas en inglés) (Ramírez-Acosta, 2017).

2. Resultados

Las universidades nacionales interculturales peruanas cuentan con un sitio web activo, para entregar información a la comunidad universitaria. Pero, debemos indicar que, existen diferencias entre sus sitios web. A continuación, vamos a analizar los resultados obtenidos, después de emplear las herramientas de evaluación del sitio web. El análisis se realizó durante el mes de enero de 2020.

Tabla 2. Herramientas para evaluar el sitio web.

Herramientas	Objetivo	Url
PageSpeed Insights de Google	Evaluar la velocidad de la página web e informa sobre el rendimiento real de una página para dispositivos móviles y de escritorio además de ofrecer sugerencias para mejorarla. Las métricas se basan en el Informe de Experiencia de Usuario de Chrome. Informa sobre la velocidad de la página y sobre la optimización de esta (PageSpeed Insight, 2020).	https://developers.google.com/speed/pagespeed/insights/?hl=es
Bankia Índicex	Analiza el nivel de competitividad digital de cualquier negocio a partir de la evaluación de su comportamiento en nueve áreas específicas a través de más de 100 parámetros. Estas áreas son: posicionamiento SEO, movilidad, experiencia de usuario, seguridad, marketing digital, contenidos, redes sociales, e-commerce y analítica web (Bankia Índicex, 2020).	https://bankiaindicex.com/
W3C Markup Validator	Verifica la validez de marcado de los documentos Web en HTML, XHTML, SMIL, MathML, etc. (W3C Markup Validator, 2020).	https://validator.w3.org/
Website Grader	Analiza el rendimiento, la adaptabilidad móvil, el SEO y la seguridad de una web (Website Grader, 2020).	https://website.grader.com/

GTMetrix	Analiza de manera específica distintos tiempos de carga como el tiempo exacto de cada request (petición), la optimización de los recursos, etc. (GTMetrix, 2020).	https://gtmetrix.com/

Fuente: Elaboración propia.

2.1. PageSpeed Insights de Google

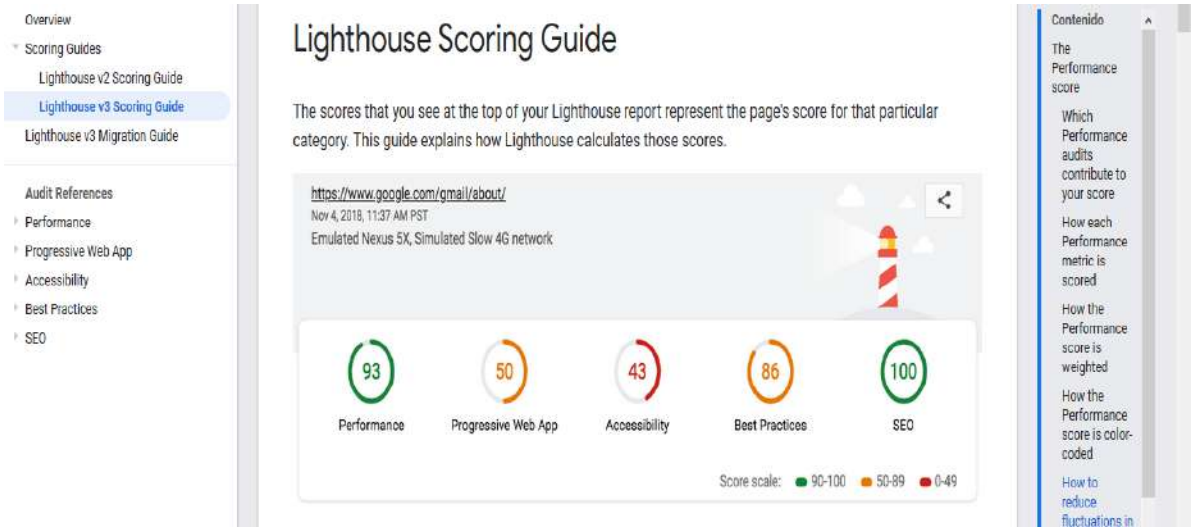

Figura 1. Guía de puntuación
Fuente: PageSpeed Insights de Google

2.1.1. Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA): http://www.uniscjsa.edu.pe

Figura 2. Resultados UNISCJSA
Fuente: PageSpeed Insights de Google

2.1.2. Universidad Nacional Intercultural de Quillabamba (UNIQ): http://www.uniq.edu.pe

Figura 3. Resultados UNIQ
Fuente: PageSpeed Insights de Google

2.1.3. Universidad Nacional Intercultural de la Amazonía (UNIA): http://unia.edu.pe

Figura 4. Resultados UNIA
Fuente: PageSpeed Insights de Google

2.1.4. Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA): http://unibagua.edu.pe

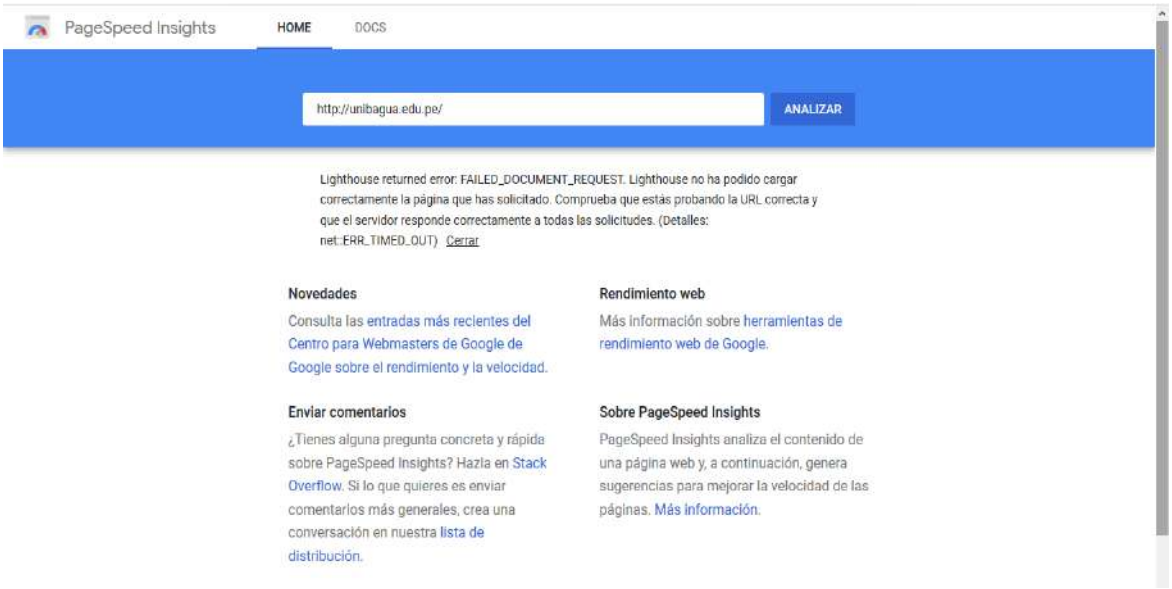

Figura 5. Resultados UNIBAGUA
Fuente: PageSpeed Insights de Google

Se observó que el mayor puntaje y rendimiento lo tiene la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 78 puntos, mientras que el menor puntaje y rendimiento, corresponde con 15 puntos a la Universidad Nacional Intercultural de la Amazonía (UNIA). Además, se debe indicar que la herramienta no pudo evaluar el sitio web de la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA).

2.2. Bankia Índicex

2.2.1. Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA)

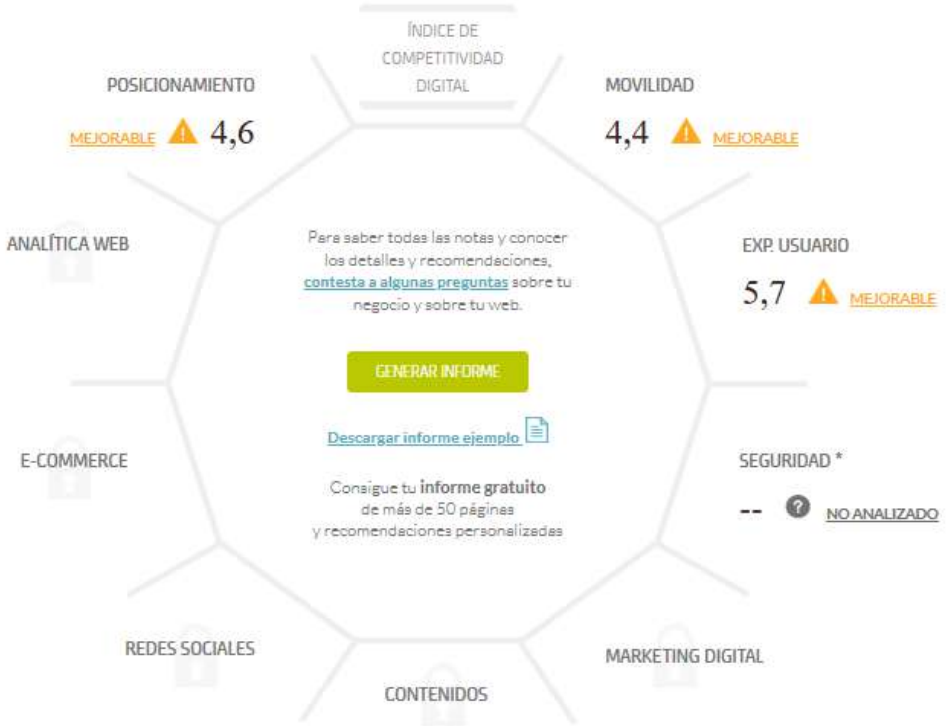

Figura 6. Índice de competitividad digital - UNISCJSA
Fuente: Bankia Índicex

2.2.2. Universidad Nacional Intercultural de Quillabamba (UNIQ): http://www.uniq.edu.pe

Figura 7. Índice de competitividad digital - UNIQ
Fuente: Bankia Índicex

2.2.3. Universidad Nacional Intercultural de la Amazonía (UNIA): http://unia.edu.pe

Figura 8. Índice de competitividad digital - UNIA

Fuente: Bankia Índicex

2.2.4. Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA): http://unibagua.edu.pe

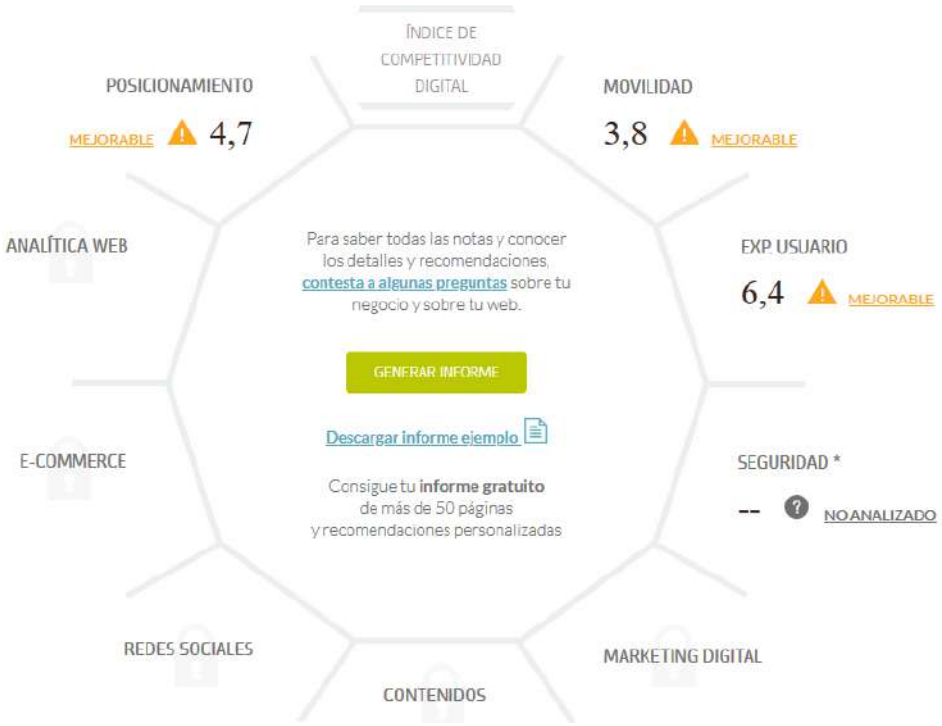

Figura 9. Índice de competitividad digital - UNIBAGUA
Fuente: Bankia Índicex

Se observó que el mayor nivel de posicionamiento lo obtuvo la Universidad Nacional Intercultural de Quillabamba (UNIQ), con 5,9 puntos. El mayor nivel de movilidad lo obtuvo la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4,4 puntos. El mayor nivel de experiencia de usuario lo obtuvieron la Universidad Nacional Intercultural de la Amazonía (UNIA) y la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA) con 6,4 puntos.

2.3. W3C Markup Validator

2.3.1. Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA): http://www.uniscjsa.edu.pe

Figura 10. Validar un documento en línea - UNISCJSA
Fuente: W3C Markup Validator

2.3.2. Universidad Nacional Intercultural de Quillabamba (UNIQ): http://www.uniq.edu.pe

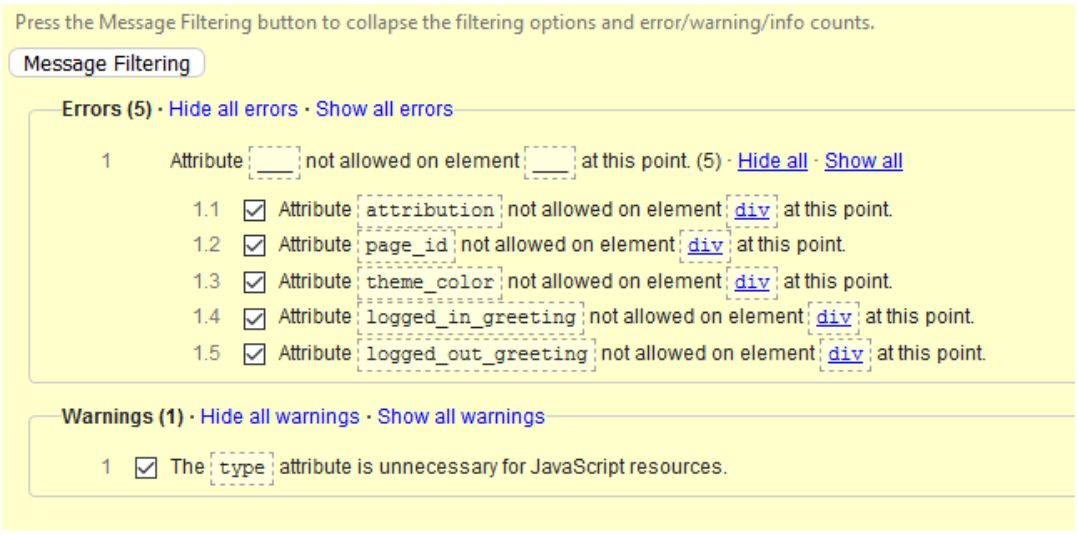

Figura 11. Validar un documento en línea - UNIQ
Fuente: W3C Markup Validator

2.3.3. Universidad Nacional Intercultural de la Amazonía (UNIA): http://unia.edu.pe

Figura 12. Validar un documento en línea - UNIA

Fuente: W3C Markup Validator

2.3.4. Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA): http://unibagua.edu.pe

Figura 13. Validar un documento en línea - UNIBAGUA
Fuente: W3C Markup Validator

Se observó que el mayor nivel de errores (51) y advertencias (98) fue el sitio web de la Universidad Nacional Intercultural de la Amazonía (UNIA), mientras que el menor nivel de errores (5) y advertencias (1) fue el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ).

2.4. Website Grader

2.4.1. Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA): http://www.uniscjsa.edu.pe

Figura 14. Análisis del rendimiento - UNISCJSA
Fuente: Website Grader

2.4.2. Universidad Nacional Intercultural de Quillabamba (UNIQ): http://www.uniq.edu.pe

Figura 15. Análisis del rendimiento - UNIQ
Fuente: Website Grader

2.4.3. Universidad Nacional Intercultural de la Amazonía (UNIA): http://unia.edu.pe

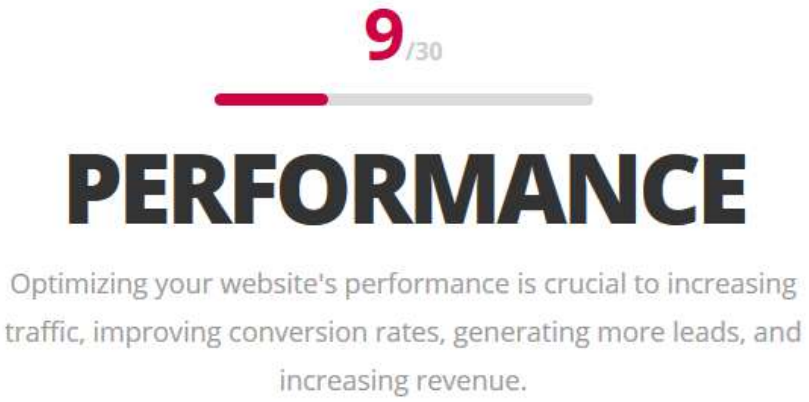

Figura 16. Análisis del rendimiento - UNIA
Fuente: Website Grader

2.4.4. Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA): http://unibagua.edu.pe

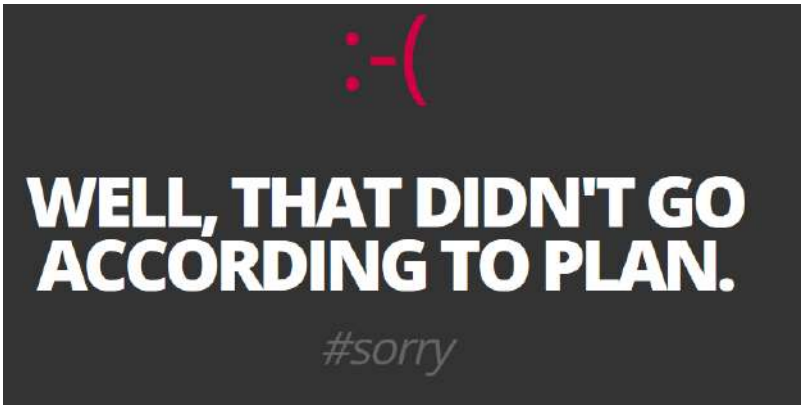

Figura 17. Análisis del rendimiento - UNIBAGUA
Fuente: Website Grader

Se observó que el mejor rendimiento lo tiene el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 30 puntos y el peor rendimiento tiene el sitio web de la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA), pues ni siquiera permite a la herramienta realizar el análisis respectivo.

2.5. GTMetrix

Figura 18. Análisis de tiempos de carga - UNISCJSA
Fuente: GTMetrix

Se observó que el mejor tiempo de carga lo tiene el sitio web de la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4.9 s, mientras que el peor tiempo de carga lo tiene el sitio web de la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA) con 35.3 s.

3. Discusión

A tenor de los resultados obtenidos en la investigación, se coincide con (Calvo & Riu, 2019) quien afirma que, el testeo de la propuesta de análisis para sitios Web ha permitido comprobar que la Web se mantiene como el principal eje comunicativo de las entidades.

Se evidencia que las características de los sitios web de las cuatro universidades interculturales, ofrecen un canal de comunicación gratuito y rápido con la comunidad universitaria, por lo tanto, se coincide con (Fuertes & Martínez, 2017), quien afirma que, en este sentido es esencial que la web facilite la integración de todas las personas

en esta nueva sociedad, evitando discriminar por razones de edad, conocimientos, idioma, formación, tecnología, cultura, religión, género y, por supuesto, discapacidad.

Conclusiones

Con respecto al primer objetivo, determinar los problemas frecuentes que presentan los sitios web de las universidades nacionales interculturales peruanas: Se concluyó que, el mayor nivel de errores (51) y advertencias (98) fue el sitio web de la Universidad Nacional Intercultural de la Amazonía (UNIA), mientras que el menor nivel de errores (5) y advertencias (1) fue el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ).

En relación con el segundo objetivo, identificar si existen diferencias específicas entre los sitios web de las universidades nacionales interculturales peruanas: Se concluyó que, el mayor puntaje y rendimiento lo tiene la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 78 puntos. Además, se debe indicar que la herramienta no pudo evaluar el sitio web de la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA). El mayor nivel de posicionamiento lo obtuvo la Universidad Nacional Intercultural de Quillabamba (UNIQ), con 5,9 puntos. El mayor nivel de movilidad lo obtuvo la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4,4 puntos. El mayor nivel de experiencia de usuario lo obtuvieron la Universidad Nacional Intercultural de la Amazonía (UNIA) y la Universidad Nacional Intercultural Fabiola Salazar Leguía de Bagua (UNIBAGUA) con 6,4 puntos. El mejor rendimiento lo tiene el sitio web de la Universidad Nacional Intercultural de Quillabamba (UNIQ) con 30 puntos. El mejor tiempo de carga lo tiene el sitio web de la Universidad Nacional Intercultural de la Selva Central Juan Santos Atahualpa (UNISCJSA) con 4.9 s.

En cuanto al tercer objetivo, examinar las ventajas importantes que ofrecen los sitios web a las universidades nacionales interculturales peruanas: Se concluyó que, facilitan la comunicación fluida con la comunidad universitaria, empleando el Internet como medio de acceso económico y amplio.

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Teaching potential of integrated learning technologies Smart, Stem and Steam

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ABSTRACT

At the current stage of digitization of the Russian economy, educational institutions urgently need new, more advanced and effective training technologies that help improve the quality of training of highly competent and competitive specialists who comply with the social order of society digital. These technologies should promote the introduction of robotic and cyber-physical systems in the training of future specialists. The article shows that SMART, STEM and STEAM integrated learning technologies that encompass the theoretical and practical components of educational programs with the help of special technological equipment: robotic complexes, virtual learning tools and cyber systems, can be used as technologies in the digital education. It is proven that the practical application of mathematical, physical, engineering and technological knowledge, modeling and design of robotic cybernetic devices and others, allow us to more effectively solve the tasks of the competition-oriented educational paradigm, create additional conditions for the development and realization of the personal potential of the students. The integrative didactic potential of SMART, STEM and STEAM technologies is determined, ensuring the achievement of the synergistic effect in the educational process and increasing the productivity of education subjects through the combination of the individual means of the technologies studied in a single system. The advantages of digital education are analyzed, which are optimized using the integrative teaching potential of SMART, STEM and STEAM technologies. Based on the characteristics of the integrative didactic potential of SMART, STEM and STEAM technologies, it is concluded that they are promising in the era of the digitization of Russian education and viable to use them in order to maintain the effectiveness of the educational process.

KEY WORDS: digitization of education; SMART, STEM and STEAM integrated learning technologies; technology; didactic properties and functions; integrative teaching potential; synergistic effect.

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Potencial didáctico de las tecnologías de aprendizaje integradas Smart, Stem y Steam

RESUMEN

En la etapa actual de la digitalización de la economía rusa, las instituciones educativas necesitan urgentemente tecnologías de capacitación nuevas, más avanzadas y efectivas que ayuden a mejorar la calidad de la capacitación de especialistas altamente competentes y competitivos que cumplan con el orden social de la sociedad digital. Estas tecnologías deberían promover la introducción de sistemas robóticos y ciberfísicos en la formación de futuros especialistas. El artículo muestra que las tecnologías de aprendizaje integradas SMART, STEM y STEAM que abarcan los componentes teóricos y prácticos de los programas educativos con la ayuda de equipos tecnológicos especiales: complejos robóticos, herramientas virtuales de aprendizaje y sistemas cibernéticos, pueden utilizarse como tecnologías en la educación digital. Está comprobado que la aplicación práctica de conocimientos matemáticos, físicos, de ingeniería y tecnológicos, el modelado y el diseño de dispositivos cibernéticos robóticos y otros, nos permiten resolver de manera más efectiva las tareas del paradigma educativo orientado a la competencia, crea condiciones adicionales para el desarrollo y la realización del potencial personal de los estudiantes. Se determina el potencial didáctico integrador de las tecnologías SMART, STEM y STEAM, asegurando el logro del efecto sinérgico en el proceso educativo y aumentando la productividad de los sujetos de educación a través de la combinación de los medios individuales de las tecnologías estudiadas en un solo sistema. Se analizan las ventajas de la educación digital, que se optimizan utilizando el potencial didáctico integrador de las tecnologías SMART, STEM y STEAM. Sobre la base de las características del potencial didáctico integrador de las tecnologías SMART, STEM y STEAM, se concluye que son prometedoras en la era de la digitalización de la educación rusa y viables para utilizarlas a fin de mantener la eficacia del proceso educativo.

PALABRAS CLAVE: digitalización de la educación; tecnologías de aprendizaje integradas SMART, STEM y STEAM; tecnología; propiedades y funciones didácticas; potencial didáctico integrador; efecto sinérgico.

Introduction

The current stage of development of scientific and technological progress has led to the urgency of digitalization of the Russian education system, which, in turn, has determined the need for educational institutions at all levels in new, more advanced and

effective technologies for training and education. Among the basic requirements for them, one can single out the need to comply with the integration requirements in the study and research of material and virtual objects, processes, phenomena, i.e. the presence of such didactic and research properties and functions that can ensure the implementation of the didactic potential of digital electronic communication tools and education systems. In addition, new digital educational technologies should fully promote and effectively accompany the introduction of robotic and cyberphysical systems, 3D-design systems, engineering, artificial intelligence in the training of future specialists.

1. Methodology

In modern pedagogy, the concept of "SMART technology" (smart or intelligent technology) has been used relatively recently, although in other sciences, primarily technical and economic, it has been used for more than forty years. There is no doubt that the main reasons that generated the inclusion of this term in the pedagogical thesaurus should be considered the achievements of scientific and technological progress in general and the development of digital means of computer science and information and communication technologies, in particular. A clear confirmation of the above can serve as the results of the work of such researchers as: N.V. Dneprovskaya, E.A. Yankovskaya (2015); Mahotin, 2018; H. Nakashima, H. Aghajan, J.C. Augusto, 2009; A.V. Zavrazhin (2015) and others.

In addition to this, along with widely known and already familiar in the field of education, intelligent SMART technologies such as: the Internet and local educational networks, interactive whiteboards SMART Board, tablets and other digital tools and devices, recently in practice educational organizations are increasingly introducing STEM- (science, technology, engineering and mathematics - science, technology, engineering, mathematics) and STEAM technology (science, technology, engineering, art and mathematics - science, technology, engineering, art being, mathematics).

2. Results

The digitalization of the Russian education system is rapidly gaining momentum, in accordance with the Digital Economy of the Russian Federation program until 2024, approved by order of the Government of the Russian Federation in July 2017, one of the goals of which is to improve the education system to provide the digital economy with competent personnel (Timofeev et al, 2019). Work to achieve this goal should contribute to improving the quality of training in educational institutions of highly qualified and competitive specialists who meet the social order of society and are able to effectively participate in the development of the digital economy.

It is known that in the narrow sense of digitalization, it represents the replacement of analog systems for collecting and processing information with technological systems that can generate, transmit and process a digital signal about their status, and in a broad sense it can be considered as: "the process of transferring functions and activities into a digital environment (business processes) previously performed by people and organizations "(Idrisov et al., 2018). Therefore, we can conclude about the advantages and benefits of digitalization in the economy, industry, energy, other areas of human activity and, accordingly, about the goals and objectives that educational institutions now face in training personnel for the digital economy.
However, the digitalization of education, as noted by I.V. Dubrovina (2018), F.F. Sharipov, S.A., (2017); Akhmetzhanova, A.V. Yuryev (2018); E.I. Klemasheva (2018) gives rise to an additional, and very significant, problem of organizing personal education on the basis of the formation and development of the level of its general cultural training through SMART technologies, rapidly penetrating into all areas of activity, gaining the status of basic ones in them and becoming the basis of the modern electronic information and educational environment, "how physical infrastructure that allows the surrounding intellect to function" (Nakashima et al, 2009) as part of cybernetic interaction in human-smart systems (intellectual) environment" (Mahotin, 2018). Obviously, according to V.A. Krasilnikova (2012); O.M. Gyshchina (2015); E.N. Bobyshev (2015); A.V. Matveeva, E.A. Krotova (2017); M. S. Ivinskaya (2017) which, along with the noted problem, the intensification of the use of new digital educational technologies will contribute to exacerbating the negatives of digitalization of the

processes of education and personal education, such as: loss of oral and written verbal communication skills; screen, gamified and social network smartphone addiction; hypertrophied virtualization of socially significant skills and competencies; visual impairment, decreased motor activity of students, etc. These and some other problems give us reason to believe that at the stage of digitalization of the educational process, STEM and STEAM technologies of mixed, integrated learning can become very relevant and practical in practice. combine theoretical and practical components of educational programs through special technological equipment, including the so-called SMART systems and environments, robotics FIR systems, virtual learning tools and cybernetic systems.

Intensification of practical application of mathematical, physical, engineering and technological knowledge, achievements of natural sciences and advanced scientific methods, modeling and designing of our own robots and other devices allows us to better solve the tasks of a competence-oriented education paradigm, creates additional conditions for the development and realization of students' personal potential , motivation for the constant expansion of their horizons, stimulating interest in learning English as the main on the language of modern science (Averin & Marko, 2017; Habib-Mireles et al., 2015).

In STEAM technology, to the first four names of scientific and subject areas that are especially significant in the development of modern technologies for the training of specialists especially in demand by society and employers, a creative direction has also been added (art - art). From the point of view of the topic of our study, this supplement can be considered as a holistic component that allows productively and diffusely integrate learning outcomes in mathematics, natural science subject areas, information technology, engineering disciplines, and robotics. And engineering, in STEAM technology is positioned as engineering art (Aniskin et al., 2016).

By the didactic potential of STEM and STEAM technologies, we mean those educational and, first of all, educational opportunities that are determined by the combination of didactic properties and functions of their implementation tools and can be used to optimize and individualize the quality training of future digital specialists, its integration and differentiation according to an algorithm defined by the

requirements of federal state educational standards (Prigogine, 2003). The didactic properties of the means for implementing STEM and STEAM technologies are their design capabilities used to solve the problems of the educational process, and the didactic functions are their external manifestation in this process. It is worth noting that, in addition to traditional computer hardware and software, the main tool base for the successful functioning of STEM and STEAM technologies includes such a top A-triad of SMART systems and environments, such as iPhone, iPad and Android, which have proved their effectiveness not only in the digital economy, but also in engineering, management, financial and economic education (Glukhov, Vasetskaya, 2017).

According to D.A. Mahotina, the further development of SMART-technologies determines not only their leading role in the development and rapid progress of "smart" environments and "smart" production industries, but also ensures intensive, almost limitless, penetration into all spheres of human activity, including education. The organization and management of constantly and continuously changing educational systems based on the introduction of new and latest promising digital computer ICTs and electronic educational resources, including STEM and STEAM education technologies, makes it possible to efficiently and productively solve the problems of the educational process at a higher intellectual level and achieve the required goals in the quality policy of upcoming digital education (Mahotin, 2018). In our opinion, it is precisely these opportunities that determine one of the most important components of the integrative didactic potential of SMART, STEM, and STEAM technologies in solving the problems of digitalization of Russian education.

The noted possibility determines the next, very significant component of the integrative didactic potential of SMART-, STEM- and STEAM-technologies.

Also, the advantages of digital SMART education (Dneprovskaya & Yankovskaya, 2015; Mahotin, 2018) can be included in the structure of the integrative didactic potential of SMART, STEM, and STEAM technologies:

- thematic interdisciplinary and design training based on the integration of natural sciences, engineering, information technology and mathematics;

- intensification and increase in the share of the practical component of the educational process in order to demonstrate to students the benefits of operational

implementation and application of modern scientific and technical results and achievements in real life;

- the possibility of studying specific projects and creating prototypes of a real product;

- the formation and development of skills and critical thinking and problem solving in the processes of modeling, 3D-designing and prototyping of the created educational and research product with its subsequent testing to achieve the goal;

- ensuring active team communications by creating a free and comfortable atmosphere for students to discuss their own opinions, present personal results and achievements that contribute to better learning of lesson materials or extracurricular activities;

- motivation and development of students' interest in natural science and engineering technical disciplines based on the game elements of SMART-, STEM- and STEAM-classes;

- phased SMART-, STEM- and STEAM-training, corresponding to the consistency of the project approach as the basis for creativity and innovativeness of the educational process;

- organization of independent work of students to operate with the knowledge gained in training sessions to strengthen them on the principle of supplementing STEM and STEAM programs with gaming, entertainment and cognitive experiments to the main educational programs (Budnyk, O. 2018).

Applicable to the digitalization of higher education, from the above components of the integrative didactic potential of SMART, STEM, and STEAM technologies, one can single out such most advantageous advantages as the possibility of activating the educational process by creating digital content to individualize the educational activities of students through the formation and development of critical thinking abilities, effective ways and methods of team and independent work. Interpreting the characteristics of STEM-technologies A.I. Prigozhin, one should also note their combinatorial innovative potential, which can provide organizational, managerial and pedagogical innovations that are beneficial for higher education (Budnyk, 2018).

Conclusions

In general, from the above components of the integrative didactic potential of SMART-, STEM- and STEAM-technologies, we can conclude that they are promising in the era of digitalization of Russian education and the advisability of applying to maintain the effectiveness of the educational process, adapting the current electronic information and educational environments to new conditions , ensuring the productive compatibility of educational and educational work in the digital educational environment.

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International tax models towards multinational companies from the perspective of national welfare

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ABSTRACT

The article is dedicated to the development of mathematical models to solve the real scientific task of supporting tax policies for counter-acting tax planning of multinational companies (MNCs) that are working in the field of production and engineering, forming the scheme international prosecutor, from the position of national welfare. Based on the analysis of the existing models of international taxes and on the peculiarities of the real mechanism of tax regulation of capital movement, new models have been developed with a balance orientation. The main points for this balance are: a) an approach aimed at determining the final results of international taxation from the perspective of national economies; b) Take as an example the gap between tax planning measures by multinationals and measures contrary to government tax planning. The approval of models with the case study of the multi-level structure in which, to counteract the tax planning of multinational companies, the Government uses rules of controlled transactions, demonstrated that due to the possibility of development of multinational companies in convenient and extraterritorial jurisdictions, for Government the final result of the application of these rules can be negative. Instead of additional income, you risk reducing the tax base and reducing budget income; And from the perspective of national welfare, this implies losing the income and capital of multinational companies. It is considered important that the rules for the taxation of multinational companies should not focus on taxes as such, but should encourage the maintenance of capital within the territory or facilitate the return of previously disinvested income.

KEY WORDS: international taxation; economic-mathematical modeling; multinational company; tax planning; controlled transaction rules; withdrawal of income; return of income; national welfare.

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Modelos tributarios internacionales hacia empresas multinacionales desde la perspectiva del bienestar nacional

RESUMEN

El artículo está dedicado al desarrollo de modelos matemáticos para resolver la tarea científica real de fundamentar las políticas tributarias para la planificación fiscal contra-actuante de las compañías multinacionales (MNC) que están trabajando en el campo de la producción y la ingeniería, formando el esquema fiscal internacional, desde la posición de bienestar nacional. Con base en el análisis de los modelos existentes de impuestos internacionales y en las peculiaridades del mecanismo real de regulación tributaria del movimiento de capital, se han desarrollado nuevos modelos con orientación hacia el equilibrio. Los puntos principales para este equilibrio son: a) un enfoque dirigido a la determinación de los resultados finales de la fiscalidad internacional desde la perspectiva de las economías nacionales; b) se toman como ejemplo la brecha entre las medidas de planificación fiscal por parte de las multinacionales y medidas contrarias a la planificación fiscal de los gobiernos. La aprobación de modelos con el estudio de caso de la estructura de varios niveles en la que, para contrarrestar la planificación fiscal de las empresas multinacionales, el Gobierno utiliza reglas de transacciones controladas, demostró que debido a la posibilidad de desarrollo de las empresas multinacionales en jurisdicciones convenientes y extraterritoriales, para Gobierno el resultado final de la aplicación de estas reglas puede ser negativo. En lugar de ingresos adicionales, corre el riesgo de reducir la base impositiva y reducir los ingresos del presupuesto; y desde la perspectiva del bienestar nacional, esto implica perder los ingresos y los capitales de las empresas multinacionales. Se considera importante que las reglas para la tributación de las empresas multinacionales no deben centrarse en los impuestos como tales, sino que deben fomentar el mantenimiento del capital dentro del territorio o facilitar el retorno de los ingresos desinvertidos anteriormente.

PALABRAS CLAVE: fiscalidad internacional; modelado económico-matemático; compañía multinacional; planificación fiscal; reglas de transacciones controladas; retiro de ingresos; devolución de ingresos; bienestar nacional.

Introduction

Problems of economic-mathematical modelling of international taxation of multinational companies (MNC) are permanently within the focus of scholars and practitioners. This is objectively conditioned by processes of globalisation and increase in

competition for capital, by huge volumes of international trade (Acuña, 2011), cross-border investments and, respectively, by the impact of taxation policy upon international flows of goods, services and capitals. One of the latest examples is a recent tax reform in the USA which is purposed, among others, for creating favourable conditions for return of capitals into the country (Feldstein, 2017).

A number of empiric assessments, which survey is represented in OECD, evidences that sensitivity to direct taxes is substantial: semi-elasticity index in the average constitutes -3.72, i.e. tax cut by 1 percent point results in growth of foreign direct investment (FDI) by 3.72%. Moreover, "...studies in which more updated data are used, demonstrate an increase in semi-elasticity, which evidences that over time FDI become more sensitive to taxation" (OECD, 2007). This means that international taxation of MNC capitals and income, along with other factors, preserves its role and, other things being equal, it is an important reason which determines their flow.

Besides, one should take into account that in connection with the digital revolution and increased development of cyber-physical production facilities, cross-border business activity has dramatically surged. It displays itself in respect of: "(i) intangible assets upon which digital economy mainly rests, (ii) users and (iii) business functions as a result of a decrease in a necessity to employ local personnel for performing certain tasks, as well as elasticity (in a number of cases) in selecting the location for servers and other resources" (OECD, 2014).

In this connection, on the one hand, new opportunities for forming more efficient "smart" systems of international trade and international taxation occur. They render essential influence over capital location and competitiveness of national economies. Whereas, on the other hand, new opportunities for cutting tax expenditures occur with subjects of international trade in goods, services and capitals. In their turn, governments of different countries and international organisations undertake measures as to counter-acting new methods of tax evasion and competition infringement (OECD, 2015; Polezharova, Lipatova, 2015).

Both of them actively employ mathematical instruments for substantiating ways of

increasing benefits and cutting expenditures which relate to new economic reality. Purposes of such modelling are different, but instruments used are often similar, so far as operation of the same economic agents is simulated (which are engaged into international economic relations or are subjected to influence of such relations) and one and the same business sphere (connected with international flows of capital, goods and services).

The purpose of this study is in development of economic-mathematical models which allow to substantiate measures of state's tax policy as to counter-acting MNCs' tax planning as well as to forming up the national scheme of international taxation which would be favourable for preservation and attraction of capitals which are necessary for modernisation of production technologies and growth of social welfare. That is, influence of international taxation of MNC is evaluated not from the perspective of interests of economic agents, but from the perspective of national welfare (subject to tax influence over MNC behaviour).

1. Methods

1. 1. Types of international taxation models

There exists a big number of very different international taxation models. Considering them in detail herein is impossible and unnecessary. Therefore, further, we will consider only key characteristics of the most important model types, which are based on the neoclassical theory of investment. They have become widely spread in economic literature and represent the greatest interest from the perspective of achieving the set goal.

The performed analysis demonstrates that the specified models may be divided into the following categories:

by the way of establishing economic equilibrium - models with equilibrium calculated, which is usually established by way of finding the extremum of function of economic agent income, depending on taxes (OECD (2007); OECD (2013); Haufler, Mardan, Schindler (2014); models with equilibrium being postulated, in which economic equilibrium is postulated instead of being calculated (Haufler, Mardan, Schindler (2014); Grubert (2003); Whalley (2001); Vishnevskiy, Grechishkin (2002);

by types of financial structure - models of bilateral or direct (direct, non-intermediated) holding structures, models of trilateral structures (i.e. structures with participation of a mediator who is usually registered in a tax haven) (OECD (2007); OECD (2013);

by kinds of economic equilibrium - models with equilibrium of tax rates, in which it is considered that values of income as obtained by companies, do not have critical significance for taking investment decisions; and the only thing which is compared is effective tax rates in different territories (Whalley (2001); Vishnevskiy, Grechishkin (2002); Sutyrin, Pogorletskiy (1998); models with equilibrium of enterprise incomes, in which the principle driver for enterprise behaviour is considered to be net (subject to taxation) income instead of taxes as such (Haufler, Mardan, Schindler (2014); Grubert (2003); models with profit equilibrium of the jurisdictions, in which not only tax rates, as well as not only enterprise income which remains within the country, are compared, but, as well, tax revenues of governments are compared (Haufler, Mardan, Schindler (2014).

It is necessary to note, that the above specified economic-mathematical models most often apply methodological approaches which are based on equilibrium of tax rates and company income (after taxation, including understated incomes). This is feasible and convenient from perspective of assessment of consequences of tax policy for companies which are the principle agent of economic relations. However, upon that, there occur problems with accounting of interests of governments of separate jurisdictions or, more generally, for interests of national economies, including subject to factors of counter-acting the outflow and/or return of profits and capitals.

For example, in the work by H. Grubert (2003) who is one of the leading global experts in the area of international taxation – as the case study of a number of scenarios, advantages and disadvantages of the worldwide tax system as well as dividend release system, are considered. In particular, situations were simulated when at payout of interest and royalties by the subsidiary to the parent company, the amount of payment is underrated and tax saving for the company is calculated, so far as in the parent company's country the tax is considerably higher. However, given that, the issue of income loss by

the domestic jurisdiction is not handled, the same as the possibility of reverse adjustment (recovery) of revenues by the government is not taken into account. Possibilities of company's manipulations with active income are not analysed. This does not allow evaluating efficiency of governments' counter-acting the MNCs' methods of tax planning, including, in terms of economic welfare of any given territory.

Work by a group of authors (Haufler, Mardan, Schindler (2014) evaluates effects of rules of a controlled company and rules of thin capitalisation per amount of MNCs' taxes and profits in terms of country's welfare. As well, an approach has been considered from the point of view of tax saving for the account of MNC capabilities use. However, this is done, firstly, under ordinary neo-classical supposition of economic agents' maximising behaviour by way of differentiation by tax rates and finding the extremum of welfare function. Secondly, there is no separation into active and passive income, to which various approaches in taxation are usually applied. Thirdly, formula (Haufler, Mardan, Schindler (2014) does not account for influence of the basic rule of controlled transactions. Besides, the model does not enable to account of the amounts of withdrawn and returned income and capitals, which handicaps true evaluation of welfare value, as well taxes on profit repatriation are not accounted of.

Approach from the point of view of return of income as earlier transacted abroad was not also fully reflected in a fundamental research carried out by Organization for Economic Cooperation and Development (OECD) (OECD (2007). 6 cases of tax planning are considered, mainly, via the use of inter-company lending methods. In general, OECD believe that "... more work should be done to investigate the implications of tax planning to forward-looking effective tax rate analysis used to infer tax reform effects on FDI. Such work could usefully draw on the insights of recent work by Grubert (2004) analysing the effects of tax-planning on backward-looking tax burden measures" (OECD (2007).

This study in which research & methodological approaches elaborated by D.W. Jorgenson (Jorgenson (1963); J. Whalley (Whalley (2001); H. Grubert (Grubert (2003) are developed, is devoted to analysis of effects of such tax-planning measures and ways to counter-act those methods D.W. Jorgenson (Jorgenson (1963); J. Whalley (Whalley

(2001); H. Grubert (Grubert (2003); but only subject to the issues not fully studied in their works. In particular, it is about evaluation of tax-planning counter-acting measures as applied by governments of different countries. Within the frames of this context, the article considers the issue of convenient jurisdictions, namely, the countries possessing such parameters of tax policies which allow MNCs to avoid taxes and to divest capitals through subsidiaries incorporated therein.

Out of the above specified model types, for the purposes hereof, we suggest that there should be used models with balance being postulated, where trilateral financial structures (with participation of intermediary subsidiaries in convenient jurisdictions and with participation of affiliated entities in offshores) are considered. These simulation models, which are not though so mathematically rigor as optimisation ones, but they allow to better take account of institutional factors and to describe economic situations in relatively simple formulae which are easier subjected to economic interpretation.

We commence with consideration of equilibrium models of enterprise profits after taxation (as basic ones), then we proceed to more complex models with profit equilibrium of jurisdictions, which is aimed achieving the set goal.

Such choice is explained by the fact that this work is not aimed at substantiation of investment solutions or tax optimisation from the point of view of economic agents. The approach suggested is aimed at more correct establishment of final results of international taxation from perspectives of national economies, when they take account of both indices of private (economic agents) and public (government) economy sectors, which characterise aggregate resources of economic development, which remain in the country and which enter from abroad. This has principle significance, so far as for many countries taxes are important not as they are, but as a tool for observing national interests and increasing citizens' welfare.

1.2. Economic statement of a complex of MNC international taxation models. General task formulation

Three tax jurisdictions (three countries) exist: one ordinary - *A*, one convenient

(with weak anti-offshore legislation) - *B*, and tax haven - *C*.

There is also some MNC - parent company which is a resident of territory A (this is by default the territory of the country we are interested in and from which perspective the situation is analysed.

This parent company incorporates a subsidiary (owns over 50% of its property) within the convenient jurisdiction *B*, which also actively operates. Whereas, it is supposed that tax planning methods may be applied by MNCs with the help of affiliated companies which are incorporated by the parent company (*A*) and subsidiary company (*B*) (indirectly) in tax haven *C*. Territory of *C* is used not for real economic operations but for defrauding of income and tax evasion (in particular, through the mediation of the subsidiary company from convenient jurisdiction B).

Companies may apply (not apply, or apply to a limited extent) conventional tax-planning methods: transfer pricing, manipulation with direct investments and dividends; thin capitalisation, concealment of ultimate beneficiaries, etc. In their turn, governments may apply respective counter-acting measures, namely *Special Anti-Avoidance Rules*, which are aimed at fighting tax evasion by using definite tax schemes: rule of controlled transactions (CT) (based on arm's length principle), rule of controlled foreign corporations or companies (CFC), controlled debt rule (CD), as well as (thin capitalisation - (TC) secondary adjustments rule (SA)[1], etc.

2. Description of economic-mathematical models

Let us enter some designations. Let the net income (profit) norm of the parent company within territory A constitute D_A. The net income (profit) norm[2] of the

[1] The sense of SA (secondary adjustment) is that the government aims for compensating the losses which resulted from income retaining by MNC abroad, considering them as imputed-income taxable assets. Usually, the withdrawn income is conditionally treated as a loan, for which late repayment the government accrues interest

[2] Net income (profit) margin may be expressed both in relative values (as a percentage ratio of income from investment to the amount of such investment), as well as in absolute values (as amount of profit as received

subsidiary within territory B constitutes D_B. Condition of economic equuilibrium is observed if

$$D_A = D_B k_B; \quad k_B > 0. \tag{1}$$

I.e. generally, as far as we have a simulation type model, $D_A \neq D_B$. And this thing may be taken into account when carrying out simulation experiments. However, so far as our task is, first of all, to study effects of tax policy, we will start analysis from the situation, when $k_B = 1 \Rightarrow D_A = D_B$.

One of the principle tools which are suggested to be used for studying effects of tax-planning measures by economic agents and counter-acting them by governments, are indices which arithmetically represent a share of the total norm of the net income (profit) by which the company (with the help of transfer pricing) and the country (by way of introducing CT rules) alter such approach:

$$\Delta\varphi = (\varphi_c - \varphi_g), \tag{2}$$

where $\varphi_c = \frac{D'}{D}$ – corrective factor which defines the fraction of income (D'), as exempted taxation by the company (which respectively decreases taxable base) relative to the total amount of its taxable income D;

$\varphi_g = \frac{D''}{D}$ – corrective factor which defines the fraction of income (D''), as returned by the government of jurisdiction (which restores taxable base) relative to the total amount of company's taxable income D;

from the preset investment amount). For convenience of economic interpretation, hereinafter we will treat *D* as some amount of net income (profit) (for example, USD 100) as generated by this fixed amount of investment

$\Delta\varphi$ – remaining difference after performing such corrections and adjustments (in ordinary situations $\varphi_c \geq \varphi_g \Rightarrow \Delta\varphi \geq 0$).

Defining, that all *D* here and hereafter are the norm of normal net income which is formed on the basis of market (ordinary, fair) prices, which subsequently may be corrected (decreased) by value D' by companies and may be reversely corrected (restored) by value D'' by jurisdictions.

Kinds of revenues:

- received totally from economic operations D (include active and passive incomes, which will be taken into account in formulae separately in connection with peculiarities in their taxation);
- passive income as: dividends D_S, royalties D_R, interest D_I.

Tax rates:

- t_{AA}, t_{BB} – effective (medium) tax rates on net income (profit)[3];
- t^n_{AA}, t^n_{BB} – nominal rates of income tax for corporations;
- $t_{S_{BAA}}$, $t_{R_{BAA}}$, $t_{I_{BAA}}$ – real tax rates for passive types of income: dividends, royalties, interest (in this case, the ones being paid out by the subsidiary company from the convenient jurisdiction *B* in favour of the parent company to jurisdiction *A*, and which are subject to taxation in jurisdiction *A* – see suffix number *BAA*); those tax rates result from adjustments of nominal rates, for whatever reason $(t_{X_{BAA}} = f(t^n_{X_{BAA}}))$;

[3] In this case, we understand the effective tax rate upon net income, as some average percent of income seizure from a typical enterprise (representative enterprise) effected by *all* the taxes as provided by the national Law (but not only the corporate income tax), i.e. as interpreted by Paying Taxes: "Paying Taxes measures all taxes and contributions that are government mandated (at any level - federal, state or local) and that apply to the standardised business and have an impact in its financial statements" (PWC, World Bank Group (2015)

- $t_{S_{BAB}}$, $t_{R_{BAB}}$, $t_{I_{BAB}}$ – nominal rates of taxes on repatriation of dividends, royalties, interest, respectively, which are collected from the source of payment (in this case - in jurisdiction *B* – see suffix number *BAB*).

As OECD officers note (OECD (2013), from perspectives of empirical analysis of tax effects upon FDI, backward-looking average effective tax rates (*AETR*) yield more relative values and are a better predictor than forward-looking marginal effective tax rates (*METR*), and by far are much better than statutory nominal tax rates which do not take into account effects of tax planning and special taxation schemes.

Based on the above said, most generally, expression of the main tool used in simulation -*AETR* (average effective tax rate) looks as follows:

$$AETR = \frac{D - D(1-\Delta\varphi)(1-t)}{D} = 1-(1-\Delta\varphi)(1-t), \quad (3)$$

provided that $D > 0$.

Thus, when comparing *AETR* of territories *A* and *B* the equilibrium formula may be represented as follows:

$$AETR_A = AETR_B,$$
$$1-(1-\Delta\varphi_A)(1-t_A) = 1-(1-\Delta\varphi_B)(1-t_B). \quad (4)$$

Similar formula was suggested by H. Grubert (Grubert (2003), however, in addition to a feature of correcting income by companies, which is accounted of in his study, in our statement a feature of reverse correction for such income by governments is added.

For the purpose of resolving the set problem, further herein we shall compare not just tax rates in interacting territories (subject to correction by companies and adjustment by governments), but rates of return (originally $D_A = D_B$) which remains in disposal of companies of different jurisdictions:

$$D_A(1-\Delta\varphi_A)(1-t_A) = D_B(1-\Delta\varphi_B)(1-t_B). \quad (5)$$

This and below formulae of income equilibrium in furtherance may be used to calculate effective tax rates, actually obtained income and justification of conclusions regarding policy directions.

The below analysis is devoted to assessment of alterations of original situations under effects of various methods of tax planning from perspectives of MNCs, as well as counter-acting measures on part of governments (starting with application of CT rules).

2.1. Findings

2.1.1. Common formula of income calculation from perspectives of MNCs subject to income exempted from taxation.

Generally, income of the parent company in territory *A* (or, similarly, a subsidiary in territory *B*) may be represented as follows:

$$D^c = D(1-\Delta\varphi)(1-t) = D - D\Delta\varphi - Dt + D\Delta\varphi\, t = D - F - T^g + T^{c+}. \quad (6)$$

Id est, company income remaining in the given territory (D^c) are determined as total income (D), less withdrawn "shadow" income (F) and paid taxes (T^g), plus funds saved by the company as a result of tax planning (T^{c+}) (which constitute, on the other hand, losses for the government).

From the point of view of MNCs' total income, this formula (6) is incomplete, meaning that it does not include the fraction of MNC income which is withdrawn from taxation. Therefore, for more correct calculation of the total volume of MNC income and evaluation of economic equilibrium subject to the factor of tax haven, expression (6) must be increased by the value F, which characterises the fraction of profit which is exempted from taxation to an offshore jurisdiction.

$$D^c_{all} = D^c + F = D(1-\Delta\varphi)(1-t) + D\Delta\varphi = (D - F) - (T^g - T^{c+}) + F. \quad (7)$$

In other words, income transferred to tax haven *C* are actually income of MNC which are withdrawn from those jurisdictions for the purpose of decreasing the taxable base.

For example, under-rating of market value by the company for a part of the total profit φ_{AC} when exporting from country *A* to country *C* allows to cut the taxable base in the home country $D_A(1-\varphi_{AC})$ and, respectively, to increase income in country *C* by the same amount $D_A\varphi_{AC}$, so far as the goods will be sold in furtherance at market price, and the taxable margin will remain in tax haven *C*. Even, taking into account, that governments which apply CT rules, can adjust income for taxation purposes; non-taxable revenue will constitute value $D_A\Delta\varphi_{ACA}$, where $\Delta\varphi_{ACA}=\varphi_{AC}-\varphi_{ACA}$, and φ_{ACA} is the amount of correction of withdrawn income by government *A*.

Besides, it is important to stress that now such revenues may act as "shadow" revenues and/or "shadow" capital which in furtherance is not returned and brings no use in the home country; instead, they are used in economy of other countries.

Thus, application of correction methods within the frames of CT rules from perspectives of national welfare may be uneffective, even if the government fully restores (corrects) taxable base. In this case, corrections will happen only for taxation purposes: $\Delta\varphi_{ACA}=\varphi_{AC}-\varphi_{ACA}=0$, whereas, in terms of counter-acting revenue outflow, or their return, they are ineffective: $\varphi_{ACA}=0$, and, therefore $\Delta\varphi_{ACA}=\varphi_{AC}$, also revenues leave the territory in full.

In such scenarios non-returned "shadow" revenues

$$F_A=D_A\varphi_{AC}+D_A\varphi_{R_{AC}}+D_A\varphi_{I_{AC}}+D_{R_{CA}}\varphi_{R_{CA}}+D_{I_{CA}}\varphi_{I_{CA}}$$

are the result of the use by MNC of transfer pricing method both in respect of active operations $(D_A\varphi_{AC})$, and passive operations $(D_A\varphi_{R_{AC}}, D_A\varphi_{I_{AC}}, D_{R_{CA}}\varphi_{R_{CA}}, D_{I_{CA}}\varphi_{I_{CA}})$.

Now the reasons due to which MNC operations adversely affect economy of territory *A* become obvious - a considerable part of capitals irretrievably remains in tax haven *C*, and the revenues which remain, are still decreased for the account of additional taxation.

However, it is necessary to mention that until now a simplified scenario was considered. In such scenario taxes on repatriation as well as peculiarities of passive income taxation are not accounted of. Therefore, further we will proceed to consideration of the situation subject to these factors.

2.1.2. Full-fledged income equilibrium model from perspectives of MNCs subject to income exempted from taxation

Let us consider a more general scenario, when:

1) parent company invested into tangible and intangible assets of a subsidiary, as well it issued a loan to the subsidiary (acquired debt securities). Profit as obtained by the subsidiary in territory *B* is repatriated as dividends D_S, royalties D_R and interest D_I to territory *A*. Besides, parent company may as well be a recipient of intangible assets and loans from a subsidiary and, respectively, pays out royalties and interest to the latest;

2) parent company and subsidiary carry out active and passive operations with affiliated companies as incorporated in a tax haven, but given that, they make no direct investments to a company in territory *C*, or their such relations are concealed (indirect), so that a company in offshore jurisdiction *C* pays no dividends to companies in countries *A* and *B*. All the economic relations in conjunctions *A-C* and *B-C* are limited by lending and transfer of intangible assets from resident-company of tax haven *C* in favour of companies in territories *A* and *B* and, respectively, by payouts of royalties and interest to jurisdiction *C*, as well as by similar counter-operations *C-A* and *C-B*;

3) parent company and subsidiary apply methods of tax planning and carry out economic operations (including, export-import operations, operations with intangible

assets, lending operations) with the help of transfer-pricing through the affiliated company which is situated in tax haven *C*. This allows correcting (decreasing) taxable base by a certain part of rate of return. In their turn, governments make corrections (restore) taxable base.

In that case, tax equilibrium model looks as follows:

$$D_A^{all} = D_B^{all} \quad (8)$$

or:

$$D_A^m + D_{S_{AB}}^p + D_{CA}^p + F_{AC} = D_{S_{BA}}^m + D_{BA}^p + D_{S_{CB}}^p + F_{BC},$$

where:

$D_A^m, D_{S_{BA}}^m$ – net income from active economic operations of parent company and subsidiary in territory *A* and *B*, respectively;

$D_{CA}^p, D_{S_{CB}}^p$ – net passive income (which are specifically separated due to peculiarities of their taxation), as obtained, respectively, by parent company and subsidiary from affiliated companies from jurisdiction *C*;

$D_{BA}^p, D_{S_{AB}}^p$ – net passive income as received by the parent company and the subsidiary (respectively) from each other;

F_{AC}, F_{BC} – the total amount of "shadow" revenues (from all the active and passive operations) as withdrawn by the parent company and the subsidiary to offshore jurisdiction *C* less taxes on passive revenue repatriation (remark 1).

The represented equilibrium model demonstrates that the amount of withdrawn passive income decrease taxes on its repatriation. For example, the total volume of income as withdrawn from jurisdiction *A* to tax haven *C* will constitute:

$$F_{AC} = D_A\varphi_{ACA} + D_A\varphi_{R_{ACA}} + D_A\varphi_{I_{ACA}} + D_{R_{CA}}\varphi_{R_{CAA}} + D_{I_{CA}}\varphi_{I_{CAA}} - \\ -(D_A\varphi_{R_{AC}}t_{R_{ACA}} + D_A\varphi_{I_{AC}}t_{I_{ACA}}). \quad (9)$$

Also, it is worth mentioning, that in this scenario we proceed from a premise of equilibrium of MNC revenues as obtained in territories *A* and *B*, irrespective of the fact to which company they belong (plus income as obtained from offshore jurisdiction *C*). Further, let us proceed to consideration of the issue from another point of view - from perspectives of the national welfare of territory *A*.

2.1.3. Model of territory welfare (in case of A government's failure to return the income as earlier withdrawn to a tax haven)

All the above considered models are tentative. In the meaning, that they estimate economic interests from MNC point of view. However, national interests are somewhat wider than interests of economic agents in the private sector. Obviously, from the perspectives of country's economic interests, not all the global revenues must be taken into account, but only those which serve its territory, being a source of labour financing and capital, job creation, financing of the social sector, science, culture, etc., i.e. everything that forms welfare of a given country.

Such statement of the question considerably alters the logics of mathematical simulation.

In the simplest case, the function of public welfare of the state may be determined as follows:

$$D^w = D\ (1-\Delta\varphi)(1-t\ ) + D\ (1-\Delta\varphi)t\ = D^c + T\,. \qquad (10)$$

The principle difference of this model from the basic one (5) is that in this case not only net income is taken into account, but also the taxes as collected by governments.

Now, let us consider a more general situation which occurs when all the three territories are taken into consideration as sources of income origin: *A*, *B* and *C*. Public welfare of territory *A* may be identified as:

$$D^w_{ABC} = D^c_{ABC} + T\,, \qquad (11)$$

where D^c_{ABC} - amount of income as obtained from the three territories (as opposed to previous scenarios, where company income was accounted of only from the territory of registration and from tax haven *C*).

Based on the above said, the total income of jurisdiction A subject to tax income of the government will constitute the following value:

$$D^w_{ABC} = D^c_{ABC} + T = \\ = D^m_A + (D^m_{S_{BA}} + D^p_{S_{CB}} + D^p_{S_{AB}} + D^p_{BA}) + D^p_{CA} + T^g_{ABC} - T^{c+}_{ABC}, \quad (12)$$

where income $D^m_{S_{BA}}, D^p_{S_{CB}}, D^p_{S_{AB}}$ is considered as dividends as obtained by the parent company from the subsidiary (income is broken into constituents, due to peculiarities of its accrual).

Taxes as collected by *A* country government consist of taxes as collected on the income as obtained from territories *A*, *B* and *C*, as well those repatriated into jurisdiction *B* and *C*, as decreased by the amounts saved by MNC as a result of tax-planning.

$$T = T^g_{ABC} - T^{c+}_{ABC} = (T^m_A + T^p_{ACA} + T^p_{ABA}) + (T^m_{S_{BAA}} + T^p_{S_{CBA}} + T^p_{S_{ABA}} + T^p_{BAA}) + T^p_{CAA} = \\ = [(T^m_{AC} - T^{m+}_{AC}) + (T^I_{I_{ACA}} + T^R_{R_{ACA}}) + (T^I_{I_{ABA}} + T^R_{R_{ABA}})] + \\ + [(T^m_{S_{BAA}} - T^{m+}_{S_{BAA}}) + ((T^{I_{CB}}_{S_{BAA}} + T^{R_{CB}}_{S_{BAA}}) - (T^{I_{CB}+}_{S_{BAA}} + T^{R_{CB}+}_{S_{BAA}}) + \\ + (T^{I_{AB}}_{S_{BAA}} + T^{R_{AB}}_{S_{BAA}}) + (T^{I_{BA}}_{I_{BAA}} + T^{R_{BA}}_{R_{BAA}})] + \\ + [(T^I_{CA} + T^R_{CA}) - (T^{I+}_{CA} + T^{R+}_{CA})]. \quad (13)$$

Thus, welfare model of country A turns into the following equation:

$$D^{w1}_{ABC} = D^{w2}_{ABC}. \quad (14)$$

Its economic significance is that they compare total income of state *A*, which originates from territories *A*, *B* and *C* at various variants of situation development, on the basis of peculiarities of application of tax-planning methods as well as measures of counter-acting them in a given situation.

In order to have a picture of how the above specified models function, let us consider specific examples.

Let us use jurisdiction *A* - Russian Federation (RF) as the parent jurisdiction. Suppose, that the parent company from RF works with a convenient territory *B* (Laos), where it has incorporated a subsidiary. Suppose also, that the parent company and the subsidiary worked with affiliated offshore companies from *C* - British Virgin Islands (BVI), where taxes on foreign income are absent completely.

In Laos taxes constitute:

- effective tax rate – $t_{BB} = 26\%$;
- on royalties as obtained from abroad $t_{I_{ABB}} = t_{I_{CBB}} = 24\%$, royalties $t_{R_{ABB}} = t_{R_{CAA}} = 24\%$;
- on repatriation of dividends $t_{S_{BAB}} = 10\%$, interest $t_{I_{BAB}} = t_{I_{BCB}} = 10\%$ and royalties $t_{R_{BAB}} = t_{R_{BCB}} = 10\%$.

In the Russian Federation:

- effective tax rate – $t_{AA} = 48\%$;
- on obtained from a foreign company: dividends $t_{S_{BAA}} = 13\%$, interest $t_{I_{BAA}} = t_{I_{CAA}} = 20\%$, royalties $t_{R_{BAA}} = t_{R_{CAA}} = 20\%$;
- on repatriation of interest $t_{I_{ABA}} = t_{I_{ACA}} = 20\%$, royalties $t_{R_{ABA}} = t_{R_{ACA}} = 20\%$.

Let us adopt, that the total amount of rate-of-return in territories *A* and *B* is equal and constitutes conditionally 100 units.

Let us also consider effects from application of CT rule (meanwhile, without taking into account CFC and TC). In connection with application of CT rule in the Russian Federation, suppose, that the government restores for taxation purposes 100% of

withdrawn income or $\varphi_g^A = 1.$. Laos Government does not apply CT rule which means that it does not adjust them, i.e. $\varphi_g^B = 0.$ Suppose also, that the parent company and the subsidiary make corrections and make "shadow" withdrawal of 20 units of active income to jurisdiction *C*, 5 units of royalty and interest payments are withdrawn for each of the following: from jurisdiction *A* to *C*, from jurisdiction *B* to *C*, from jurisdiction *C* to *A*, as well as from jurisdiction *C* to *B*. Besides, suppose that, 5 units of passive income (royalties, interest) are remitted from jurisdiction *A* to *B* and from jurisdiction *B* to *A*.

Also, it is worth mentioning that in case of entering into force a double tax treaty between Russia and Laos, it will be nulled with the use of tax-credit method.

From MNC perspective, by substituting to (8) we obtain the following:

$$D_A^m + D_{S_{AB}}^p + D_{CA}^p + F_{AC} = D_{S_{BA}}^m + D_{BA}^p + D_{S_{CB}}^p + F_{BC} + \Delta;$$

$$(70,0 - 30,0 - 33,6) + (10,0 - 3,4) + (20,0 - 10,0 - 4,0) + (40,0 - 2,0) =$$
$$= (70,0 - 30,0 - 24,9 + 10,7) + (10 - 2) + (20 - 10 - 5,4 + 2,7) + (40,0 - 1,0) + \Delta;$$
$$6,4 + 6,6 + 6 + 38,0 = 25,8 + 8 + 7,3 + 39,0 + \Delta;$$
$$19,0 + 38,0 = 41,0 + 39,0 + \Delta$$
$$\Delta = -23,0.$$

Calculation outcomes demonstrate that at such source data, it has direct economic sense to invest into a subsidiary in Laos, so far as the income which remains after taxation constitutes a value which is substantially larger than the same when operating in the home country (41.0>19.0 units). When accounting of "shadow" revenue (38.0 and 39.0 units), delta remains practically unchanged (23.0 units, while it constituted 22.0 units).

In such situation advantages of opening a subsidiary in Laos are conditioned by the fact that the jurisdiction of the parent company, having applied CT rules, additionally attracts to taxation the income withdrawn in the amount of 16.4 units (or does not allow to save on taxes as Laos does), as well as by a less effective tax rate in Laos. At the same time, the amount of withdrawn revenues is equal (it is insignificantly decreased by taxes on repatriation: in jurisdiction *A* - by 2 units, in jurisdiction *B* - by 1 unit).

As well, due to subsidiary's manipulations with taxes the government of jurisdiction B receives to its budget taxes by 12.7 units less than due. Besides, the government of country *A* also loses 0.7 unit of tax on dividends. As a result, totally MNC saves 13.4 units which constitutes approximately 7% of all their income from three territories (total revenue is 200 units).

On the basis of the above said, a conclusion can be made that the amount of income which remains in the parent company's disposal was not effected by counter-acting measures represented as CT rules as applied by the government of country *A*. Amounts of the income withdrawn by the economic agent are somewhat equal to subsidiary's operating results in Laos, although its government is loyal to such transactions and does not enter restricting rules. Besides, for the parent company the situation is getting complicated due to additional taxation on part of the government of country *A*.

However, if analysing the situation in terms of national welfare, one can come to substantially other conclusions.

For that purpose, let us make a calculation with variable parameters as identical to a previous scenario, substituting them to (14) (see also remark 1):

$$D_{ABC}^{w1} = D_{ABC}^{w2} + \Delta;$$

$$6,4 + (25,8 + 7,2 + 6,6 + 8) + 6 + (44,5 - 0,7) =$$
$$= 20,8 + (25,8 + 7,2 + 6,6 + 8) + 8 + (44,5 - 17,1) + \Delta;$$
$$6,4 + 47,6 + 6 + 43,8 = 20,8 + 47,6 + 8 + 27,4 + \Delta;$$
$$60,0 + 43,8 = 76,4 + 27,4 + \Delta;$$
$$103,8 = 103,8 + \Delta;$$
$$\Delta = 0.$$

In the first case (if *A* applies CT rules) the total revenues of territory A from operations in jurisdictions *A*, *B*, *C* constitute 103.8 units, including:

- tax revenues of the government - 43.8 units;

- revenues of the parent company - 60.0 units (obtained from territories *A* – 6.4, *B* – 47.6, including dividends 39.6, *C* – 6.0).

In the second case (if *A* does not applies CT rules) the total income of territory *A* from operations in jurisdictions *A*, *B*, *C* have not changed in general and constituted 103.8 units, but they are re-distributed between MNC and government:

- tax revenues of the government - 27.4 units;

- revenues of the parent company - 76.4 units (obtained from territories *A* – 20.8, *B* – 47.6, (including dividends 39.6), *C* – 8.0).

Thus, it becomes obvious that CT rules in perspective of country *A* welfare are ineffective, so far as in general revenues have not changed $(\Delta = 0)$. Total "shadow" revenues in both scenarios as withdrawn to jurisdiction *C* remained unchanged and constituted 77.0 units (from territories *A* – 38.0, *B* – 39.0).

It is worth mentioning, that if jurisdiction *A* would be able not to lose or to return revenues from territory *C*, the global revenues of the country from territories *A*, *B* and *C* would constitute 180.8 units.

The performed calculations allow to make a conclusion that in case if the government of the parent company is unable to return capitals or to prevent their outflow, the total revenue of territories *A* and *B* without taxes would constitute 60.0 units, which is considerably less than volumes of "shadow" revenues within offshore jurisdiction *C* - 77 units. Besides, governments of countries *A* and *B* lose 13.4 units of taxes (and this is considering that government of country A applies CT rules which somewhat restore the taxable base, however, in general, they are uneffective as a "shadow" revenue return method).

This evidences that when applying CT rules, jurisdiction *A* returned 16.4 units of income as taxes; but this is incomparable with the fact that territory *A* lost 77 units of withdrawn "shadow" revenues (inluding the revenues not-returned to country *B*, which would have finally returned to country *A* as dividends). As a result, income of territory A,

notwithstanding introduction of CT rules, shall shrink almost twice (from 180.8 to 103.8 units).

It is also necessary to point out that in connection with problems relating to establishment of market values and, respectively, with efficiency of CT rules application in operations with intangible assets - $\varphi_g^A \to 0,$, which means that jurisdiction *A* may also lose income as reconstituted taxes. This states about a necessity to improve CT rules in this direction.

3. Discussion

The given calculations demonstrate a difference in the considered statements:

a) from perspective of MNC - there are assessed net and "shadow" revenues of MNC, where they were not obtained;

b) from perspective of country welfare - only those revenues of MNCs and governments are assessed, which work for demands of the given territory.

From perspective of revenues of territories - return of withdrawn "shadow" revenues has the most substantive significance. So far as from perspective of total MNC income, the income is not only exempted from taxation, but it is also transferred to other territories; however, given that, MNC income does not shrink, but vice versa - it increases for the account of saved taxes. Therefore, from perspective of country welfare the exempted income considerably reduces it, whereas, restored taxes (even when restored in full) cannot reimburse those losses.

Predecessors (see for example, Grubert (2003); Vernon (1998); Krasnov (2013); Celestin (2000); Bhat (2009)), have already provided substantiated recommendations as to improvement of MNC taxation. In particular, in their works, some scholars stated suggestions about proceeding to fractional method of MNC taxation. European Commission's draft report "Company taxation in the internal market" as was originally

edited in 2001, actually substantiated fractional method for MNC taxation in EU countries (European Commission (2016).

However, they were focused on the matters of tax evasion and income correction by companies. However, our aspect of view is different, so far as it is not only about and not merely about tax revenues of the state, but it is about income and capitals of MNCs which are withdrawn and do not participate in improvement of national welfare.

The main conclusion by H. Grubert (Grubert (2003), which proceeded from establishing the company income equilibrium, was that multinational MNC strategies with the use of aggressive tax-planning schemes (and first of all, in operations with intangible assets) have the determinative effects upon effective tax burden over trans-border investments. And that such approach from governments may be definitive in the behaviour of the host country, when imposition of tax burden upon different types of companies depends on their coontribution to the national welfare. We agreed with the statement and proceeded further, but, given that, firstly, we focused on evaluating acts of MNC from perspectives of national welfare and, secondly, we considered efficiency of measures of tax-planning counter-acting rules on part of governments (these are not considered by H. Grubert).

From perspective of the presented approach, there is stressed the importance of forming-up such rules for MNC tax-planning counter-acting, which would focus not on taxes as such, but would foster keeping capitals within the territory and/or would facilitate the return of earlier divested income. Within this context, it is expedient to pay more attention, for example, to secondary adjustments rule (SA) in combination with the minimal taxation at income return. That is, the task is to sacrifice taxes, but to receive foreign-currency proceeds for country's benefit and, specifically, from high-tech companies which have digital capacities for income withdrawal.

Conclusion

One of the main problems of international taxation of MNC is tax-free outflow of

capitals and income of MNCs, as a result of their use of tax-planning methods, including those connected with development of digital economy.

In order to justify ways on counter-acting MNCs' tax planning as well as on forming up the national scheme of international taxation which would be favourable for preservation and attraction of capitals, there have been developed economic-mathematical models which develop predecessors' approaches.

Out of various model types which are usually applied in this area, for the purposes hereof, we have selected and suggested that there should be used models with balance being postulated, where trilateral financial structures (with participation of intermediary subsidiaries in convenient jurisdictions and with participation of affiliated entities in offshore jurisdictions) are considered.

The models allow analysing various tax-planning methods on part of MNC as well as various ways to counter-act tax-planning on part of governments. But their principle peculiarities are that, firstly, there is suggested an approach that is aimed at establishment of final results of international taxation from perspectives of national economies, when they take account of both indices of private (economic agents) and public (government) economy sectors, which characterise aggregate resources of economic development, which remain in the country and which inflow from abroad. And, secondly, that both measures of tax planning on the part of MNCs and counter-acting measures to tax planning on the part of governments, are taken into account as a complex.

Approbation of developed models (case study - CT rule which has fundamental significance for counter-acting MNC tax-planning) has evidenced the following.

(1) From perspective of MNC's economic interests, government's strict measures, like CT rules, may have direct negative effect. I.e. the more effective the rules function, the less income remains in company disposal in the home jurisdiction, so far as it is re-distributed in government's favour as taxes. As a consequence, MNC is interested to widen its activity in convenient and offshore jurisdictions in prejudice of the home one, which helps it to evade the effect of CT rules. Thus, for the government the final outcome of CT rules may be negative, so far as instead of additional revenues, it is at a risk of getting

a shrinking tax basis and a reduction in budget revenues. From the perspective of national welfare, the outcome is much more negative, so far as the country can lose both revenues and capitals of MNCs (as a consequence - jobs, production volume, etc.) and tax revenues.

And there is another important matter. Principally, CT rules function poorly with respect to intangible assets, so far as under advanced development of digital economy it is very difficult to justify conventional "market" price for them. This means that MNCs can always find mechanisms of exemption of a part of income from taxation with the use of transfer pricing method for intangible assets, and therefore, country's welfare will decline even more also due to tax reasons. In this relation, it is compulsory to improve them, including with the use of features of artificial intellect which is able to analyse large-volume databases and which will provide necessary information to competent agencies of the states concerned therein. However, given that, it is necessary to thoroughly consider whether it is expedient to invent more rigid CT rules, or to provide considerable tax relief for certain kinds of activities, because taxes will be lost anyway, but besides that, income will also be withdrawn.

(2) National tax policy with respect to MNC to a great extent depends on tax policies of other countries with which it is tied by economic relations, so that under conditions when in the world there exist convenient jurisdictions and offshores which are engaged, in particular, in conjunctions *A-C* and *B-C*, strict anti-evasion measures in jurisdiction *A* (conjunction *A-C*) may not work, so far as capitals have a possibility to outflow through *A-B-C*; in its turn, this puts a question regarding global agreement of taxation rules;

(3) The problem is not only in taxes as such and their distribution among national jurisdiction. If, for example, taxes upon MNC are additionally charged in jurisdiction *A*, but the earlier withdrawn capital is not factually returned to country *A* from jurisdictions *B* and *C*, this has no great economic sense so far as this does not increase national welfare of territory *A*, but merely re-distributes GDP between the private sector and government in favour of the government (which usually results in crowding-out effect of private

capitals with governmental ones);

(4) For substantiating the international taxation scheme as favourable for economic growth, there should be further developed an approach from perspective of national welfare, which requires account of global income of MNC and its distribution by jurisdictions (including with the use of fractional method). So far as, as noted before, after all, it is not the taxes which are important, but where the real capital settles down and works, where jobs and production facilities are created, innovations are generated, etc.

But these conclusions are tentative and further studies are necessary.

Their general logic may be to widen model parameterisation for the purpose of performing a complex of computational experiments with various typical variants of changes in state regulation rules by taxation agencies (CT, CFC, TC, SA) and based on results, to perform economic interpretation of obtained outcomes (consequences of various regulation variants);

Upon outcomes of such widened experimenting, it will be possible to substantiate additional suggestions in the area of national tax policies as to capital attraction, retain and return with the use of a special combination of available tax tools (tax rates, rules, methods, benefits, etc.). Its use will also allow to update the real taxable base and its current distribution by jurisdictions.

But in general, it is important in further researches to focus specifically on income and capital flow as well as on public welfare, but not on taxes as such.

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Annexes

Remark. Decryption of formula elements in equilibrium models

$$D_A^m = D_{AC}^m - F_{AC}^m - T_{AC}^m + T_{AC}^{m+} =$$
$$= \{D_A(1 - d_{R_{AB}} - d_{I_{AB}} - d_{R_{CA}} - d_{I_{CA}})\} - \{D_A\varphi_{AC} + D_A(\varphi_{R_{AC}} + \varphi_{I_{AC}})\} -$$
$$-\{[D_A(1 - d_{R_{AB}} - d_{I_{AB}} - d_{R_{CA}} - d_{I_{CA}})]t_{AA}\} + \{D_A\Delta\varphi_{ACA}t_{AA} + D_A(\Delta\varphi_{R_{ACA}} + \Delta\varphi_{I_{ACA}})t_{AA}\};$$

$$D^{p}_{S_{AB}} = D^{p}_{S_{AB}} - T^{p}_{ABA} - T^{p}_{ABB} - T^{p_{AB}}_{S_{BAB}} - T^{p_{AB}}_{S_{BAA}} =$$
$$= [D^{I}_{S_{AB}} + D^{R}_{S_{AB}}] - [T^{I}_{I_{ABA}} + T^{R}_{R_{ABA}}] - [T^{I}_{I_{ABB}} + T^{R}_{R_{ABB}}] - [T^{I}_{S_{BAB}} + T^{R}_{S_{BAB}}] - [T^{I}_{S_{BAA}} + T^{R}_{S_{BAA}}] =$$
$$= \{D_{R_{AB}} + D_{I_{AB}}\} - \{D_{R_{AB}} t_{R_{ABA}} + D_{I_{AB}} t_{I_{ABA}}\} - \{D_{R_{AB}} t_{R_{ABB}} + D_{I_{AB}} t_{I_{ABB}}\} -$$
$$-\{D_{R_{AB}}(1 - t_{R_{ABA}} - t_{R_{ABB}}) t_{S_{BAB}} + D_{I_{AB}}(1 - t_{I_{ABA}} - t_{I_{ABB}}) t_{S_{BAB}}\} -$$
$$-\{D_{R_{AB}}(1 - t_{R_{ABA}} - t_{R_{ABB}}) t_{S_{BAA}} + D_{I_{AB}}(1 - t_{I_{ABA}} - t_{I_{ABB}}) t_{S_{BAA}}\};$$

$$D^{p}_{CA} = [D^{p}_{CA} - F^{p}_{CA} - T^{p}_{CA}] = [D^{I}_{CA} + D^{R}_{CA}] - [F^{I}_{CA} + F^{R}_{CA}] - [T^{I}_{CA} + T^{R}_{CA}] + [T^{I+}_{CA} + T^{R+}_{CA}] =$$
$$= \{D_{R_{CA}} + D_{I_{CA}}\} - \{D_{R_{CA}} \varphi_{R_{CA}} + D_{I_{CA}} \varphi_{I_{CA}}\} - \{D_{R_{CA}} t_{R_{CA}} + D_{I_{CA}} t_{I_{CA}}\} +$$
$$+\{D_{R_{CA}} \Delta\varphi_{R_{CAA}} t_{R_{CA}} + D_{I_{CA}} \Delta\varphi_{I_{CAA}} t_{I_{CA}}\};$$

$$F_{AC} = [(F^{m}_{AC} - T^{p}_{ACA} + F^{p}_{CA})] = [(F^{m}_{AC} - (T^{I}_{I_{ACA}} + T^{R}_{R_{ACA}}) + F^{I}_{CA} + F^{R}_{CA})] =$$
$$= \{[D_A \varphi_{AC} + D_A \varphi_{R_{AC}} + D_A \varphi_{I_{AC}}] - (D_A \varphi_{R_{AC}} t_{R_{ACA}} + D_A \varphi_{R_{AC}} t_{R_{ACA}})\} + \{D_{I_{CA}} \varphi_{I_{CA}}\} + \{D_{R_{CA}} \varphi_{R_{CA}}\}$$

$$D^{m}_{S_{BA}} = D^{m}_{BC} - F^{m}_{BC} - [T^{m}_{BC} - T^{m+}_{BC}] - [T^{m}_{S_{BAB}} - T^{m+}_{S_{BAB}}] - [T^{m}_{S_{BAA}} - T^{m+}_{S_{BAA}}] =$$
$$= \{D_B(1 - d_{R_{BA}} - d_{I_{BA}} - d_{R_{CB}} - d_{I_{CB}})\} - \{D_B \varphi_{BC} + D_B \varphi_{R_{BC}} + D_B \varphi_{I_{BC}}\} -$$
$$-\{[D_B(1 - d_{R_{BA}} - d_{I_{BA}} - d_{R_{CB}} - d_{I_{CB}}) t_{BB}] - [D_B \Delta\varphi_{BCB} t_{BB} + D_B \Delta\varphi_{R_{BCB}} t_{BB} + D_B \Delta\varphi_{I_{BCB}} t_{BB}]\} -$$
$$-\{[D_B(1 - d_{R_{BA}} - d_{I_{BA}} - d_{R_{CB}} - d_{I_{CB}})(1 - t_{BB}) t_{S_{BAB}}] -$$
$$-[D_B \Delta\varphi_{BCB}(1 - t_{BB}) t_{S_{BAB}} + D_B \Delta\varphi_{R_{BCB}}(1 - t_{BB}) t_{S_{BAB}} + D_B \Delta\varphi_{I_{BCB}}(1 - t_{BB}) t_{S_{BAB}}]\} -$$
$$-\{[D_B(1 - d_{R_{BA}} - d_{I_{BA}} - d_{R_{CB}} - d_{I_{CB}})(1 - t_{BB}) t_{S_{BAA}}]$$
$$-[D_B \Delta\varphi_{BCB}(1 - t_{BB}) t_{S_{BAA}} + D_B \Delta\varphi_{R_{BCB}}(1 - t_{BB}) t_{S_{BAA}} + D_B \Delta\varphi_{I_{BCB}}(1 - t_{BB}) t_{S_{BAA}}]\};$$

$$D^{p}_{BA} = D^{I}_{S_{BA}} + D^{R}_{S_{BA}} - [T^{I}_{I_{BAB}} + T^{R}_{R_{BAB}}] - [T^{I}_{I_{BAA}} + T^{R}_{R_{BAA}}] =$$
$$= D_{I_{BA}} + D_{R_{BA}} - \{D_{I_{BA}} t_{I_{BAB}} + D_{R_{BA}} t_{R_{BAB}}\} - \{D_{I_{BA}} t_{I_{BAA}} + D_{R_{BA}} t_{R_{BAA}}\};$$

$$D^{p}_{S_{CB}} = D^{I}_{CB} + D^{R}_{CB} - [F^{I}_{CB} + F^{R}_{CB}] - [T^{I}_{CB} + T^{R}_{CB}] +$$
$$+[T^{I+}_{CB} + T^{R+}_{CB}] - [T^{I_{CB}}_{S_{BAB}} + T^{R_{CB}}_{S_{BAB}}] + [T^{I_{CB}+}_{S_{BAB}} + T^{R_{CB}+}_{S_{BAB}}] - [T^{I_{CB}}_{S_{BAA}} + T^{R_{CB}}_{S_{BAA}}] + [T^{I_{CB}+}_{S_{BAA}} + T^{R_{CB}+}_{S_{BAA}}] =$$
$$= D_{I_{CB}} + D_{R_{CB}} - \{D_{I_{CB}}\varphi_{I_{CB}} - D_{R_{CB}}\varphi_{R_{CB}}\} - \{D_{I_{CB}}t_{I_{CB}} + D_{R_{CB}}t_{R_{CB}}\} +$$
$$+\{D_{I_{CB}}\Delta\varphi_{I_{CBB}}t_{I_{CB}} + D_{R_{CB}}\Delta\varphi_{R_{CBB}}t_{R_{CB}}\} -$$
$$-\{[(D_{I_{CB}} - D_{I_{CB}}t_{I_{CB}} - D_{I_{CB}}\Delta\varphi_{I_{CBB}})t_{S_{BAB}}] + [(D_{R_{CB}} - D_{R_{CB}}t_{R_{CB}} - D_{R_{CB}}\Delta\varphi_{R_{CBB}})t_{S_{BAB}}]\} +$$
$$+\{[(D_{I_{CB}}\Delta\varphi_{I_{CBB}}t_{I_{CB}})t_{S_{BAB}}] + [(D_{R_{CB}}\Delta\varphi_{R_{CBB}}t_{R_{CB}})t_{S_{BAB}}]\} -$$
$$-\{[(D_{I_{CB}} - D_{I_{CB}}t_{I_{CB}} - D_{I_{CB}}\Delta\varphi_{I_{CBB}})t_{S_{BAA}}] + [(D_{R_{CB}} - D_{R_{CB}}t_{R_{CB}} - D_{R_{CB}}\Delta\varphi_{R_{CBB}})t_{S_{BAA}}]\} +$$
$$+\{[(D_{I_{CB}}\Delta\varphi_{I_{CBB}}t_{I_{CB}})t_{S_{BAA}}] + [(D_{R_{CB}}\Delta\varphi_{R_{CBB}}t_{R_{CB}})t_{S_{BAA}}]\}$$

$$F_{BC} = [(F^{m}_{BC} + F^{I}_{CB} + F^{R}_{CB})] = [(F^{m}_{BC} - (T^{I}_{I_{BCB}} + T^{R}_{R_{BCB}}) + F^{I}_{CB} + F^{R}_{CB})] =$$
$$= \{[D_B\varphi_{BC} + D_B\varphi_{R_{BC}} + D_B\varphi_{I_{BC}}] - (D_B\varphi_{R_{BC}}t_{R_{BCB}} + D_B\varphi_{R_{BC}}t_{R_{BCB}})\} + \{D_{I_{CB}}\varphi_{I_{CB}}\} + \{D_{R_{CB}}\varphi_{R_{CB}}\}$$

Convergencia a NIIF: impactos en estructura financiera de los fondos de empleados del Departamento de Sucre – Colombia

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RESUMEN

En la presente investigación se evaluó el efecto de aplicar las Normas Internacionales de Información Financiera para Pymes en los fondos de empleados del Departamento de Sucre – Colombia, mediante la comparación de los principales indicadores financieros tanto para la norma internacional como en la norma local colombiana. Para lograr la comparación de las dos normas contables y para evitar los problemas de desempeño de los fondos, se tomaron los estados financieros al 31 de diciembre de 2014 bajo norma colombiana y el estado financiero para propósitos de conversión bajo norma internacional al 1 de enero de 2015. Adicionalmente se realizó una modelación para medir el impacto de la norma original NIC 32, en donde se reclasificaron los aportes sociales al pasivo. La investigación fue de carácter descriptiva, y para ello se tomó como base la información reportada por los fondos a la Superintendencia de la Economía Solidaria. Dentro de las principales conclusiones se encuentra que no se visualizan impactos significativos en la estructura financiera de los fondos de empleados de Sucre por el cambio de regulación contable hacia NIIF.

PALABRAS CLAVE: Fondos de empleados; Normas Internacionales de Información Financiera; convergencia; indicadores financieros; aportes sociales

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Convergence to IFRS: impacts on financial structure of employee funds of Sucre Department - Colombia

ABSTRACT

In the present investigation, the effect of applying the International Financial Reporting Standards for SMEs in the employee funds of the Department of Sucre - Colombia was evaluated, by comparing the main financial indicators for both the international standard and the Colombian local standard. To achieve the comparison of the two accounting standards and to avoid the performance problems of the funds, the financial statements were taken as of December 31, 2014 under Colombian standard and the financial statement for conversion purposes under international standard as of January 1, 2015. Additionally, a modeling was carried out to measure the impact of the original IAS 32 standard, where social contributions to the liabilities were reclassified. The investigation was descriptive, and the information reported by the funds to the Superintendence of the Solidarity Economy was taken as a basis. Among the main conclusions is that there are no significant impacts on the financial structure of Sucre employee funds due to the change in accounting regulation towards IFRS.

KEY WORDS: Employee funds; International Financial Reporting Standards; convergence; financial indicators; social contributions

Introducción

La convergencia de normas locales en Colombia, hacia Normas Internacionales de información financiera (en adelante NIIF), ha generado diferentes reacciones entre los sectores y usuarios de la información financiera, debido entre otros, a los cambios que estas generan en las bases de reconocimiento, medición y revelación con respecto al GAAP local, pudiendo alterar la estructura financiera y por ende los diferentes indicadores económicos (Arias y Sánchez 2014).

Este escenario no es ajeno a las empresas del sector solidario, que a partir 1 de enero de 2015 deben converger en forma obligatoria a NIIF, de acuerdo a la| Circular Externa 5 de 2014 de la Superintendencia de Economía Solidaria. Por ser los Fondos de Empleados entidades de carácter social y solidario que propende por satisfacer las necesidades colectivas de sus asociados y desde luego, preservar los aportes de los mismos, "las cooperativas y en general, las entidades del sector solidario, como las asociaciones

mutuales, han adquirido recientemente gran relevancia por su contribución en la economía del país, toda vez que estas instituciones son consideradas un elemento importante de desarrollo social, económico, cultural y ambiental" Morales, M. (2014 p.132)

Sin embargo, el sector cooperativo es el que levantó todo el revuelo, ya que originalmente la NIC 32 obligaba a que los aportes de los socios no se contabilizaran como capital social de la cooperativa, sino que dichos aportes deberían ser llevados como pasivos, porque existe un derecho del socio para, en caso de retiro, reclamar su reembolso, golpeando la estructura del patrimonio de las cooperativas (Álvarez B. y Suarez E. 2015). Finalmente, la norma colombiana decidió no aplicar este lineamiento de NIC 32, y dejar los respectivos aportes de los socios en el patrimonio. En este sentido bajo una metodología de investigación descriptiva, se pretende describir los posibles efectos del cambio a NIF, incluyendo la modelación con los preceptos originales de NIC 32.

La estructura del artículo empieza por describir algunos de los principales impactos a nivel mundial por la implementación de NIIF en el mundo y luego especificándolos en la economía solidaria, para continuar con la descripción del sector de la economía solidaria en Colombia finalizando con el análisis de los impactos en los indicadores financieros seleccionados por la implementación de NIIF, incluyendo la modelación por la aplicación de NIC 32.

1. Metodología

Este trabajo se desarrolla con una metodología de tipo descriptiva, ya que el análisis de la información lleva a cabo un análisis estructural, entendido como el estudio que permite tener una panorámica general de los distintos componentes de los estados financieros, es decir, el comportamiento de los elementos que constituyen cada uno de esos componentes y que se identifican como activos, pasivos, patrimonio, gastos e ingresos. Además, "la descripción científica se basa en el propósito de dar a conocer una información, un hecho, simplemente un dato, tal cual es, depurando al máximo las apreciaciones subjetivas del sujeto" (Cerda, 2002, p.75). Para lograr la medición de impactos por el cambio a NIIF, se tomaron los balances de transmisión a la superintendencia de economía

solidaría al 31 de diciembre de 2014 bajo (COLGAAP) y el estado de situación financiera de apertura para propósitos de conversión bajo NIIF (ESFA) al 1 de enero de 2015, de los fondos de empleados del Departamento de Sucre.

Para la medición de los impactos se realizaron análisis financiero, de los dos estándares a la misa fecha de corte, lo anterior para eliminar incongruencias en los resultados de los indicadores debido desempeño de las cooperativas. Los indicadores financieros utilizados son de liquidez, estructura y endeudamiento, cuyos resultados son comparados por los arrojados bajo COLGAAP y NIIF. Adicionalmente, para el análisis de los impactos de NIC 32 se realizaron una modelación, en donde se reclasificaron los aportes sociales al pasivo.

2. Evolución de las NIIF a nivel mundial

Una de las intenciones de los reguladores contables con la implementación de NIIF, es homologar las políticas contables, con el propósito de reducir problemas de comparabilidad, adicionalmente se pretende mejorar la calidad de la información contable, situación que se ha logrado con el proceso de implementación (Barth Landsman y Lang, 2008). Este proceso se inició en el año 1973, por iniciativa de algunos países europeos, sin embargo, la aceptación de las NIIF por parte de muchos países depende de la aceptación de los mercados de valores, situación que fortalecerá la expansión de las NIIF a nivel mundial. (Restrepo 2011).

De esta forma las NIIF han adquirido una verdadera connotación internacional, principalmente por el apoyo de instituciones como la Comunidad Económica Europea, el G20 y la Organización Internacional de Comisiones de Valores IOSCO. Inclusive la bolsa de valores de Nueva York (NYSE) permitió la presentación de los estados financieros bajo NIIF para los emisores foráneos. Es así como las recientes convergencias hacia las NIIF, que han sido llevadas a cabo por más de 100 países, se convierten en el hito más importante de los cambios de regulación en la historia de la contabilidad (Dasker, Hail, Leuz & Verdi, 2008).

Algunos de los estudios sobre el proceso de implementación de NIIF muestran resultados mixtos sobre la calidad e impactos sobre los estados financieros, se destacan el trabajo de Callao, S., Ferrer, C., Jarne, J., y Laínez, J. (2010) en el Reino Unido y en España, concluyeron que la aplicación de NIIF afectó negativamente la relevancia de los reportes financieros de estos países, entre otros, por la incapacidad de identificar los valores de mercado en los estados financieros de las distintas compañías. Por otro lado, se encuentran estudios como el de Pérez, R., Urquía, E. y Muñoz, C. (2009) acerca de la relación de éxito que tienen las pymes que se interesan por la implementación de las NIIF en España, por la connotación de que en ese país la implementación de NIIF para Pymes es voluntaria.

En Latinoamérica, las pymes venezolanas, Zapata, G., Hernández, A. (2010) indicaron que la problemática de implementación, gira alrededor de la norma tributaria y del cómo evitar sanciones más que en la línea de aspectos financieros o administrativos; lo anterior se evidencia por la estructura administrativa que tienen las pymes que es diferente a la de las empresas que cotizan en bolsa. Mientras tanto, Lima, R. (2007) argumenta que las pymes son un importante grupo de empresas que recoge la mayoría de las organizaciones, por lo que desde la academia se han tomado decisiones para profundizar más en las pymes y con ello fortalecer este sector de la economía e influir en instaurar normas contables que vayan acordes con las características que estas tienen.

Las variedades de estudios pasan también con la implementación por primera vez, es así como el trabajo realizado por Vásquez, N. (2013) en México sobre la NIIF 1, evidencian que las excepciones obligatorias que más aplicaron las empresas fueron las relacionadas con: estimaciones, contabilidad de coberturas y participaciones no controladoras.

En Chile, Silva, B. y Garrido, C. (2006) concluyen que la implementación de NIIF, busca ser el insumo para inversionistas de cualquier lugar del mundo para poder tomar adecuadas decisiones y así traer inversión extranjera. Adicionalmente, según Yáñez, V, Pilar, F. e Inestrosa, C. (2010), el proceso de implementación de NIIF implica para el profesional contable y financiero un desarrollo mucho más profundo de sus competencias y habilidades profesionales.

Uno de los estudios más amplios de implementación de NIIF, realizados en Latinoamérica, incluyendo a Colombia, es el realizado por Vásquez, N., Carril, M. y Pascual, M. (2013) en donde refuerzan que uno de los factores que influye para la adopción de NIIF es la existencia de una bolsa de valores fuerte, debido a la necesidad de los usuarios de la información financiera confiable.

Entretanto, Cañibano, L. y Gisbert, A. (2007) presentan un panorama de la obligatoriedad de algunos países vs el carácter voluntario y su impacto en las grandes empresas que cotizan en bolsa, mostrando que se mejora la presentación de información financiera bajo NIIF.

Finalmente, se encuentran trabajos como el de Torres, F. y Rodríguez, B. (2008) que evidencia más consecuencias desde el punto de vista conceptual y teórico, como el impacto de la nueva información financiera para su uso por parte de los distintos usuarios de la información, sin trascender al análisis de casos o eventos prácticos de aplicación de estándares en alguna temática cercana a las pymes del país.

En cuanto al proceso de adopción de NIIF en Colombia, a diferencia de países como los europeos, ha sido lento en la actualización de la normatividad contable, en especial, por parte del Consejo Permanente para la Evaluación de las Normas sobre Contabilidad, retrasando la incorporación a diversos tratados internacionales que exigen la preparación de estados financieros rigurosos, consistentes con indicadores de alta calidad y transparencia.

3. Impacto de las NIIF en el sector de la economía solidaria

La primera gran preocupación de la aplicación de NIIF para el sector solidario, es que las estas normas no pueden ser tomadas como base para la aplicación a los diferentes tipos de industrias o de sectores de la economía (Gómez, 2004), recordando que ni las sociedades cooperativas, son entidades que coticen en mercados bursátiles. De esta forma su implementación puede traer impactos financieros importantes de no tomarse un proceso serio de adaptación de las normas a la economía solidaría. (Castaño, C., Zamarra, J. y Correa, J., 2014) Estas incertidumbres se encuentran también en varios escritos de

carácter internacional, siendo la más importante de ellas la clasificación de las aportaciones sociales realizadas por los socios como pasivo financiero, cambiando así la actual estructura de capital social de las cooperativas ya que dichos aportes se contabilizan como patrimonio. A nivel nacional Rendón, B., Montaño, E. Gaitán, G. (2013) y Correa, J. y Ojeda, N. (2014), en sus investigaciones evalúan el efecto de aplicar la norma internacional de contabilidad (NIC 32), especialmente en lo relacionado con instrumentos financieros y los aportes sociales reconocidos y revelados por las entidades cooperativas redundando en el efecto de la estructura patrimonial de las mismas. Lo anterior ha generado mucha sensibilidad en el sector cooperativo y especialmente a los responsables de estas empresas ya que la estructura, composición del capital social y de los fondos propios a la luz de las NIIF cambiaría, generando un giro de ciento ochenta grados en su calificación patrimonial. (Polo, F., Cubedo, M., 2007); (Molina, R. 2007). La interpretación CINIC2 queda corta ante esta problemática ya que el reembolso de las aportaciones al capital social en caso de retiro del socio (implicando una reducción del capital) es una de las características de las cooperativas (Vargas Vasserot, 2007).

En este mismo sentido, Martínez, F. (2014), refiriéndose al caso de las cooperativas panameñas, deja sentada su preocupación de buscar un modelo, que sea propio a las cooperativas en cuanto a la implementación de las NIIF, este nuevo modelo debe desarrollar nuevas mediciones de instrumentos financieros ya que las exigibles por NIIF no aplican al sector, ya que han sido desarrolladas para el mercado de capitales. Así mismo, las sociedades cooperativas están jugando un rol importante en el proceso de convergencia contable internacional, en las cuales deberían tener en cuenta la realidad del sector con los principios y valores fundamentales como los solidarios (Alianza Cooperativa Internacional para las Américas, ACI-Américas, 2012).

Otro aspecto importante según Castaño, C., Correa, J. y Zamarra J. (2014) en el sector solidario es el cálculo de deterioro de la cartera, que se determina de acuerdo con el tiempo vencido a la tasa de referencia, contabilizándose el mencionado deterioro, mediante una provisión, según el mecanismo de la administración de riesgo crediticio (SARC). El estándar internacional exige que al final de cada periodo, se debe realizar una evaluación

para determinar la provisión por deterioro de cartera, medida al costo o al costo amortizado. Ahora, al entrar en vigencia el SARC, quedaría eliminada la clasificación por edades de acuerdo con la Circular Básica Contable y Financiera, no obstante, se podría presentar la cartera en una condición de mayor riesgo, de acuerdo a los criterios señalados en la norma. Para Cardozo, H. (2015), las normas o estándares internacionales obligan a establecer el deterioro individual de cada deudor mitigando la posibilidad de existir alguna contingencia de pérdida, en donde la entidad solidaria debe dejar evidencia en un formato especial en la cédula de cada deudor.

Por todo lo expuesto y ante solicitudes expresadas por la Superintendencia de la Economía Solidaria, en Colombia , se contempla una salvedad en la aplicación de las NIIF en relación con el tratamiento y deterioro de la cartera de las entidades sujetas a su inspección y vigilancia (NIC 39 y NIIF 9), el Consejo Técnico de Contaduría Pública (C.T.C.P), plantea que, dado que las estructuras financieras y de negocios de las cooperativas de ahorro y crédito vigiladas por la S.E.S., son similares a las cooperativas financieras y a las compañías de financiamiento, se le dé el mismo tratamiento señalado en el Decreto 1851 de 2013 para las entidades de crédito vigiladas por la Superintendencia Financiera, en aras de la equidad, que luego de un análisis de impacto de la aplicación de las NIIF en este sector solidario, el día 27 de julio de 2015, el (C.T.C.P), emitió el documento, llamado propuesta de excepción a la aplicación integral de las NIIF en el tratamiento de la cartera de crédito de las entidades vigiladas por la S.E.S., en la cual determina que es viable el establecimiento de una excepción en los estados financieros individuales o separados que permita a la S.E.S. mantener el modelo de provisión actual de la cartera de préstamos, mientras se implementa el modelo de administración de riesgo crediticio.

3.1. Economía solidaria en Colombia

Según los datos de la Superintendencia de Economía Solidaria., se estima que en Colombia el sector solidario cerró en 2014 con 4.708 entidades vigiladas, 5,67% menos que

en 2013. Según Cenicoop y Confecoop, la principal explicación a la reducción del número de entidades fue la salida de algunas cooperativas de trabajo asociados, debido a la implementación de medidas por parte de los entes de control con el fin de regular el uso indebido de este modelo cooperativo.

Del total de entidades que reportaron información en 2014, las más importantes son las cooperativas con el 57,3% y los fondos de empleados con el 35%. Véase (Tabla 1).

Las Cooperativas de Ahorro y Crédito que son solo el 4% tienen el mayor número de asociados con el 42%, sin embargo, generan menos empleos que las Cooperativas que con 42% de los asociados tienen el 37% de empleados.

En cuanto al tamaño, las mayores participaciones son las cooperativas con activos que representa el 43% del total, y a su vez son las que tienen mayores ingresos con 87%. En resultados las cooperativas también son las de mayores excedentes con el 41%; en cuanto a los excedentes resaltamos el comportamiento de los fondos de empleados que a pesar de tamaño pequeño (20%) generan excedentes que equivalen al 21% del sector.

Tabla II. Cifras Economía solidaria Colombia, 2004

(en millones de pesos)

Categoría	Activo	Pasivo	Patrimonio	Ingresos	Excedentes y/o pérdidas
Cooperativas	12.439.863	5.950.508	6.489.355	15.464.610	213.211
Cooperativas de Ahorro y Crédito	10.037.428	6.199.974	3.837.454	1.465.141	198.350
Fondos de Empleados	6.403.644	4.350.745	2.052.899	771.144	110.986
Asociaciones Mutuales	173.605	123.341	50.264	47.676	-673
Otras Organizaciones	30.820	6.607	24.213	44.448	717
Total	29.085.360	16.631.175	12.454.185	17.793.019	522.592

Fuente: Elaboración propia.

3.2 Fondos de empleados

Los fondos de empleados son empresas asociativas, de derecho privado, sin ánimo de lucro, constituidas por trabajadores dependientes y subordinados en donde la asociación y el retiro son voluntarios.

Cardozo, H. (2008) expresa que, "la disparidad de los Fondos de Empleados con las instituciones que ejercen actividad financiera radica en que sus asociados capitalizan su empresa, regularmente, a través de descuentos de nómina, dándole permanente liquidez a su función de intermediación, a la vez que reduce sus riesgos. Además, los Fondos de Empleados pueden imponer sanciones, incluso de orden social, a sus asociados, lo cual le da una ventaja sobre los bancos comerciales" (p.2). Dentro de las ventajas de los Fondos de Empleados, existe el hecho de estar cerca del trabajador y conocer sus problemas y necesidades. A diferencia de las entidades financieras que desconocen aspectos claves de la situación de sus clientes, generando asimetría en la información.

En Colombia, están registrados 1.646 fondos de empleados con 976.466 asociados los cuales generan 17.000 empleos aproximadamente, con un ratio de un empleado por cada 56 asociados, en la región Caribe este ratio parece excesivo, con una relación de un empleado por cada 22 asociados, a diferencia de la región Pacífica que tiene por cada 94 asociados un empleado.

La Región Caribe ocupa el tercer lugar en cuanto a presencia de fondos de empleados, con una participación en activos de $400.162 millones, siendo el 6,2%, del total país, en cuanto a excedentes reportan $10.524 millones y participan con el 9,48%. Dentro de la región Caribe el Departamento del Atlántico es el líder en cuanto a participación por tamaño de los fondos con el 65%.

Destacamos la relación activo-excedentes que muestra Sucre ya que posee el triple de excedentes que el Magdalena con la misma cantidad de activos, y el 18% más de excedentes que Córdoba que tiene el doble de activos. También es de anotar que, los fondos del Atlántico necesitan menor inversión de activo para generar excedentes.

Tabla III. Fondos de empleados, Regiones 2014

Región	# Fondos empleados	%	Asociados	%	Empleados	%
Amazonía	6	0,4%	1.232	0,1%	12	0,1%
Andina	1.247	75,8%	770.285	78,6%	13.460	77,3%
Caribe	121	7,4%	50.750	5,2%	2.276	13,1%
Orinoquía	12	0,7%	4.010	0,4%	50	0,3%
Pacífica	260	15,8%	153.189	15,6%	1.625	9,3%
Total	1.646	100%	979.466	100%	17.423	100%

Fuente: Elaboración propia.

Tabla IV. Resultados financieros de Fondos de Empleados, región Caribe, 2014

(en millones de pesos)

Departamento	Activo	Pasivo	Patrimonio	Ingresos	Excedentes y/o pérdidas
Atlántico	$ 260.922	$ 150.423	$ 110.499	$ 32.044	$ 7.571
Bolívar	$ 84.779	$ 63.700	$ 21.079	$ 9.681	$ 1.706
Cesar	$ 28.814	$ 12.465	$ 16.349	$ 3.400	$ 472
Córdoba	$ 12.539	$ 6.255	$ 6.284	$ 2.475	$ 287
Sucre	$ 5.763	$ 1.559	$ 4.203	$ 902	$ 351
Magdalena	$ 5.327	$ 2.400	$ 2.927	$ 663	$ 112
Guajira	$ 2.018	$ 670	$ 1.348	$ 273	$ 26
Total	$ 400.162	$ 237.472	$ 162.689	$ 49.438	$ 10.524

Fuente: Elaboración propia.

En cuento a los fondos de empleados del Departamento de Sucre, para el año 2014, cuenta con 5 fondos al cual pertenecen 645 asociados, generado 8 empleos directos con un ratio de 80 asociados por empleo. Poseen activos totales por $5.763 millones y excedentes de $351 millones. (Tabla 7).

Destacamos que FEHORES tiene el 71% más de excedentes que FEPEC que tiene 51% más de activos; y tiene aproximadamente los mismos excedentes que LICAPEFE que cuenta con el 25% más de activos, sin embargo, el FEUS es el fondo más importante en todas sus variables.

Además, se observa que el activo de FEHORES es financiado el 63% por el pasivo, debido a que gran parte de la cuota periódica obligatoria es destinada a depósito de ahorro permanente, más los ahorros voluntarios. Caso contrario ocurre con FEDECATOL, FEUS, FEPEC y LICAPEFE donde el patrimonio financia el 61,55%, 82,48%, 72,94% y 63,89%, respectivamente.

Tabla V. Fondos de Empleados del departamento de Sucre, 2014 (millones de pesos)

Sigla	Asociados	Empleados	Activo	Pasivo	Patrimonio	Ingresos	Excedentes y/o Perdidas
FEDECATOL	93	1	$1.056	$407	$650	$148	$68
FEUS	285	4	$3.225	$565	$2.660	$500	$209
FEHORES	103	1	$393	$248	$145	$66	$29
FEPEC	106	1	$595	$161	$434	$126	$17
LICAPEFE	58	1	$493	$178	$315	$61	$28
Total	645	8	5.763	1.559	4.203	902	351

Fuente: Elaboración propia.

4. Análisis financiero NIIF - Col GAAP y Modelación

En un entorno competitivo para la empresa de hoy, independientemente del sector al que pertenezca, es importante conocer su situación financiera para tomar decisiones que le permitan alcanzar sus objetivos y metas fijadas. Por lo que no es suficiente contar solo con la información contable, sino que se requiere interpretarla y analizarla para entender el origen y comportamiento de los recursos de la empresa; es por esto, que surge la necesidad del análisis financiero. De acuerdo a García, O. (1999), Castaño, C. y Arias, J. (2013) y Correa, J. y otros (2010), el diagnóstico financiero o análisis financiero comprende el estudio e interpretación de la información proporcionada por la contabilidad, e inclusive toda la información disponible, contextualizada y estructural, que sea cuantitativa y cualitativa, histórica y proyectada, para tratar de determinar la situación económico-financiera de la empresa o de un área específica de ésta, haciendo uso de técnicas, entre otras, de los indicadores financieros para llegar a conclusiones más complejas en un entorno dinámico de la empresa.

Para el caso concreto de los Fondos de Empleados y de acuerdo a la Circular Contable y Financiera N° 004 de 2008, el análisis financiero para una organización solidaria, debe evaluar el desempeño financiero y operacional, es necesario la aplicación de indicadores, lo que permitirá a los administradores tomar decisiones en cualquier momento del ejercicio contable. Según García, O., Legis Editores S.A. (2015), los indicadores financieros de propósito especial, permiten conocer aspectos como la liquidez, rotación, solvencia, rentabilidad y endeudamiento del ente evaluado.

En este capítulo se describen los resultados de los indicadores financieros bajo COLGAAP y NIIF, aplicable en Colombia a los fondos de empleados del Departamento de Sucre, tanto par el riesgo de liquidez, cartera, financiero, estructura y operacional, con el propósito de observar el resultado bajo Colgaap y por la convergencia a NIIF.

Adicionalmente se describe los resultados de la modelación realizada por los autores, que consiste en el re cálculo de los indicadores financieros, tomando como base las NIIF

FULL, es decir considerando entre otros los aportes sociales como pasivo y no como patrimonio.

Los indicadores aplicables a los fondos de empleados, hacen uso de umbrales que reflejan la presencia o ausencia de amenazas que afectan el nivel de salud financiera, y se presentan como indicadores de color. Los tres colores que permite la Superintendencia de Economía Solidaria son: el verde, el amarillo, y rojo. El verde indica que la entidad tiene vía libre para desarrollar sus actividades, y se considera como buena "salud" financiera, el color amarillo indica precaución y análisis de probables situaciones que afectan el desarrollo de las actividades y el color rojo, indica posee problemas en la viabilidad o desarrollo de sus actividades, es decir tiene amenazas contundentes o definitivamente cesa de sus intenciones operacionales

4.1. Indicadores de Riesgo de Liquidez

Según los resultados arrojados por los indicadores de riesgo de liquidez, los fondos en estudio están dentro del umbral VERDE en el fondo de liquidez y el nivel de disponible e inversiones, en los tres análisis. (Véase tabla VI). Hay una variación en número de veces en razón corriente, en prueba ácida y solidez por la reclasificación de las cuentas convenios por cobrar, intereses, responsabilidades pendientes. Al implementar las NIIF la capacidad para responder a sus obligaciones a corto plazo ha disminuido, por ejemplo, en razón corriente bajo COLGAAP los fondos contaban con $3,40 por $1 adeudado al corto plazo como respaldo de sus obligaciones, y bajo NIIF contaban con $3,26 por $1 adeudado. Por otra parte, los indicadores de prueba ácida y de solidez bajo COLGAAP muestra que los fondos contaban a corto y largo plazo con $2,97 y $3,70 respectivamente por $1 adeudado, y bajo NIIF mejoró a $3,03 y $3,71 respectivamente. Pero al hacer la modelación, según el indicador de solidez la capacidad de los fondos para cubrir sus obligaciones a corto y largo plazo desmejoró significativamente, disminuyendo a $1,31 por cada peso que adeuda.

Sin embargo, los resultados finales de los índices del grupo de liquidez prácticamente no cambian por el efecto de la implementación de NIIF, ni tampoco en la respectiva modelación de NIIF FULL.

Tabla VI. Indicadores de Riesgo de Liquidez

Indicador	Cálculo	Colgaap	Umbral Colgaap	NIIF	Umbral NIIF	Modelación NIIF	Umbral Modelación
Fondo de Liquidez	Disponible / Total Depósitos	5.18%	Verde	5.18%	Verde	5.18%	Verde
Nivel de Disponible e Inversiones	Disponible + Inversiones / Total de Activos	12.01%	Verde	12.03%	Verde	12.03%	Verde

Fuente: Elaboración propia a partir de datos de fondos de empleados del depto. de Sucre que reportaron información de convergencia a NIIF para Pymes a la Superintendencia de economía solidaria. (La modelación se realizó tomando los aportes de capital como pasivos).

4.2. Indicadores de Riesgo de Cartera

De acuerdo a los indicadores de riesgo de cartera aplicados bajo COLGAAP, NIIF y modelación, los fondos de empleados en estudio se encuentran en el umbral AMARILLO en cuanto a la cobertura de provisión general, presentando una leve disminución debido al aumento de la cartera de créditos. La cobertura de inversión de ahorros arroja un aumento de 0,1 veces debido a los ajustes por convergencia en la cuenta créditos de consumo, otras garantías - con libranza y reclasificación de los intereses. Para los indicadores de Cartera el impacto de NIIF y modelación con referencia a COLGAAP no es evidente ya que el indicador queda en umbral VERDE en los tres escenarios y su variación no es significativa

Sin embargo, teniendo en cuenta los resultados del indicador de cobertura de provisión general, es necesario que los fondos hagan un replanteamiento de la recuperación de la cartera.

Tabla VII. Indicadores de Riesgo de Cartera

Indicador	Cálculo	Colgaap	Umbral Colgaap	NIIF	Umbral NIIF	Modelación NIIF	Umbral Modelación
Cobertura Provisión General	Provisión Cartera / Total Cartera Bruta	0.55%	Amarillo	0.54%	Amarillo	0.54%	Amarillo
Cobertura de inversión de ahorros	Cartera Bruta / Depósitos	3.7	Verde	3.8	Verde	3.8	Verde

Fuente: Elaboración propia a partir de datos de fondos de empleados del depto. de Sucre que reportaron información de convergencia a NIIF para Pymes a la Superintendencia de economía solidaria. (La modelación se realizó tomando los aportes de capital como pasivos).

4.3. Indicadores de Riesgo Financiero

El indicador de disminución patrimonial refleja una leve variación de COLGAAP a NIIF debido al aumento en los excedentes y/o pérdidas acumulados por adopción por primera vez. Pero en cuanto al resultado de la modelación que es de 59,11 siendo la variación significativa, lo anterior es debido principalmente a la reclasificación de los aportes sociales temporalmente restringidos al pasivo, sin embargo, no afecta el umbral en el que se encuentran los escenarios antes indicados, es decir, VERDE, posiblemente debido a que los fondos de empleados del departamento de Sucre, tienen suficientes recursos en otros rubros de patrimonio como son la cuenta de reservas con $768.3 millones y fondos de destinación específica con $216.3 millones, adicionalmente para el año de estudio los fondos obtuvieron resultados del periodo representativos dentro del total de patrimonio siendo de $350.3 millones. Sin embargo, como parte de las estrategias de cada fondo, estos

dineros pueden ser distribuidos en reservas fortaleciendo el componente patrimonial o se pueden usar en distintos beneficios para los asociados.

Por otra parte, el indicador de activo productivo muestra una leve disminución debido al aumento del activo por los ajustes mencionados en indicadores anteriores.

En resumen, los indicadores de riesgo financiero están en el umbral VERDE en los tres escenarios, lo que es favorable para estos fondos, sin mostrar impactos importantes por la convergencia a NIIF

Tabla VIII. Indicadores de Riesgo Financiero

Indicador	Cálculo	Colgaap	Umbral Colgaap	NIIF	Umbral NIIF	modelación NIIF	umbral modelación
Disminución patrimonial	Patrimonio / Capital Social	1.47	Verde	1.46	Verde	59.11	Verde
Activo productivo	Activos productibles / Total de Activos	88%	Verde	89%	Verde	89%	Verde

Fuente: Elaboración propia a partir de datos de fondos de empleados del depto. de Sucre que reportaron información de convergencia a NIIF para Pymes a la Superintendencia de economía solidaria. (La modelación se realizó tomando los aportes de capital como pasivos).

4.4. Indicadores de Riesgo de Estructura

En los indicadores de riesgo de estructura aplicados bajo Colgaap, NIIF y modelación, existe variaciones importantes, debido a los ajustes por convergencia a NIIF y en la modelación de NIIF FULL, realizados en los rubros cartera de créditos y activos materiales, y en la cuenta aportes sociales temporalmente restringidos, el cálculo de

aportes sociales mínimos no reducibles, y la reclasificación de aportes sociales temporalmente restringidos, para el caso de la modelación.

En cuanto al indicador de Endeudamiento el resultado del umbral es VERDE tanto para Colgaap como NIIF, sin embargo, en el caso de la modelación el resultado del umbral es ROJO el cual desmejora por la reclasificación de los fondos sociales. En cuanto al indicador aporte social sobre activos, para los casos Colgaap y NIIF es ROJO, y en la modelación mejora sustancialmente, pasando al umbral VERDE. Debido principalmente a la maximización de los activos no circulantes.

En este conjunto de indicadores y especialmente en el de endeudamiento se ve muy afectado en el proceso de modelación por lo que se considera que fue adecuada la medida tomada por la Superintendencia de Economía Solidaria de dejar los aportes sociales temporalmente restringidos en el patrimonio.

4.5. Indicadores de Riesgo de Endeudamiento

El indicador de endeudamiento total muestra que los activos de los fondos están siendo financiados en un 27% con los pasivos, con la implementación de las NIIF esta financiación tiene una disminución debido a ajustes en cuentas del activo, mencionados en indicadores anteriores. Dicho indicador aumenta significativamente al hacer la modelación ubicándose en 76% por la reclasificación de los aportes sociales temporalmente restringidos al pasivo. En cuanto al indicador índice de propiedad se refleja un aumento, pasando de 72,94% bajo Cogaap a 73,04% bajo NIIF, como resultado del incremento del activo y de la cuenta excedentes y/o pérdidas acumuladas por adopción por primera vez, reflejando que el apalancamiento con el patrimonio es mayor. Caso contrario sucede con la modelación, donde el apalancamiento con patrimonio es de 24%.

Teniendo en cuenta que el indicador de endeudamiento ideal debe estar situado entre el 40% y el 60%, podemos decir que para los dos primeros escenarios los fondos pueden estar incurriendo en un exceso de capital ocioso, con la consiguiente pérdida de rentabilidad de sus recursos. Por el contrario, para el caso de la modelación el indicador de

endeudamiento arroja un resultado mayor al 60% lo que significa que los fondos están soportando un excesivo volumen de deuda.

Adicionalmente, destacamos que, con la modelación el apalancamiento de los activos se invierte, en el entendido de que bajo Colgaap y NIIF estaba mayormente financiado por el patrimonio, y bajo modelación son financiados mayormente por el pasivo.

Tabla IX. Indicadores de Riesgo de Estructura

Indicador	Cálculo	Colgaap	Umbral	NIIF	Umbral	Modelación NIIF	Umbral modelación
Endeudamiento sin Ahorro Permanente	Total Pasivo - Fondos sociales + Depósitos / Total Activo	1.78%	Verde	1.78%	Verde	50.96%	Rojo
Depósitos sobre Activos	Depósitos / Total Activos	23.09%	Rojo	23.01%	Rojo	23.01%	Rojo
Aporte Social sobre Activos	Aporte Social / Activo Total	49.77%	Rojo	49.59%	Rojo	1.22%	Verde
Capital Institucional sobre Activos	Patrimonio - Capital Social) / Activo Total	23.18%	Verde	23.45%	Verde	23.45%	Verde

Fuente: Elaboración propia a partir de datos de fondos de empleados del depto. de Sucre que reportaron información de convergencia a NIIF para Pymes a la Superintendencia de economía solidaria. (La modelación se realizó tomando los aportes de capital como pasivos).

Tabla X. Indicadores de Riesgo de Endeudamiento

Indicador	Cálculo	Colgaap	NIIF	Modelación NIIF
Endeudamiento total	Pasivo Total / Activo Total	27.06%	26.96%	76.14%
Indice de Propiedad	Patrimonio / Activo	72.94%	73.04%	23.86%

Fuente: Elaboración propia a partir de datos de fondos de empleados del depto. de Sucre que reportaron información de convergencia a NIIF para Pymes a la Superintendencia de economía solidaria. (La modelación se realizó tomando los aportes de capital como pasivos).

Conclusiones

El contenido de la NIC 32 plantea un cambio en la forma tradicional de contabilización del capital social en las entidades de la economía solidaria, de acuerdo a la modelación realizada, este tratamiento contable de las aportaciones de los socios como pasivos en vez de patrimonio neto, aumenta el endeudamiento y deterioro de su solvencia, con efectos negativos en las calificaciones de riesgos, adicionalmente se afecta negativamente la estructura financiera de los fondos. Este aspecto es especialmente relevante para las grandes cooperativas, en las que tienen gran importancia los indicadores de solvencia o las calificaciones de las agencias. En este mismo sentido deduce que, debido a un incremento a causa de recibir los aportes sociales como pasivo exigible y pasar a convertirse en depósitos, estos causarán un mayor costo de interés por la prima de seguro de los depósitos, lo cual implica gastos que se verán reflejados en el Estado de Resultados y terminarán afectando los excedentes. Adicionalmente este tipo de entidades se van a

encontrar en una situación de desventaja frente a otras formas de asociación cooperativa que desde su constitución cuentan con una determinada cifra de recursos propios.

Desde este punto de vista, consideramos acertada la decisión de la Superintendencia de Economía Solidaría de dejar los aportes sociales dentro del patrimonio modificando la NIC 32 y la IFRIC 2. Evitando impactos en su estructura y endeudamiento. Adicionalmente consideramos procedente recomendar que estas entidades, en su proceso de convergencia a NIIF, realicen una actualización de sus estatutos con el fin de adecuar y aumentar el capital mínimo irreducible, de tal manera que permitan o posibiliten que su estructura de financiación y, por tanto, sus posibilidades de operación y márgenes de liquidez no se vean afectadas duramente al disminuirse de manera considerable el patrimonio, vía traslado de aportes sociales a pasivos exigibles y el posterior retiro de estos. En definitiva, los fondos de empleados deben asumir el proceso de convergencia a NIIF con disciplina ya que es necesario ser muy precisos en la definición de sus políticas contables. Por lo que se infiere una vez analizados los diferentes indicadores para los tres escenarios, a manera de sugerencia para los diferentes fondos, como organismos de control y supervisión, es que los aportes sociales temporalmente restringidos permanezcan en el patrimonio como lo establece la normativa colombiana.

De otro lado el cambio de Colgaap a NIIF no se observan variaciones importantes en cuento a los indicadores de liquidez, cartera, riesgo financiero, estructura y endeudamiento ya que en los dos escenarios todos los indicadores se mantienen en el umbral verde, por lo que se infiere que no hubo ningún impacto por el cambio de política contable.

Ahora, a manera de ahondar aún más en la problemática, sería pertinente plantear una investigación del comportamiento de los entes pertenecientes al sector solidario, de los países latinoamericanos, en donde se socialice los resultados obtenidos como experiencia, de haber adoptado la NIC 32.

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Organizational modeling in production processes of cluster profiles for urban environments

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ABSTRACT

One of the most important aspects of the development of the urban environment is the comprehensive reconstruction of the municipal development territories, with the aim of creating favorable living conditions and the effective use of the production, engineering, scientific, and other potentials of the complex of edification. The structural condition of many industrial buildings means that they can be operated for more than a decade. This coefficient sparks great interest in industrial buildings precisely for the purpose of their redistribution, rather than reconstruction or demolition combined with new construction. The objective of this study is to define an algorithm for organizational and technological construction, in order to determine the redistribution of industrial facilities. The methodology used refers to the dependency graphs of the relative time loss, versus the redistribution coefficient and also the economic efficiency of the project, versus the actual duration of the construction and installation. From this methodology an adequate mathematical model is introduced.

KEYWORDS: production organization, redistribution organization methods, redistribution coefficients, redistribution of industrial territories, the effectiveness of organizational and technological solutions.

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Modelado organizacional en procesos de producción de perfiles de clusters para entornos urbanos

RESUMEN

Uno de los aspectos más importantes del desarrollo del entorno urbano es la reconstrucción integral de los territorios del desarrollo municipal, con el objetivo de crear condiciones de vida favorables y el uso efectivo de los potenciales de producción, ingeniería, científicos, y otros del complejo de edificación. La condición estructural de muchos edificios industriales significa que pueden ser operados por más de una década. Este coeficiente provoca un gran interés en los edificios industriales precisamente con el propósito de su redistribución, en lugar de la reconstrucción o demolición combinada con una nueva construcción. El objetivo de este estudio consiste en definir un algoritmo para la construcción organizacional y tecnológica, a fin de determinar la redistribución de instalaciones industriales. La metodología utilizada se refiere a los gráficos de dependencia de la pérdida de tiempo relativa, versus el coeficiente de redistribución y también la eficiencia económica del proyecto, versus la duración real de la construcción y la instalación. A partir de esta metodología se introduce un modelo matemático adecuado.

PALABRAS CLAVE: organización de producción, métodos de organización de redistribución, coeficientes de redistribución, redistribución de territorios industriales, la efectividad de las soluciones organizativas y tecnológicas.

Introduction

The article deals with the principles of creating a unified system of modules interacting with each other in the implementation of projects for the conversion of industrial facilities. The authors describe the main criteria of forming a complex organizational system, which includes a large number of functional subsystems and modules related to investment, design, production and information components of the project structure. For decades, urban planning of various cities and megacities in the Soviet Union and later in Russia was formed on the same basic principles providing clearly distinguished contours of residential buildings, industrial areas, as well as forest areas and urban infrastructure. Over time, the urban environment absorbed new territories, developing not only geographically, but also forming new modern social requirements. Thus, new principles to design space-planning solutions of residential premises of apartment buildings and requirements for the arrangement of "green"

urban areas were formed. In addition, the approach to the preservation and development of urban Geoecology has changed significantly. Basically, this factor served as a basis for the formation of municipal programs for renovation of industrial areas that have an impact on the urban environment (Aliakbar et al., 2019; Daeyoung & Park, 2006; Sugiantiningsih et al., 2019; Zeibote et al., 2019).

By creating qualitative and quantitative characteristics of individual elements of the system under consideration, it is possible to formulate the basic requirements for the source data necessary to create a structured model of organizational design and project management. At the same time, the system should function reliably in the interaction of all integrated structures of the project under the influence of the external environment. The principles and nature of urban clusters are described in detail, their separate types, as well as the relationship and the main criteria for their functioning are highlighted.

1. Literature review

Organizational and technological models of re-profiling using expert assessments can be classified as follows:

1) Full redevelopment. This type of redevelopment implies a radical redevelopment of the territory and real estate, starting with the change in the purpose of the land, the approval of a new project and ending with the laying of new engineering networks and the organization of new transport interchanges (Eddelani et al., 2019). Full redevelopment involves a complex of marketing research, development of the project concept and its coordination, as well as elaboration of the architectural idea. Exclusively land is used in this type of redevelopment.

2) Partial redevelopment. This type of redevelopment involves the redevelopment of urban areas and some facilities, with the modernization or renewal of existing transport interchanges and utilities. In this case, it is not always carried out to change the purpose of the land, and the future project is often designed within the existing purpose, in some cases applying small adjustments. As a rule, office warehouse or logistics complexes with administrative buildings are developed in this way. In the case of partial redevelopment, existing land and some existing facilities are

used, which are usually undergoing reconstruction or modernization.

3) Surface redevelopment. This type of redevelopment, as a rule, does not imply serious, fundamental changes to the existing facilities. Either administrative buildings or separate workshops are subject to such redevelopment. According to this option, as a rule, warehouse complexes are built in cases where a radical change in transport routes, access roads and engineering infrastructure facilities is not required.

To get acquainted with the current state of affairs in the issue under study, as well as to study the latest developments, it is necessary to refer to scientific publications of domestic and foreign format.

According to Abramov who stresses the relevance of the topic adopted for the study, at present, well planned and competently staffed integrated structural construction units will help achieve a high level of reliability and labor productivity and avoid negative (extraordinary) situations during the construction period eventually ensuring improved project performance (Abramov, 2019).

In general redesigning is worthy of attention by the method of reforming the structures and management functions in an enterprise in order to solve the problems of adapting to the conditions of uncertainty and rapid changes in the external environment.

The process of enterprise re-profiling can be represented in three stages:

1) Situational analysis and planning of the program for restructuring measures;

2) Implementation of the enterprise re-profiling program;

3) Monitoring the process of re-profiling and evaluating the effectiveness of ongoing activities.

This study is aimed at improving and facilitating the first stage of the life cycle of industrial re-profiling and planning. The methods and algorithms developed in the paper will allow for more efficient analysis and planning of future events.

As noted by Lapidus and Topchiy, neither at the stage of planning nor at the stage of implementation there are effective, scientifically based systems in Russia (Lapidus & Topchiy, 2019). The processes on object repurposing that started in the 1990s were chaotic and non-systemic. Development companies did not form structured hierarchical systems of management and control over such projects.

Besides, there was no system analysis and assessment of a possibility of a form, type and techniques for carrying out similar works. The systematization of management and monitoring in the implementation of re-profiling projects is also not structured and has no scientifically sound deterministic form (Newton, 2016).

In order to solve the mentioned problem, the authors consider the use of an information complex interaction system consisting of a large number of different functional subsystems and modules, including investment, organizational-technological and informational ones. In addition, the main elements of this information system should be grouped into four main functional and informational macroblocks, one of which is aimed to develop the design framework, allocate resources, and calculate the project life and costs necessary for the implementation of the project (Sung & Lee, 2015).

Such parameters as the project cost, number of working shifts a day, number of working days a week, coefficient of combination of works, financing conditions are specified as the most general factors influencing the re-profiling process planning and being interrelated (Zueva et al., 2019). It is advisable to establish relationship between these parameters using the mathematical theory of experiment planning, which is a fundamental part of experimental and statistical modeling theory (Menelyuk & Lobakova, 2016).

Thus, the literary analysis confirms the relevance of the topic accepted for study and enables to identify the most important factors determining the process of re-profiling at the planning stage and the possibility of finding a relationship between them. The main indicators, based on the scientific sources discussed above, include economic efficiency, intra-shift loss of time, the amount of work in the conversion. Dependencies between them will be established by using the known graphs of the relationship between the values under consideration, or on the basis of the study, if there is no known relationship.

2. Methodology

The main study models will be the dependency graphs of values:

1. The relative time loss versus the redeployment coefficient;

2. The project economic efficiency versus the actual construction and installation duration (Zueva et al., 2019)

As a result of the study, we plan to obtain an experimental graph of the project economic effect dependence on the redeployment coefficient.

The time loss is determined by the following formula (1) (Topchiy et al., 2019):

$$P = \frac{t_{loss}}{T_{cr}}, \quad (1)$$

where P is the relative value of time loss; t_{loss} is the number of shifts in which it is impossible to carry out construction and installation due to the characteristics of the redeployed facility, given, for instance, its location or duration of an activity during construction; T_{cr} is the critical path value (in shifts) determining the construction duration planned, regardless of the working time loss.

The redeployment coefficient is determined by formula (2) (Abramov, 2019):

$$C_{red} = \frac{S_{pwa}}{S}, \quad (2)$$

where C_{red} is the redeployment coefficient; S_{pwa} is the industrial facility area subject to construction; in other words, the planned work area; S is the total industrial facility area.

Economic efficiency is determined by formula (3):

$$E = \frac{C_{est}}{C_{act}}, \quad (3)$$

where E is the economic project efficiency determined by the degree of decrease in the actual estimated construction cost compared to the project cost; C_{est} – the estimated cost of construction works; C_{act} – the actual cost of construction works.

The actual work duration is determined by formula (4) (Newton, 2016):

$$T_{act} = \frac{t_{loss}+T_{cr}}{T_{cr}}, \quad (4)$$

where T_{act} is the relative actual work duration defined as the ratio of actual duration regarding the time loss to the critical path value.

It must be noted that the project economic efficiency dependence on the actual construction and installation duration is an element of a probabilistic approach to the estimation of organizational and technological construction indicators considered in some scientific literature sources (Jensen et al., 2018).

The most probable duration, compared to the critical path value reflecting the

planned duration, is determined by formula (5):

$$T_{mp} = T_{cr} + 3\sigma, \quad (5)$$

where T_{mp} is the most probable construction duration; σ is the mean-square error of duration planning.

Based on construction experience and its planning (Joblot et al., 2019), we can assume (6) that:

$$\sigma = 0.05\, T_{cr} \quad (6)$$

With regard to the assumption (6), formula (5) can be transformed into equation (7):

$$T_{mp} = T_{cr} + 3 \times 0.05\, T_{cr} = 1.15\, T_{cr} \quad (7)$$

With two critical points corresponding to the critical path value and the most probable construction duration, the project economic efficiency dependence on the actual construction and installation duration may be built using the data from Appendix 1.

The result is shown in Figure 1.

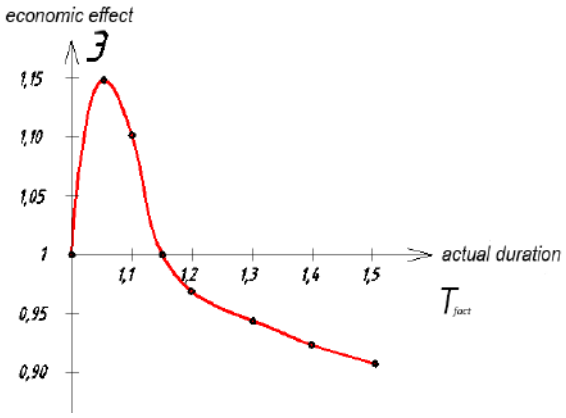

Figure 1. The project economic efficiency versus the actual work duration

Dependence of the relative time loss on the redeployment coefficient is an unknown value; it is this relationship that will be the main subject of this scientific study. This ratio is known only for its nature, which is an inverse relationship (Figure 2) (Abramov et al., 2016).

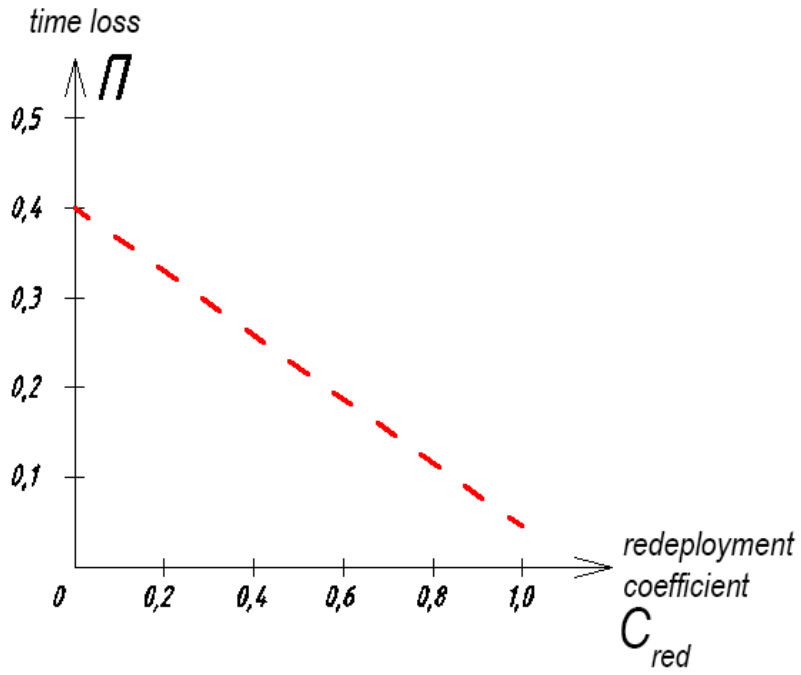

Figure 2. The nature of the relative time loss dependence on the redeployment coefficient.

In what follows a flow chart where can introduce the procedure has been done through this study is schematically depicted (figure 3).

3. Results and discussion

To accurately determine the points on graph 2 and draw up a curve, an expert survey must be conducted. The survey will be performed according to specially prepared questionnaires given in Figure 4. The experts' aim will be to determine the relative time loss during construction at various redeployment coefficient values. The values varying from 0 to 1 with an interval of 0.2 are shown in the questionnaire in the table to create a statistically representative data array equal to six points.

Figure 3. System model

To determine the required number of experts who must participate in the study to create a representative statistical data array, we shall use formula (8) obtained during the generalization of the mathematical data statistical analysis basics (Pukhkal & Mottaeva, 2018):

$$m = \frac{h^2 \cdot r_a \cdot r_o}{\Delta^2}, \qquad (8)$$

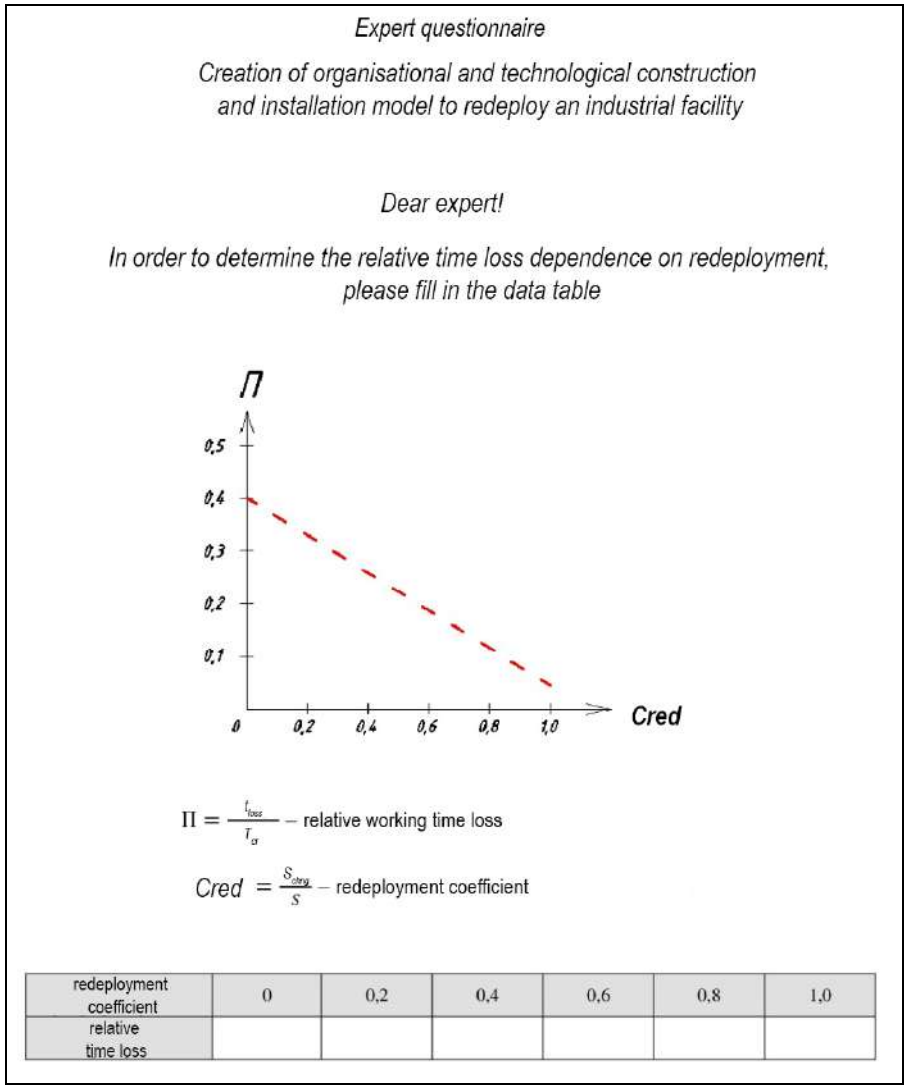

Figure 4. Expert survey questionnaire.

Where m is the required minimum number of experts; h is the confidence coefficient; r_a is the proportion of sample elements with this attribute; r_o is the proportion of sample elements without this attribute; Δ is the representativeness error.

The confidence coefficient study is expressed as a percentage indicating an assessment degree of the confidence interval boundaries for the studied values and is usually equal to 80-99% (Lapidus & Abramov, 2018).

Taking the confidence coefficient value equal to 90%, we will get:

$h = 0.9$;

$r_a = h = 0.9$;

$r_o = 1 - r_a = 1 - 0.9 = 0.1;$

$\Delta = 1 - h = 1 - 0.9 = 0.1;$

$$m = \frac{h^2 \cdot r_a \cdot r_o}{\Delta^2} = \frac{0.9^2 \cdot 0{,}9 \cdot 0.1}{0.1^2} \approx 8 \qquad (8)$$

A study with a known representativeness error not exceeding 10% must be conducted by 8 experts having the necessary competencies in the study subject.

After determining the study methods, models and parameters, as well as the required number of experts, it was possible to obtain statistical data.

The data of questionnaires of the expert survey participants were summarized in Table 1

Table 1. Expert survey data.

Redeployment coefficient	0	0.2	0.4	0.6	0.8	1.0
Expert 1	0.4	0.35	0.3	0.25	0.2	0.1
Expert 2	0.45	0.4	0.33	0.25	0.15	0.05
Expert 3	0.5	0.47	0.37	0.27	0.1	0
Expert 4	0.44	0.45	0.4	0.22	0.1	0
Expert 5	0.5	0.42	0.35	0.28	0.12	0.05
Expert 6	0.42	0.4	0.35	0.2	0.1	0.03
Expert 7	0.5	0.44	0.4	0.27	0.12	0.05
Expert 8	0.47	0.4	0.35	0.23	0.1	0.04

After collecting the data, one must proceed to process it mathematically. The Kolmogorov criterion is designed to verify that the analyzed data sample belongs to a certain distribution law. If this criterion meets the verification condition, the statistical hypothesis about the consistency of expert opinions will be confirmed, i.e. the survey results will be considered representative and the data may be subject to further study.

Step 1. We shall define cumulative expert survey results (Table 2).

Table 2. Cumulative expert survey results.

No.	Expert 1	Expert 2	Expert 3	Expert 4	Expert 5	Expert 6	Expert 7	Expert 8
1	0.40	0.45	0.50	0.44	0.50	0.42	0.50	0.47
2	0.75	0.85	0.97	0.89	0.92	0.82	0.94	0.87
3	1.05	1.18	1.34	1.29	1.27	1.17	1.34	1.22
4	1.30	1.43	1.61	1.51	1.55	1.37	1.61	1.45
5	1.50	1.58	1.71	1.61	1.67	1.47	1.73	1.55
6	1.60	1.63	1.71	1.61	1.72	1.50	1.78	1.59

Step 2. We shall calculate the relatively accumulated frequency differences in the opinions of experts (Table 3).

Table 3. Calculation of parameters for data analysis.

No.	f1	f2	f3	f4	f5	f6	f7	f8	D
1	0.250	0.281	0.313	0.275	0.313	0.263	0.313	0.294	0.063
2	0.469	0.531	0.606	0.556	0.575	0.513	0.588	0.544	0.138
3	0.656	0.738	0.838	0.806	0.794	0.731	0.838	0.763	0.181
4	0.813	0.894	1.006	0.944	0.969	0.856	1.006	0.906	**0.194**
5	0.938	0.988	1.069	1.006	1.044	0.919	1.081	0.969	0.163
6	1.000	1.019	1.069	1.006	1.075	0.938	1.113	0.994	0.175

Table 3 presents the following data:

f is the relatively accumulated frequency (relationship of the current value of *n* to the maximum);

D is the difference between the maximum and minimum values relative to the accumulated frequencies in each interval.

The accumulated results are calculated by formula (9):

$$n_i = n_i + n_{i-1}, \quad (9)$$

where *n* is the accumulated expert survey result; *i* is the interval number.

The relative accumulated frequency is calculated by formula (10):

$$f_i = \frac{n_i}{\max(n_i)}, \quad (10)$$

where *f* is the relative accumulated frequency; *i* is the interval number; *max (n)* is the maximum value of the accumulated result.

The difference is calculated by formula (11):

$$D_i = \max(f) - \min(f), \quad (11)$$

where *D* is the difference relative to the accumulated frequencies; *i* is the interval number; *max (f)* is the maximum value relative to the accumulated frequency in this interval; *min (f)* is the minimum value relative to the accumulated frequency in this interval.

Step 3. Subsequently, the maximum value of the difference *D* is determined compared to the empirical critical difference value D_{crit} calculated according to the table of critical difference values in relative frequencies

$$D_{crit} = 0.325,$$

where D_{crit} is the critical value of the difference in relative frequencies.

$N = 13.14$ is the sample size of the analyzed data defined as the sum of all the expert survey results.

The largest estimated value is equal to $D_{max} = 0.194$ (Pezeshki & Ivari, 2018).

Since

$$D_{max} < D_{crit},$$

$$0.194 < 0.325.$$

The assumption of the consistency of expert opinions in the survey results is confirmed.

Since, as a result of statistical analysis, the expert survey data given in Table 1 is recognized as representative, we shall use it as a mathematical basis for determining the previously unknown dependence of relative time losses on the redeployment coefficient. The average expert survey data from Summary Table 1 is given in Table 4 (Hasik et al., 2019).

Table 4. The average expert survey values.

Redeployment coefficient	0	0.2	0.4	0.6	0.8	1.0
Relative time loss	0.46	0.42	0.36	0.25	0.12	0.04

A graph of the desired dependence was plotted according to Figure 5.

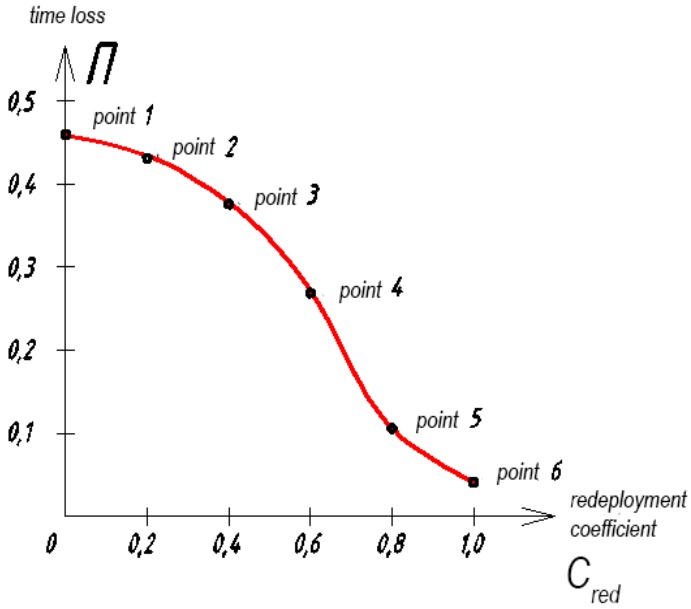

Figure 5. The relative time loss versus the redeployment coefficient.

By summarizing the graphs presented in Figures 1 and 4, the project economic effect relationship with the redeployment coefficient may be determined.

To determine the key point of the graph, we shall use Figure 5. The economic efficiency graph (Figure 1) goes over a value of 1 at a point corresponding to a time loss of 0.15 T_{cr}. For the redeployment volume, this value will be 0.74.

Thus, the coefficient value of 0.74 accounting for time losses due to the redeployment process characteristics does not affect the quality and accuracy of the organizational and technological model determining the planned construction and installation duration.

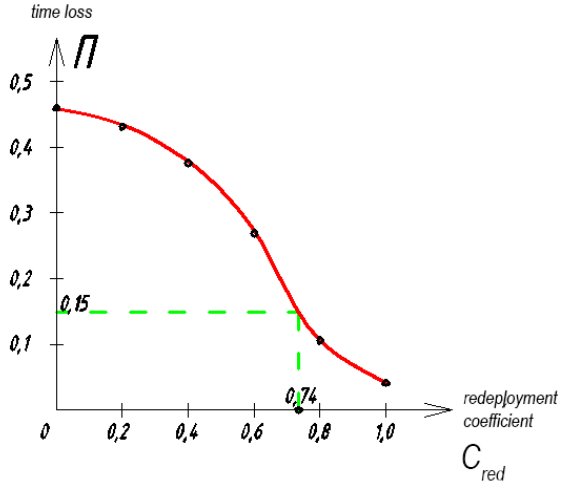

Figure 6. Determining the key value of the redeployment coefficient.

The final graph of the project economic effect dependence on the redeployment coefficient is given in Figure 7.

The values on the graph are obtained in the following way:

According to a dependence of 1, with construction duration of 1.1, the economic effect is 1.1, which means that, according to a dependence of 4, for the relative time loss of 0.1, the redeployment coefficient will be 0.85. Further calculations are summarized in Table 5.

Table 5. Determining the economic effect.

Dependence	Figure 1		Figure 4	
Indicator	T_{act}	E	P	C_{red}
Point 1	1.00	**1.00**	0.00	**1.00**
Point 2	1.10	**1.10**	0.10	**0.85**
Point 3	1.15	**1.00**	0.15	**0.74**
Point 4	1.20	**0.97**	0.20	**0.68**
Point 5	1.30	**0.93**	0.30	**0.55**
Point 6	1.40	**0.91**	0.40	**0.32**

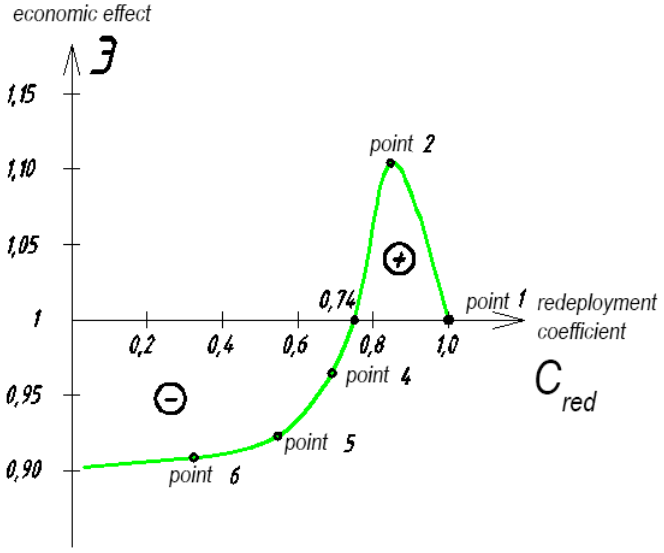

Figure 7. Experimental dependence of the project economic effect on the redeployment coefficient.

According to the dependence graph, with a redeployment coefficient ranging from 0.74 to 1, the use of standard organizational and technological models does not negatively affect the economic project efficiency due to insignificant losses of working time because of work peculiarities during the redeployment of an industrial facility. Redeployment gives employees whose jobs are at risk the chance to find a new job at the University. Hiring managers can use redeployment to find current employees to fill their jobs.

There are a number of reasons why an employee's job can be at risk, including limited funding and organisational change. If your job is at risk and you have 12 months or more continuous service at the University you can use the Redeployment service. The service has an online register for hiring managers to use and a jobs portal where jobs are advertised to redeployees only.

Redeployment is committed to helping to maintain job security for employees. By hiring a redeployee we can keep the knowledge, skills and experience of an employee who is already loyal to the University.

When the coefficient value ranges from 0 to 0.74 (most facility redeployment cases), standard models have a negative impact on economic efficiency, since they do not consider the specifics of the work. In this case, the redeployment features are

considered by the planned increase in the work duration determined by the redeployment coefficient dependence on the loss of working time (Figure 4).

As a result of a scientific study conducted using the expert assessment method by means of a questionnaire, including statistical data analysis according to the Kolmogorov criterion, an interconnection between such industrial facility parameters as relative time losses → redeployment coefficient, as well as the project economic effect → redeployment coefficient was established.

In this paper, we considered the problem of surveillance coverage evaluation undertaken by measuring the dispersion of an redeployment network and that of a redeployment method for maximizing coverage. In the former perspective, this paper describes deployment entropy as a novel quantitative measurement of distribution of redeployment s when they execute surveillance coverage mission. The properties of deployment entropy make it a reasonable method to measure the distribution. In the later perspective, the two-level redeployment method is developed to relocate the redeployment s to achieve an even distribution. Some simulation results reveal that the proposed algorithm can improve the coverage percentage of the redeployment s network no matter when the redeployment is randomly deployed in the interested region or the redeployment.

The simulation also shows that our proposed two-level redeployment scheme has a lower movement cost when achieving the same coverage percentage as the one-level scheme.

Conclusions

According to the study results, the following algorithm for the organizational and technological construction and installation model development may be presented:

1. Determination of the industrial facility redeployment coefficient.

2. If the coefficient ranges from 0.74 to 1, the organizational and technological model is developed in the same way as for a new construction project.

If the coefficient ranges from 0 to 0.74, to develop an accurate organizational and technological model, the relative time loss due to the peculiarities of a construction work must be considered. Time loss is determined graphically from the

curve given in Figure 4. Regarding the time loss increasing the planned work duration at the construction preparation stage, there is no need to make emergency decisions during a redeployment project if the work duration increases due to unforeseen circumstances. This coefficient is responsible for the increase in the economic effect.

The identified dependencies made it possible to create a tool for evaluating the effectiveness of organizational methods for re-profiling industrial areas. The absence of such methods for designing organizational structures previously did not provide an opportunity to calculate optimal, rational and effective methods of construction and installation work.

Conflicts of Interest

The authors declare no conflict of interest.

Acknowledgement

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Diversidad fenotípica de aves criollas de postura basada en caracteres zoométricos

Rafael Galíndez *
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Omar Colmenares **

RESUMEN

Con la finalidad de analizar la diversidad fenotípica de aves criollas venezolanas de postura del Laboratorio Sección de Aves, Instituto de Producción Animal, Facultad de Agronomía, Universidad Central de Venezuela, se tomaron medidas zoométricas de 220 gallos y gallinas de las razas FAGRO (n = 33), GDB (n = 65), IPA (n = 36) y Maracay (n = 86). Se consideró el peso vivo, perímetro torácico, longitud corporal, muslo, pierna, tarso, ala, orejilla, barbilla, plumas de cola, altura de cresta y ancho de orejilla. Se realizaron análisis de varianza incluyendo los efectos de sexo y raza, comparando los promedios con la prueba de Duncan. Se calcularon los coeficientes de correlación de algunas medidas corporales. Se ejecutó un análisis discriminante, se calcularon las distancias de Mahalanobis y se graficaron los centroides de cada raza. Todas las medidas resultaron superiores ($P<0,05$) en los machos con diferencias entre 1 y 57%. Se detectaron divergencias ($P<0,05$) entre razas, siendo Maracay e IPA las que expresaron mayores valores. La mayoría de las correlaciones de las medidas corporales resultaron altamente significativas, observándose magnitudes superiores en la raza IPA. Las distancias de Mahalanobis basadas en seis caracteres discriminantes, revelaron que las razas más alejadas son Maracay y FAGRO. Se concluye que existe marcado dimorfismo sexual en las aves estudiadas; asimismo, se detectó alta diversidad entre los grupos analizados.

PALABRAS CLAVE: centroides, distancia de Mahalanobis, gallinas.

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Phenotypic diversity of native laying birds based on zoomometric characters

ABSTRACT

In order to analyze the phenotypic diversity of Venezuelan Creole bird layers of the Laboratorio Sección de Aves, Instituto de Producción Animal, Facultad de Agronomía, Universidad Central de Venezuela, zoometric measures were taken of 220 male and female of the FAGRO (n = 33), GDB (n = 65), IPA (n = 36) and Maracay (n = 86) breeds. The traits considered were live weight, thoracic perimeter, body length, thigh, leg, tarsus, wing, ear lobe, wattle, tail feathers, comb height and ear lobe width. Variance analysis were performed including sex and breed effects, comparing the average through Duncan test. Relationship coefficients of some body measurements with live weight were calculated. On the other hand, discriminant analyses and Mahalanobis distances were calculated, the centroids of every breed were plotted. All measurements were higher ($P<0.05$) in males with differences between 1 and 57%. Differences were detected ($P<0.05$) between breeds, Maracay and IPA expressed higher values. Most correlation of the body measurements were highly significant, with higher magnitudes observed in IPA breed. Mahalanobis distances based in six discriminant trait, revealed that Maracay and FAGRO are the breeds more distances. It is concluded that there is high divergences between sexes moreover, it is detected high diversity between analyzed groups.

KEYWORDS: centroids, Mahalanobis distance, hens.

Introducción

Es imprescindible caracterizar los recursos genéticos de interés zootécnico disponibles antes de diseñar y ejecutar cualquier programa de conservación o mejora genética de las poblaciones locales de animales. En este sentido, la descripción de estos recursos se ejecuta compilando tres tipos de información: histórica, fenotípica y genética (FAO, 2012). Asimismo, se ha establecido que la caracterización fenotípica es fundamental para definir el inventario de individuos pertenecientes a las razas, líneas o grupos genéticos presentes en una determinada región, condición medioambiental o manejo específico (FAO, 2012).

Para el caso de las gallinas criollas venezolanas, si bien es cierto, que se han recabado muchos datos de caracteres productivos y funcionales (Galíndez *et al*., 2012;

2014; Galíndez y Blanco, 2017), son pocos los estudios que se han realizado para dilucidar la diversidad morfométrica y genética de las poblaciones. Dentro de los estudios relacionados a la diversidad fenotípica, se ha explorado un poco con el análisis de los caracteres cualitativos (color del plumaje, orejilla, tarsos, tipo de cresta, etc.), los cuales son muy eficientes para definir las razas (Lucas y Galíndez, 2017). Por otro lado, no se han estudiado los rasgos zoométricos que, en algunos casos, no son suficientes para delimitar las razas, teniendo que recurrir a menudo al auxilio de caracteres productivos, cualitativos o el análisis genético molecular para separar con precisión los individuos de una raza, línea o grupo poblacional de los otros. En este orden de ideas, el uso de herramientas estadísticas como el análisis discriminante paso a paso ofrece un enorme potencial para definir las características que separan a las poblaciones, y clasificar por supuesto, los grupos de individuos.

El objetivo del presente trabajo fue estudiar la diversidad fenotípica de aves criollas venezolanas de postura basada en caracteres zoométricos.

1. Materiales y Métodos

Los datos se recolectaron de los ejemplares de gallos y gallinas presentes en el Laboratorio Sección de Aves del Instituto de Producción Animal de la Facultad de Agronomía de la Universidad Central de Venezuela (Laboratorio Sección de Aves), el cual tiene una altitud de 455 m.s.n.m, precipitación promedio de 1135 mm, temperatura promedio de 25,5 °C y humedad relativa promedio de 74,0 % (INIA, 2019).

Las aves estaban ubicadas en el galpón "A", que posee piso de concreto, tiene 64 m de largo, 6 m de ancho, altura mínima de 2,7 m y máxima de 5,0 m. Está dividido en 60 corrales con dimensiones de 2,0 m de largo, 2,0 m de ancho y 2,0 m de alto (0,43 m de pared de concreto y 1,57 m de malla metálica). El piso de cada corral estaba cubierto de concha de arroz, los bebederos eran de tipo campana (32) y en otros corrales de tipo copa (28). Los comederos eran tipo tolva con una capacidad de alimentación máxima de veinte (20) aves por cada uno.

Para medir el peso se utilizó un equipo electrónico marca Salter Brecknell, con capacidad máxima de 45 kg y apreciación de 50 g. Para cuantificar las longitudes se

hizo uso de un vernier marca INOX con una amplitud máxima de 15,1 cm (apreciación de 1 mm) y una cinta métrica con una extensión máxima de 150 cm.

Se tomaron medidas de 220 aves, conformados por gallinas y gallos adultos; distribuidos por raza de la siguiente manera:

FAGRO: 33.

GDB: 65.

IPA: 36.

Maracay: 86.

Total: 220.

La alimentación se basó en el suministró de balanceado comercial para ponedoras a razón de 100 g por animal, con las siguientes características: proteína cruda (16%), fibra cruda (5%), extracto etéreo (3%), extracto libre de nitrógeno (50%).

Se consideraron 14 caracteres cuantitativos: peso corporal, longitud corporal, muslo, pierna, tarso, ala, orejilla, barbilla, plumas de la cola; perímetro pectoral; ancho de ala, orejilla, barbilla y altura de cresta (Tabla 1).

Se realizaron análisis de varianza para comparar las medidas zoométricas entre sexo y razas, utilizando el programa estadístico SAS (Littell *et al*., 2002). El modelo usado fue el siguiente:

$Y_{ijk} = \mu + Sex_i + R_J + \varepsilon_{ijk}$; donde:

Y_{ijk} = medida zoométrica.

μ = media teórica de la población.

Sex_i = efecto del sexo del ave (macho, hembra).

R_j = efecto de raza (FAGRO, GDB, IPA, Maracay).

ε_{ijk} = residual con media "0" y varianza "σ", normal e independientemente distribuido.

En análisis preliminares se comprobó la ausencia de la interacción sexo*raza, por tal motivo se excluyó de los análisis finales. Para verificar la diferencia entre los promedios se realizó la prueba de medias de Duncan (Steel *et al*., 1997). Se calcularon los coeficientes de correlación para determinar posibles relaciones entre el peso vivo (PV), perímetro torácico y la longitud corporal, muslo, pierna y tarso.

Tabla 1. Descripción de mediciones corporales en aves criollas de postura/Description of body measurements in Creole birds of lay

Longitud corporal	Distancia entre la punta del pico y la base de la cola (sin las plumas).
Perímetro torácico	La circunferencia del pecho tomada hasta la punta posterior de la pechuga
Longitud del muslo	Distancia entre la articulación coxofemoral a la articulación de la rodilla
Longitud de la pierna	Distancia entre la articulación de la rodilla hasta la articulación del tarso
Longitud del tarso	Distancia entre la articulación del taso y el origen del cuarto dedo
Longitud del ala	Distancia medida desde la unión del húmero con las vértebras dorsales hasta la punta de las plumas primarias (el ala debe estar extendida).
Ancho del ala	Longitud medida entre la unión del húmero con el cubito hasta la última pluma secundaria (el ala debe estar extendida).
Altura de la cresta	Distancia entre la sierra más alta a la inserción de la cresta en el cráneo
Longitud de orejilla	Distancia entre la parte superior y la inferior de la orejilla.
Ancho de orejilla	Longitud entre la parte rostral y la caudal de la orejilla.
Longitud de barbilla	Distancia desde la base de la barbilla hasta el final de la misma.
Ancho de barbilla	Longitud entre la parte rostral y caudal de la barbilla (sin estar extendida).
Longitud de plumas de cola	Distancia desde la base del pigostilo (hueso de cola) hasta el final de la misma.

Fuente: Gutiérrez, 2013; Pérez *et al*., 2004.

Se realizó un análisis discriminante por pasos (stepwise) con el programa estadística SAS, con la finalidad de determinar las variables que serían usadas en el análisis de agrupamiento, este procedimiento establece las variables que tienen más poder discriminante (Littell *et al.*, 2002).

Finalmente, se computaron las distancias de Mahalanobis entre razas y la representación gráfica de las mismas usando el complemento para Microsoft Excel XLSTAT (XLSTAT, 2018).

2. Resultados y discusión

La Tabla 2 muestra los promedios por sexo para gallinas y gallos criollos del Laboratorio Sección de Aves (LSA). Todas las variables consideradas resultaron superiores (P<0,05) en los machos, con diferencias que oscilan entre 1% (ancho de orejilla) y 57% (longitud de barbilla).

Las diferencias entre sexo en cuanto a medidas zoométricas ha sido reportado con anterioridad (Lázaro *et al.*, 2012; Cabarles, 2013; Guni *et al.*, 2013; Sanmartin, 2014; Chincoya *et al.*, 2016;), comentado los autores que las divergencias entre machos y hembras obedecen al dimorfismo sexual producto del control que ejercen algunas hormonas sobre estos caracteres. Asimismo, algunos investigadores asocian la mayor longitud de la cresta y barbilla de los machos con el desarrollo de las gónadas y la secreción de hormonas sexuales (Duguma, 2006; Bembide *et al.*, 2013).

De manera general, los caracteres medidos tanto en machos como hembras superan algunos reportes de la literatura (Duguma, 2006; Chincoya *et al.*, 2016); sin embargo, son inferiores a otro trabajo publicado (Bembide *et al.*, 2013), pudiendo aseverar que las diferencias genéticas entre los grupos de aves del presente estudio y los trabajos citados se expresa en los valores fenotípicos mencionados, como consecuencia de los procesos de selección artificial aplicados en estas poblaciones, de la adaptación de los individuos a las condiciones ambientales, edad y estado fisiológico (Bembide *et al.*, 2013).

Por otra parte, se ha mencionado que el dimorfismo sexual en esta especie está relacionado a altos niveles de poligamia social, que a su vez es consecuencia de la

competencia de los machos para acceder al apareamiento y la selección artificial dirigida hacia animales más grandes, pesados y con caracteres secundarios (tamaño de la cresta, orejillas y barbillas) muy bien definidos (Alabi *et al*., 2012).

Tabla 2. Medidas zoométricas para machos y hembras de cuatro razas de gallinas criollas/Zoometric measurements for male and female of four Creole hens breeds.

Variable	Promedio		Desviación estándar	Coeficiente de variación
	Macho	Hembra		
Peso vivo (g)	2595,0 a	1800,5 b	408,4	21,4
Longitud corporal (cm)	44,8 a	39,5 b	3,4	8,3
Perímetro pectoral (cm)	37,8 a	30,9 b	4,2	13,6
Longitud de muslo (cm)	10,5 a	8,9 b	0,9	10,4
Longitud de pierna (cm)	14,7 a	12,4 b	1,3	9,6
Longitud de tarso (cm)	9,6 a	7,9 b	1,1	12,3
Longitud de ala (cm)	38,9 a	34,0 b	3,5	9,7
Ancho de ala (cm)	20,1 a	17,5 b	2,9	15,7
Altura de cresta (cm)	6,4 a	3,4 b	1,6	39,5
Longitud de orejilla (cm)	3,5 a	2,1 b	0,7	32,6
Ancho de orejilla (cm)	1,6 a	1,1 b	0,15	15,2
Longitud de barbilla (cm)	6,5 a	2,8 b	1,6	42,1
Ancho de barbilla (cm)	3,8 a	1,7 b	0,7	34,7

Letras diferentes en la misma fila reflejan diferencias (P<0,05).

Con excepción de la longitud corporal (Tabla 2) todas las demás variables tienen coeficiente de variación superior al 9%, por tanto se está en presencia de elevada variabilidad, situación que es descrita en la literatura como: una población sin uniformidad para los caracteres considerados (Matola, 2016), lo cual resultaría lógico, puesto que el grupo de animales evaluados incluye varias razas, por tanto, es probable

que existan sub-divisiones por ésta causa. La aseveración anterior se corrobora con los resultados presentados en la Tabla 3, en la cual se aprecian diferencias (P<0,05) en magnitudes entre razas para todos los caracteres medidos.

Diferencias entre razas, líneas o grupos han sido reportadas (Duguma, 2006; Al – Atiyat, 2009; Galíndez *et al.*, 2012; Cabarles, 2013; Galíndez *et al.*, 2014), tanto para caracteres zoométricos como para rasgos productivos, coincidiendo los autores que las divergencias observadas tienen su origen en el genoma diferencial de las aves. De manera general, las razas Maracay e IPA expresaron mayores (P<0,05) valores para los rasgos morfométricos con muy pocas diferencias entre ellas (longitud corporal, ancho de ala, altura de cresta, longitud de orejilla, ancho y longitud de barbilla) (Tabla 3).

En promedio las razas mencionadas superan a las restantes en el peso corporal en un poco más de 290 g; estos valores, combinados con las longitudes corporales, muslo, pierna y tarso demuestran que las dos primeras razas son de mayor tamaño que las razas FAGRO y GDB.

Las similitudes entre las últimas razas mencionadas sugieren que pudiesen existir ancestros comunes; sin embargo y como se ha evidenciado, es necesario realizar estudios a nivel molecular para estudiar la diversidad de las poblaciones (Alabi *et al.*, 2012).

En otro orden de ideas y a pesar que las condiciones de explotación, edad de los animales, clima, etc., son disímiles entre esta investigación y otros trabajos, algunas comparaciones pudiesen establecerse. Por ejemplo, el peso adulto de las razas Maracay e IPA es similar al de la raza española de gallinas Menorquina; mientras que las razas FAGRO y GDB son semejantes a la raza Mallorquina (Méndez, 2010). Asimismo, la longitud de las extremidades para este estudio es inferior a las razas españolas mencionadas, lo que supone que estas últimas son animales más altos, situación que responde a la selección dirigida hacia caracteres ornamentales realizada con anterioridad.

La Tabla 4 muestra los coeficientes de correlación y regresión lineal simple ente el peso vivo y las medidas morfométricas más importantes de gallos y gallinas del Laboratorio Sección de Aves. Sólo las correlaciones de peso vivo – longitud de pierna en GDB y peso vivo – longitud del tarso en FAGRO resultaron no significativas. Las

correlaciones de menor magnitud se observaron en la raza FAGRO (peso vivo – longitudes de muslo y pierna); mientras que las de mayor valor se evidenciaron en la raza IPA (peso vivo – longitud del muslo, corporal y pierna).

Tabla 3. Medidas zoométricas para varias razas de gallinas criollas venezolanas/Zoometric measurements for several breeds of Venezuelan Creole hens.

	Grupo Racial			
Variable	Maracay	IPA	FAGRO	GDB
Peso vivo (g)	2050,6 a	2005,8 a	1751,7 b	1723,0 b
Longitud corporal (cm)	41,3 a	40,0 b	40,0 b	38,7 c
Perímetro pectoral (cm)	32,1 ns	32,0 ns	31,9 ns	31,1 ns
Longitud de muslo (cm)	9,4 a	9,2 a	8,8 b	8,8 b
Longitud de pierna (cm)	13,0 a	13,1 a	12,5 b	12,2 b
Longitud de tarso (cm)	8,3 a	8,4 a	8,1 b	7,7 c
Longitud de ala (cm)	35,1 a	35,8 a	33,8 b	33,7 b
Ancho de ala (cm)	18,8 a	17,7 b	17,5 b	16,4 c
Altura de cresta (cm)	3,6 c	4,5 a	4,1 b	3,6 c
Longitud de orejilla (cm)	2,2 c	2,4 b	2,6 a	2,2 c
Ancho de orejilla (cm)	1,1 b	1,2 a	1,1 b	1,1 b
Longitud de barbilla (cm)	3,2 b	3,7 a	3,7 a	3,2 b
Altura de barbilla (cm)	1,9 b	2,0 a	2,0 a	1,9 b

Letras diferentes entre filas expresan diferencias (P<0,05), ns: no significativo.

Las relaciones observadas coinciden con reportes anteriores (Pérez *et al.*, 2004; Méndez, 2010; Méndez *et al.*, 2011; Guni *et al.*, 2013). Asimismo, en una caracterización de los fenotipos de las gallinas locales en Dekina, descubrieron correlaciones

significativas para los parámetros peso vivo – largo corporal (0,596), peso vivo – perímetro pectoral (0,704), peso vivo – largo de tarso (0,641) (Daikwo *et al.*, 2011).

Los resultados sugieren que el aumento de cualquiera de estos parámetros corporales causará incremento en el peso del cuerpo, por tanto, pueden ser usadas cualquiera de estas medidas para estimar el peso corporal con elevada precisión (Alabi *et al.*, 2012; Guni *et al.*, 2013).

Por otra parte, estas relaciones resultan particularmente útiles en zonas, principalmente rurales, donde no existe la disponibilidad de equipos de medición del peso corporal (Alabi *et al.*, 2012).

En la Tabla 5 se presentan los resultados del análisis discriminante paso a paso (stepwise) realizado con el programa estadístico SAS. De catorce variables originales, se seleccionaron seis, de acuerdo al procedimiento sugerido, estas son: altura de la cresta, longitud del muslo, longitud del tarso, longitud corporal, longitud de la barbilla y longitud del ala; el resto de las variables son retiradas del análisis, pues según el análisis discriminante, poco se diferencian las razas utilizando estas medidas (De la Fuente, 2011).

La variable que mejor discrimina es altura de la cresta, debido a que posee el mayor R^2 parcial y el mayor valor de "F" (de la Fuente, 2011), el resto de las variables sigue el orden en el cual son mencionadas anteriormente. Cabe mencionar que el peso corporal no discrimina de manera eficiente las razas estudiadas, tal cual ha sido reportado para gallinas jordanas (Al – Atiyat, 2009). Sin embargo, largo corporal, largo del muslo, largo de tarso, largo de la barbilla y del ala son características que definen bien el tamaño de las gallinas (Chincoya *et al.*, 2016).

Tomando como criterio la distancia de Mahalanobis, las razas más disímiles serían FAGRO y Maracay, seguidas de IPA – Maracay, luego GDB – Maracay, FAGRO – IPA, GDB – IPA y FAGRO - GDB (Tabla 6).

Las distancias de Mahalanobis son adimensionales, por tanto, mientras mayor sea el valor, la distancia entre los grupos es superior (Salas y Escobedo, 2008). En este orden de ideas, es lógico pensar que existen diferencias apreciables, no sólo morfológicas (color de plumaje, tarsos, etc.), sino en algunas medidas zoométricas

entre las razas, lo que coincide con el análisis de varianza anterior, en el cual se observan algunas diferencias entre estas razas (Tabla 3).

Tabla 4. Coeficientes de correlación lineal simple entre el peso vivo (PV), longitud corporal (LC), perímetro pectoral (PP), longitud del muslo (LM), pierna (LP) y tarso (LT) en cuatro razas de gallinas criollas venezolanas/Simple lineal correlation coefficients between live weight (PV), body length (LC), pectoral perimeter (PP), thigh length (LM), leg (LP), and tarsus (LT) in four breeds of Venezuelan Creole hens.

	Raza			
	Maracay	IPA	FAGRO	GDB
Parámetros	Correlación			
PV-LC	0.66 **	0.70**	0.49**	0.42**
PV-PP	0.57**	0.59**	0.62**	0.67**
PV-LM	0.68**	0.83**	0.39*	0.67**
PV-LP	0.66**	0.70**	0.39*	0.2lns
PV-LT	0.63**	0.67**	0.29ns	0.56**

** (P<0,01), * (P<0,05), ns: no significativo

Tabla 5. Análisis discriminante para los caracteres zoométricos de gallinas criollas venezolanas/Discriminant analyses for the zoometric characters of Venezuelan Creole hens.

Paso	Variable introducida	R^2 parcial	F	λ de Wilks
1	Longitud del muslo	0,1305	10,81**	0,8695**
2	Altura de la cresta	0,1849	16,26**	0,7087**
3	Longitud corporal	0,0640	4,88**	0,6633**
4	Longitud del tarso	0,0667	5,08**	0,6190**
5	Longitud de Barbilla	0,0553	4,14**	0,5848**
6	Longitud del ala	0,0528	3,92**	0,5540**

**P<0,01

Las divergencias entre las razas estudiadas considerando algunos aspectos productivos (producción y peso de huevos) y reproductivos (fertilidad) han sido reportados en la literatura (Galíndez *et al.*, 2012; 2014).

Tabla 6. Distancia de Mahalanobis para cuatro razas de gallinas criollas venezolanas/Mahalanobis distances for four breeds of Venezuelan Creole hens.

	FAGRO	GDB	IPA	MARACAY
FAGRO	0	0,948	1,592	3,194
GDB	0,948	0	1,285	1,821
IPA	1,592	1,285	0	2,038
MARACAY	3,194	1,821	2,038	0

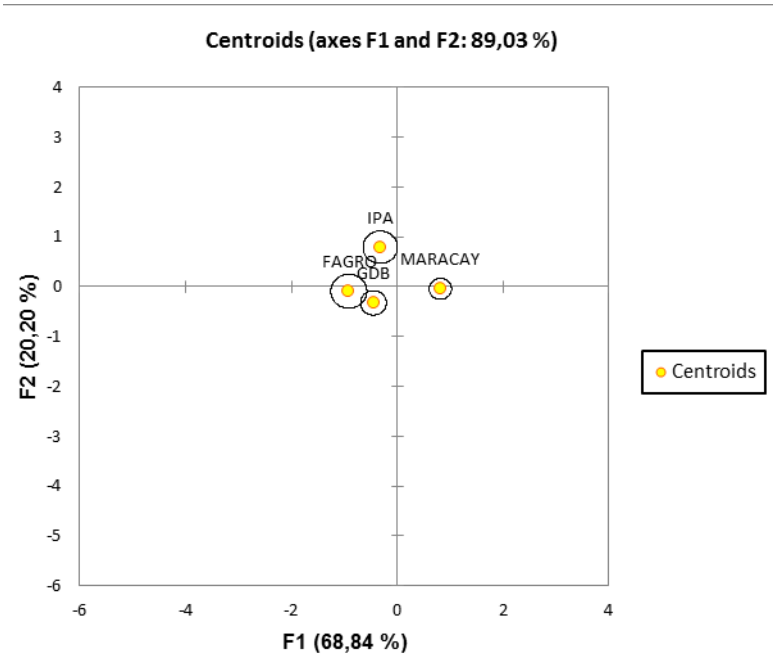

Figura 1. Representación gráfica de las distancias entre los centroides de cuatro razas de gallinas criollas venezolanas/Graphic representation of the distances between the centroids of four breeds of Venezuelan Creole hens.

La mayor distancia entre las razas FAGRO y Maracay es de esperar y se corresponde con la historia genealógica de estas razas, ya que, no comparten ancestros comunes (en el espacio de tiempo próximo que dio origen a las razas); asimismo, la cercanía detectada entre las razas GDB y FAGRO probablemente sea consecuencia de que los individuos de la primera raza son ancestros de la segunda (Galíndez, 2008). Aun así, se observa diversidad en los caracteres medidos entre las razas, lo cual representa una oportunidad para la conservación y mejora de los recursos zoogenéticos avícolas disponibles en Venezuela. Resultados homólogos han sido evidenciados (Abdelqader *et al.*, 2008; Al – Atiyat, 2009) en poblaciones de gallinas criollas de Jordania, en las cuales, con la ayuda de la metodología del análisis discriminante se clasificaron exitosamente varios grupos genéticos de aves.

En la Figura 1 se observan de manera más clara las distancias entre las razas estudiadas. Los centroides para las razas FAGRO y GDB son graficados muy próximos, mientras que las razas IPA y Maracay son representadas más distantes de las dos anteriores, y estas a su vez, separadas entre sí.

A pesar de que algunos individuos mostraron rasgos morfométricos similares a una raza cuando pertenecen a otra, se pueden separar grandes grupos coincidentes con los promedios raciales (Figura 1), tendencia que es similar a lo señalado en estudios anteriores (FAO, 2009; Chincoya *et al.*, 2016), en gallinas de Camboya y México, respectivamente, en los cuales lograron separar los grupos de gallinas, a pesar que entre un grupo y otro existieron similitudes para algunos caracteres, pero divergían en la mayoría de los otros rasgos zoométricos.

En este orden de ideas, se observa la diferenciación clara de la raza Maracay, mientras que las otras razas son mostradas con mayor cercanía. Tal resultado conduce a pensar que los caracteres a incluir en el análisis deben ser más determinantes o disímiles entre las razas.

Conclusiones

Las medidas zoométricas consideradas confirman la aseveración sobre el marcado dimorfismo sexual en estas aves, observando valores superiores para los machos. Se

detectó alta diversidad entre los grupos analizados, siendo ésta más pronunciada entre las razas Maracay y FAGRO. Por otra parte, a pesar que la herramienta de análisis discriminante es muy útil para clasificar las poblaciones animales, se recomienda que los caracteres a incluir en la investigación posean un alta poder de separación para obtener resultados satisfactorios.

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Theoretical methods for measuring chemo-physical properties of nucleic acids during the oxidation of DNA and the incidence of cancer

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ABSTRACT

The purpose of this papers is to investigate theoretical methods to measure the chemo-physical properties of nucleic acids during DNA radicalization and cancer incidence. For this purpose, structures consisting of DNA nucleotides were considered and all structures were optimized using DFT at the CAM-B3LYP / 6-31G level and spatial parameters such as bond length, HOMO and LUMO orbitals, and thermodynamic parameters were obtained, as well as NMR spectroscopy. The results showed that the guanine base had better conditions for oxidation compared to other bases. Also in the NMR calculations using the GIAO method we were able to examine the single and double chain structure in different states when it is natural and abnormal. Therefore, in this work, we try to find a normal relationship between chemical displacement and the rate of natural state DNA aberration, by studying the comparison of isotropic and anisotropic parameters with respect to DNA bases such as adenine, guanine, cytosine, thymine. It was concluded that the skewness (η) is between (0.1) and the skewness is between (1-1), which can be correlated with the abnormalities of the DNA base from the normal to abnormal state. It was also found that the phosphate group oxygen atom in the abnormal form showed most of the changes in these parameters compared to the natural form.

KEYWORDS: Cancer, Mutation, Chemo-physical properties, Nucleic acid, DNA, NMR.

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Métodos teóricos para medir las propiedades quimio-físicas de los ácidos nucleicos durante la oxidación del ADN y la incidencia de cáncer

RESUMEN

El propósito de este trabajo es investigar los métodos teóricos para medir las propiedades quimio-físicas de los ácidos nucleicos durante la radicalización del ADN y la incidencia de cáncer. Para este propósito, se consideraron las estructuras que consisten en nucleótidos de ADN y se optimizaron todas las estructuras utilizando DFT a nivel CAM-B3LYP / 6-31G y se obtuvieron parámetros espaciales tales como longitud de enlace, orbitales HOMO y LUMO y parámetros termodinámicos, así como espectroscopía de RMN. Los resultados mostraron que la base de guanina tenía mejores condiciones para la oxidación en comparación con otras bases. También en los cálculos de RMN utilizando el método GIAO pudimos examinar la estructura de cadena simple y doble en diferentes estados cuando es natural y anormal. Por lo tanto, en este trabajo, intentamos encontrar una relación normal entre el desplazamiento químico y la tasa de aberración del ADN del estado natural, mediante el estudio de la comparación de parámetros isotrópicos y anisotrópicos con respecto a bases de ADN como adenina, guanina, citosina, timina. Se concluyó que la asimetría (η) está entre (0,1) y la asimetría está entre (1-1), lo que puede correlacionarse con las anomalías de la base de ADN desde el estado normal a anormal. También se encontró que el átomo de oxígeno del grupo fosfato en la forma anormal mostró la mayoría de los cambios en estos parámetros en comparación con la forma natural.

PALABRAS CLAVE: Cáncer, mutación, propiedades quimio-físicas, Ácido nucleico, ADN, RMN.

Introduction

The importance of public health of society and attention to the health of the people causes a society to be healthy and progressive. Also with the fast improvement of genetic knowledge in recent years and the recognition of the role of nucleic acids and DNA in various diseases, and in particular the refractory disease of cancer has caused special attention to be paid to its various applications in various fields of sciences and

industry such as chemistry, biochemistry and medical, pharmaceutical industries and for the treatment of diseases.

In recent years, with the help of computers and quantum methods, the achievement of the physical, chemical parameters of nucleic acids has been made possible to radicalize DNA and has been caused to know more the complex behavior of this vital component of body of living organisms. Using chemical accounting methods and QM / MM method in this research, it has been tried to use this extraordinary possibility in addition to filling the existing voids of experiential and experimental methods with a better knowledge of changes in the physiochemical structure of DNA, especially in conditions of radicalized and mutation agents that this knowledge will make DNA changes in cancer disease recognized and will lead to the treatment of this disease. The idea can also be a new independent opinion in the field of medical sciences which can be the basis for many future researches and studies, as well as it can be a big step for advancing scientific knowledge of scientists and researchers in molecular cell biology, biochemistry, chemistry, medicine, physiology science researchers and all subfield of the sciences above.

In a healthy living, there is always a balance between the rate of cell division and the natural death of the cell. A natural cell may be changed to a cancerous cell without any clear reason, but in most cases, the changing is made due to repeated confrontation with carcinogenic substances such as alcohol and tobacco and free radicals. The apparent form and the cancerous cells function with the normal cells are significantly different. A mutation or alteration made occurs in DNA or a genetic material of the cell. DNA is responsible for controlling and preserving apparent form and function of the cell. When the DNA of a cell changes and becomes cancerous, that cell differs from healthy cells (Aghelan and Panjehpour, 2016) and does not do the other tasks on the normal cells of the body. The modified cell is detached from its nearby cells and does not know when its growth should finish and die. In other words, the modified cell does not follow the instructions and internal signals that control other cells and acts independently instead of coordinating with other cells. Researchers found in their studies that non-genetic imbalances of protein lead to out-of-control growth and cancer (Lari et al., 2016).

Researchers concluded that the two proteins Plcy1 and Grb2 were in competition with the Akt for binding during pathway while performing laboratory studies on the mice. When the Plcy1 protein binds to this pathway, it activates cell proliferation, and protein Grb2 controls the cell proliferation. For any reason, cells which include (instruction of mistake and error of messenger RNA of nucleic acids and DNA deficit of protein Grb2), normal growth of cell is out of control and resulting in a probability of cancer. In addition, the protein p53 also plays vital and important role in controlling and preventing the growth of cancer cells as an inhibitor of tumor and cancer. Mutation in the gene DNA causes a disorder in the formation or production of the protein, and in most types of cancers, mutation in the gene is obvious, and biological studies in computations method due to special attention paid to the gene in recent decades by biomedical methods that can be indicated in computations methods as a way to confront with the laboratory and research constraints in this field (Zhai et al., 2012).

There are various mutation factors in the environment that can cause mutation and various diseases in humans such as high energy radiation, chemicals and stress. According to new analysis in scientist studies, consuming tobacco can averagely make mutation in DNA of a lung cell and make 17 types of cancer. In theory, each DNA mutation can provide the potential needed for the progressive activation of cellular degeneration, and ultimately these changes will lead to cancer. The main role of types of DNA polymerase enzymes is genome proliferation. The task of these enzymes is very important and vital, as any factor which make a disorder for these enzymes damage people's health (Yan et al., 2002).

One of the cases that can be considered for identifying DNA damages is identifying probable DNA damages against the oxidizing agents, including oxidizing chemicals and various incidence rays. Which result in present base's oxidation in the DNA and in particular, the present guanine base in DNA sequencing, which will be oxidized easier than bases (Steenken and Jovanovic, 1997), and has less oxidation potential. DNA somewhat has ability to restore itself, but when the number of this (Sun et al., 2015) the property of charges transport in DNA, in addition to creating ideal properties to identify the DNA sequencing in electrical and electrochemical biosensors,

facilitates the oxidation capability of its present bases, genetic mutation and disorder in genetic process (Hall and Barton, 1996). Two mechanisms of electron transport and transport of electron hole were suggested for charge transport and oxidation transport of organic bases in two-strand. In transporting electron hole, mechanism of DNA bases oxidation, particularly guanine base is desired, but in electron transport should consider the role of all bases in charge transporting. Among the present two-strand bases, guanine property for charge transporting is better than other bases, so that the percentage of base guanine present in two-strand, will have a direct effect on the charge transport property in two-strand (Prat et al., 1998), the tendency for electron absorbing in guanine, is lesser than other present two-strand bases, in the other hand oxidation potential, makes guanine more favorable than other bases (Hume et al., 2013).

1. Literature Review

Larry et al. (2017), in a research utilized computer computational methods and molecular modeling on achieving new anti-cancer drugs. Anti-cancer drugs from the factors of Cytotoxic, which is specifically destroys the DNA, by the help of computational methods affects the drugs for genetic and epigenetic disorders and more specifically tended to process of convert and development of malignant cells. Accessing to information of human genome and targeting vulnerable genes of cancer, by the use of computational modeling and prognosis, makes diagnosis and treatment of cancer possible with lesser cost and time. In recent years, the use of computational chemistry and molecular modeling for designing drug by the help of computer attracted pharmaceutical specialists. Initially, by computational modeling method the key factors that are not attainable through examination, computed by simplifying concept of cancer to the four level of atomic, molecular, microscopic, and macroscopic. The computational activity of the MTT assay showed that Atorvastatin, which is a cholesterol synthesis inhibiting, has a significant effect on inhibiting growth of HeLa's cancer cells. Molecular dynamic studies of anti-tumor activity on Nelfinavir anti-aids drug in inhibiting cellular kinase protein and inhibiting growth of cancer cell showed that, docking of Thalidomide derivatives in multiple Myeloma was evaluated and showed that, the Pomalidomide Derivate has greatest effect on inhibiting alpha-beta

Tubulin Mitosis and inhibiting proliferation of cell division. Computational studies of Hydralazine, which is antihypertensive drug, showed that this compound by DNA methylation and inhibiting proliferation of growing cells has anti-cancer effect.

Asadi et al. (2018), in a research examined effect of complex Manganese (II) andits bound to DNA and molecular docking by the use of DFT computational method and IR & UV theory studies. In this research, the interaction amount of related complex of metallic center to DNA by the use of CD spectroscopy methods and UV-Vis spectroscopy method, Electrophoresis gel, viscosity and Cyclic voltammetry were studied. The interaction of this compound with two types of DNA in Leukemia indicates excellent interaction of this compound similar to Cisplatin anti-cancer drug. Then in the theory section, electron density theory was used to computation and optimization of geometry. Theoretical computations showed that, the complex interaction with the small DNA screws had a higher interaction.

Bandiopyas et al. (2016), in a research surveyed the link structure and molecular singularity between DNA and Ligands based on oxime and Palladium complexes by using DFT computational method. In this study, interaction of Palladium complex (II) with Phenyl (Pyridine-2- hydrazine) Acetaldehyde oxime (LH) and pair of two-stranded base of DNA were studied by using DFT computational method. Spectral, electrochemical and biophysics behavior of this set were evaluated. In terms of physicochemical parameters, the following binding constants were resulted. For Ligand of binding constant 3.93×10^4 and for consonant complex $1.38 \times 10^3\ M^{-1}$ were resulted.

Hume et al. (2013), in a research surveyed the formation of Mitomycin as an alkylating agent through DFT computational method. The mechanism of DNA complex formation with other complexes has been very successful with DFT computational method, particularly for simple models. By comparing obtained results of computations, mechanical properties were predicted with high accuracy. Reduction of one and two-electron of system strongly depends on ph.

The property of charge transfer in the DNA, not only creates ideal properties to detect the sequence of DNA in the electrical and electrochemical biosensors, but also

facilitates the oxidation capability of bases existing in it and also leads to genetic mutation and disorder in the genetic process (Gray, 2006).

Two mechanisms of the electron transfer and electron hole are recommended for transferring of charge and oxidation of organic bases in two strands. In transmitting the electron hole, the oxidation mechanism of the DNA, especially the base of the guanine, is intended; but in the transmission of electron, the role of transferring the charge of all the bases should be considered. Among the bases existing in double strands, the property of guanine charge transfer is better than other bases; so that the percent of guanine base existing in the double strands have a direct effect on the property of charge transfer in the double strands (Forshew et al., 2012). The tendency for electron absorption in the guanine is less than other bases existing in the double strands. On the other hand, it makes the potential of guanine oxidation more susceptible than other bases (Bensimon et al., 2011).

2. Computaional methods

The molecular structure, quantum mechanics and Theoretical computations, charges distribution for RNA and DNA calculated using standard GIAO and B3LYP level of theory with 6-31 G(d) basis set with the gaussian 09 program to performed to study chemical and physical properties of nuclei and NMR chemical shift data [15] .Gaussian 09 is a computational chemistry software package appropriate to demonstration interaction of electrons in atoms and molecules. Molecular orbital energies, bond energies, molecular geometries and energies, and vibrational frequencies are the other features can be found in this program. The chemical shift refers to aspect dependent on the secondary magnetic field created by the induced motions of the electrons surrounding nucleus [16] .The NMR analysis have been fulfilled with four parameters including, magnetic isotropic (σiso) and magnetic anisotropic (σaniso) shielding,σ_{11},σ_{22},σ_{33} as shown in the following result for its fundamental importance in chemistry and biochemistry studies ,in which the σ defined as magnetic shielding tensor(ppm) and (η) defined as shielding asymmetry .σ also refers to the differential resonance shift due to the induced motion of the electrons [17] . Kinetic and thermodynamic investigations, geometry optimization, Monte Carlo and vibrational

analysis done by using HyperChem 8.0.8 software which is a sophisticated molecular modeling environment that is familiar for its quality, Flexibility, and ease of use. 3D embodiment with quantum calculations, molecular mechanics, and dynamics are other capability of this tool [18]. For Mont Carlo in molecular mechanic method we optimized Potential, kinetic and total energy with 10 steps in 310 k degree (the most stable and important temperature) and 298 k degree (environment temperature) and for Semi empirical the Am1 method with all parameters (Total Energy, Binding Energy, Isolated Atomic Energy, Electronic Energy, Core–Core Interaction and Heat of Formation) is the best vibration analysis of molecules using a quantum mechanical approach that was obtained Semi empirical (Mollaamin and Monajjemi, 2015).

3. Results and Discussion

3.1. Examination of Double-stranded NBO with sequences of AAAAA, GACTG and GGGGG

The energy levels and orbital shape of HOMO and LUMO from Gaussian Software and DFT calculations of this sequence are presented further. Table 1 presents the energy values of the single-stranded molecule with sequences of AAAAA, GACTG and GGGGG. The energy of formation for these sequences is also given in Table 2.

Table 1: HOMO and LUMO Energy in different double-strands

Structure	HOMO(ev)	LUMO(ev)
double-strand GGGGG	-0.30895	-0.30401
double-strand AAAAA	-0.31190	-0.31093
double-strand GACTG	-o.31037	-0.30931

Table 2: The formation energy in different double-standard

Structure	HF of formation energy (Hartree–Fock)	symmetry

GGGGG double-strand	299.80268	C01
AAAAA double-strand	2449.25418	C01
GACTG double-strand	2756.235487	C01

3.2. LUMO orbital

The orbital shape of double-stranded HOMO with the GGGGG sequence is presented in the following figure. Due to the resonance of π-bond in natural molecular orbital structure, this molecule is very large and uninterrupted.

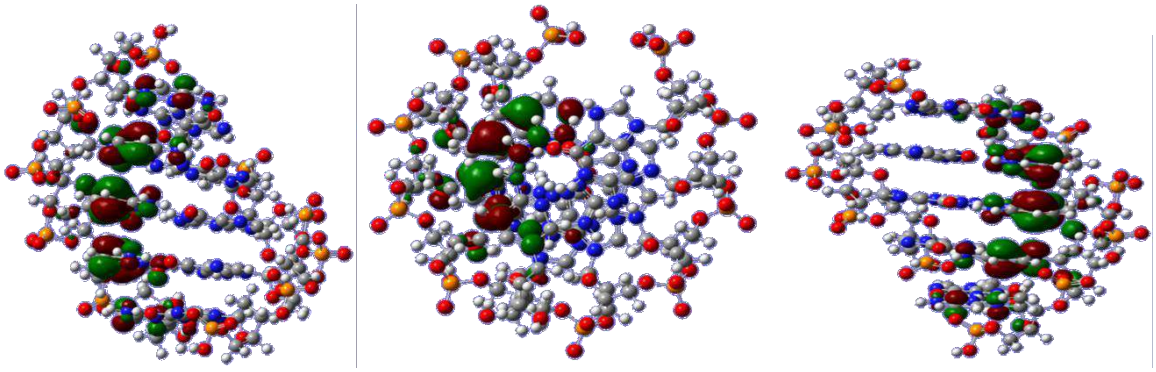

Fig 1: LUMO orbital with GGGGG sequence

3.3. HOMO orbital

The orbital shape of double-stranded HOMO with the AAAAA sequence is presented in the following figure.

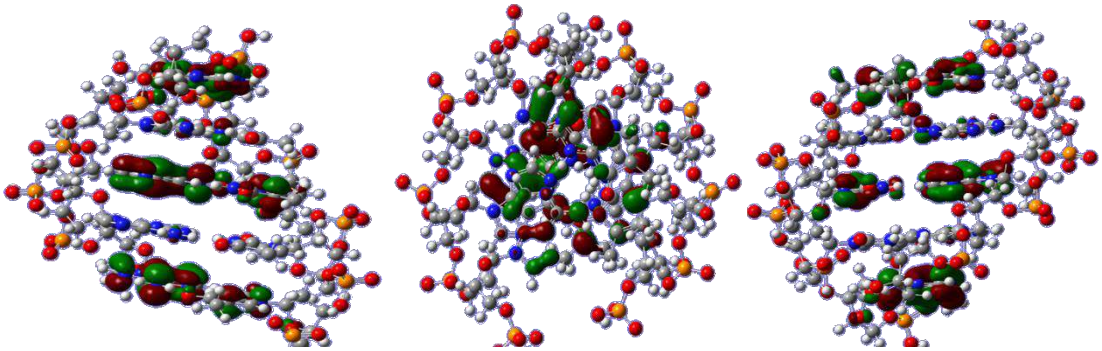

Fig 2: HOMO orbital with AAAAA sequence

Due to the calculations and also examination of the structure and arrangement of the LUMO and HOMO orbitals, it was found that the sequences with the largest number of guanine base are oxidized earlier and the charge transfer and oxidation process performed easier.

3.4. Investigation of isotropic and anisotropic parameters for bases and nucleotides.

According to the data and NMR calculations for isotropic and anisotropic parameters for the bases and nucleotides, a comparison was performed between the oxidized and normal states. In bases, according to data comparison, it was found that the highest difference between the oxidized and the normal state for the adenine, guanine, cytosine and thymine bases is in the N_3, N_3 ,N_1, N_{10} atoms, respectively, that is corresponding to the experimental results.

In nucleotides, according to data comparison, it was found that for isotropic and anisotropic parameters, the highest difference between the normal and oxidized state for adenosine, guanosine, cytidine, and thymidine in O_2 atoms related to the phosphate group, that is corresponding to the experimental results.

3.5. Investigation of isotropic and anisotropic parameters for single-stranded and double-stranded DNA

The purpose of this project is to investigate the theoretical methods for measuring chemo-physical properties of nucleic acids during the radicalization of DNA and the incidence of cancer. For this purpose, structures consisting of DNA nucleotides were considered and all structures were optimized using DFT at CAM-B3LYP / 6-31G

level and spatial parameters such as bond length, HOMO and LUMO orbitals and thermodynamic parameters as well as NMR spectroscopy were obtained. The results showed that guanine base had better conditions for oxidation compared to other bases. Also in NMR calculations using the GIAO method we were able to examine the single-strand and double-strand structure in different states of thesis when natural and abnormal.

Therefore, in this thesis, we attempted to find an normal relationship between chemical displacement and the rate of aberration of DNA from the natural state, by studying the comparison of isotropic and anisotropic parameters with respect to DNA bases such as adenine, guanine, cytosine, thymine, and concluded that asymmetry (η) is between (0,1) and skew is between (1-1) which can be correlated to the abnormalities of the DNA base from the normal state to abnormal.

It was also found that the oxygen atom of the phosphate group in the abnormal form showed the most changes in these parameters compared to the natural form. Also it can be seen by examining the chemical displacement spectra and anisotropy of the latency tensor in the Double-stranded DNA with GC sequence, the oxygen atom of the phosphate group in the guanosine nucleotide of the abnormal form has the highest value than the natural form and oxygen atoms belonging to the phosphate group in the cytotine nucleotide changed with less intense than guanine in these parameters. Also it can be seen by examining the spectra of Double-stranded DNA with AT sequence that the oxygen atom of the phosphate group in the abnormal form of the adenine nucleotide has the highest value than the natural form of DNA. Also the oxygen atom of the phosphate group in the thymidine nucleotide changed with less intense than adenine in these parameters, as shown in Fig 3 and 4. NMR calculations are also performed using the relations of 4-1 and 4-3.

$$\Omega = \sigma_{33} - \sigma_{11}$$
$$K = \frac{3(\sigma_{iso} - \sigma_{22})}{\Omega} \qquad (4\text{-}1)$$

$$\Delta\sigma = \sigma_{11} - \frac{\sigma_{22}+\sigma_{33}}{2} \qquad (4\text{-}2)$$

$$\eta = \frac{\sigma_{22}-\sigma_{33}}{\delta}$$

$$\sigma^{iso} = \frac{3}{trace\,\sigma} = \frac{3}{\sigma^{11}+\sigma^{22}+\sigma^{33}} \qquad (4\text{-}3)$$

Table 3: The values of adenosine nucleotide overlay parameters

Atom's type	σ aniso ppm	σ iso ppm	K rad	Ω ppm	σ33 ppm	σ22 Ppm	σ11 ppm	Muliken atomic charge
O	137.0079	218.6819	0.091	69.8588	152.4007	281.3853	222.2595	-0.647948
p	258.0445	335.1564	-0.021	224.7894	254.8455	270.9890	479.6349	1.495780
O	961.7359	66.3624	0.013	695.9465	440.8199	13.3940	-255.1266	0.5930299 -
O	6166.7607	-3973.4408	0.043	6865.7552	-8554.032	-1678.0117	-1688.2777	- 0.335427
O	231.2869	268.2188	-0.132	85.7005	274.7038	169.5483	360.4043	- 0.613474
C	34.4208	142.1014	0.097 -	13.2991	144.5186	150.5660	131.2195	- 0.160717
N	68.5388	189.4703	-0.069	33.9149	192.8832	216.5594	.158.968	- 0.706129
N	380.1567	31.8259	0.069	427.6186	285.0197	-46.9430	-142.5989	- 0.574808
C	121.3123	67.2695	0.036	143.4229	147.8067	49.6178	4.3838	0.639564

Table 4. The values of adenosine oxide nucleotide overlay parameters

Atom's Type	σ aniso ppm	σ iso ppm	K ppm	Ω ppm	σ33 Ppm	σ22 Ppm	σ11 ppm	Muliken atomic charge
O	164.6387	199.2350	0.0952	42.9872	200.5285	153.6607	243.5157	-0.6410
P	326.7443	399.1740	0.054	185.1866	349.9045	312.5155	535.0911	1.6368
O	202.1424	107.6228	0.033	181.2749	10.0672	121.4590	191.3421	-0.3178
O	188.7454	136.1039	-0.045	42.8396	119.3799	126.7124	162.2195	- 0.3400
O	185.1566	249.3519	-0.053	70.9462	244.1889	188.7317	315.1351	- 0.5626
C	54.7438	144.1590	0.014	22.0528	155.3159	143.8738	133.2631	- 0.1979
N	59.1531	181.3394	-0.432	18.7078	192.0187	141.2731	210.7265	-0.7618
N	241.7861	95.3768	0.011	174.9972	202.6740	55.7796	27.6768	- 0.7750
C	122.4604	71.3949	0014	72.1281	113.8931	58.5268	41.7650	0.7061

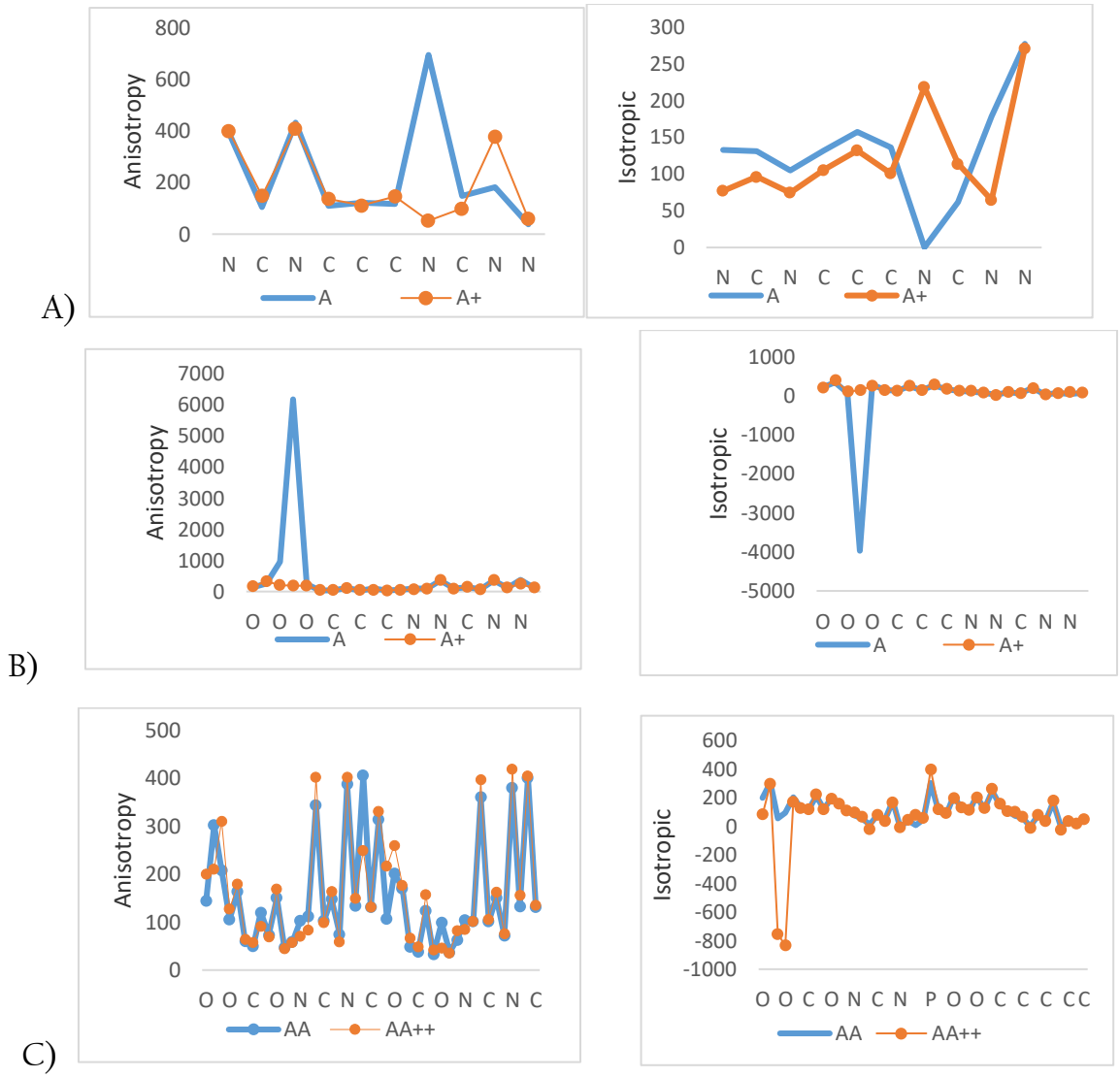

Fig 3: Charts Isotropic and Anisotropy A) Adenine B) Adenosine C) Single-strand and Oxidation form

Also it can be seen by examining the chemical displacement spectra and anisotropy of the latency tensor in the Double-stranded DNA with GC sequence, the oxygen atom of the phosphate group in the guanosine nucleotide of the abnormal form has the highest value than the natural form and oxygen atoms belonging to the phosphate group in the cytotine nucleotide changed with less intense than guanine in these parameters. Also it can be seen by examining the spectra of Double-stranded DNA with AT sequence that the oxygen atom of the phosphate group in the abnormal form of the adenine nucleotide has the highest value than the natural form of DNA. Also

the oxygen atom of the phosphate group in the thymidine nucleotide changed with less intense than adenine in these parameters.

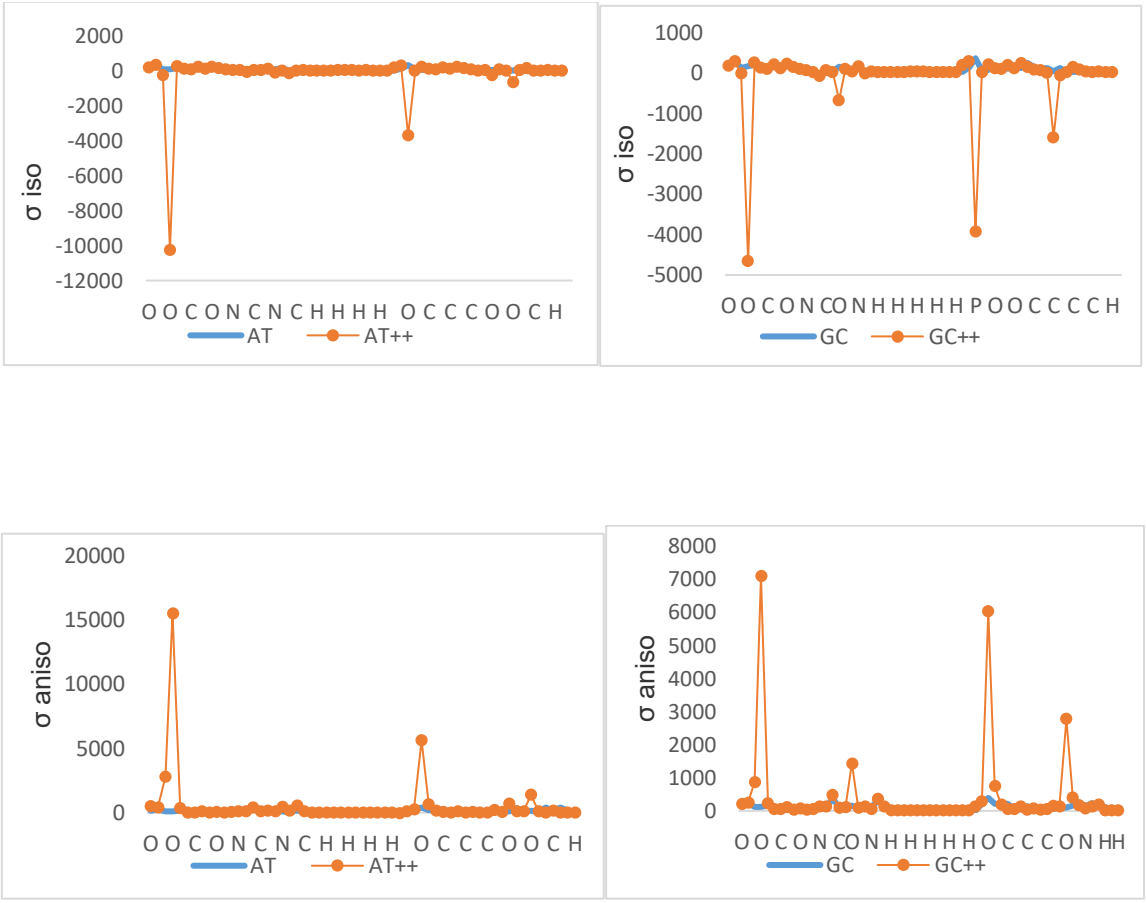

Fig 4: Isotropic and Anisotropy graphs of GC and AT Sequence and their double-stranded oxide form

3.6. Comparison of the anisotropy parameter of the latency tensor for DNA nucleotides

By examining the anisotropy parameter of the nucleotide lattency tensor, it was found that phosphate group oxygen has major changes in the natural and abnormal state that these parameters describe sample width and shape and with this a comparison can be made between the two states that shown in Fig 5.

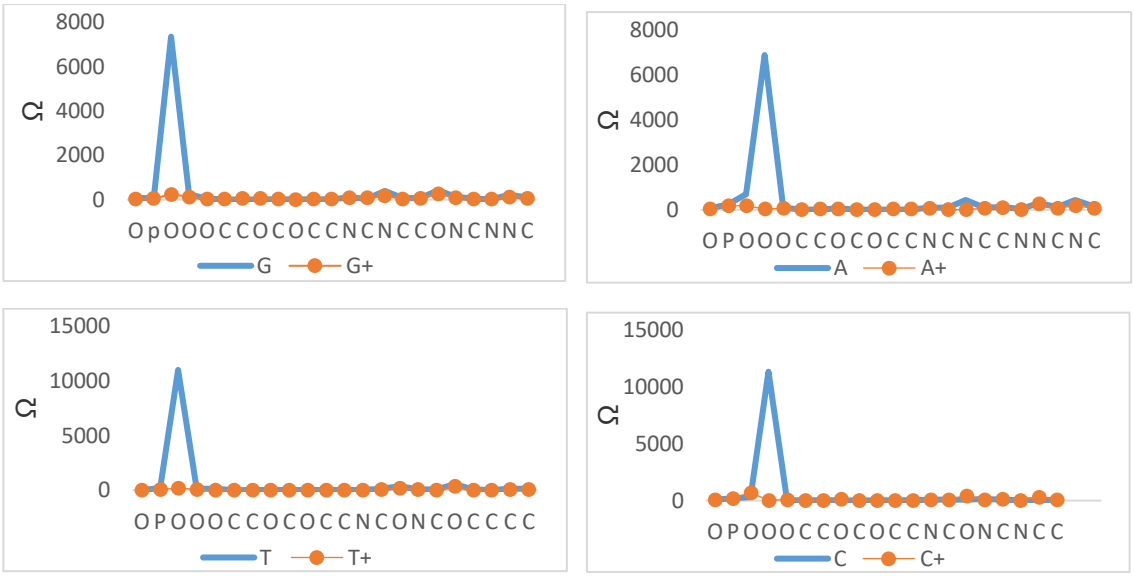

Figure 5: Comparision of Overaly Parameters for Nucleotide

3.7. Investigation of Thermodynamic Parameters of DNA Nucleotides

By studying the thermodynamic parameters much information can be obtained about how chemical reactions proceed and progress. In the present study, using the B3LYP / 6-31G FREQ order, we obtained thermodynamic parameters for DNA nucleotides, the values of which are reported in tables 5 to 7. Thermodynamic properties including internal energy, enthalpy change, entropy change, Gibbs free energy change and specific heat capacity change were calculated for all DNA bases in different states at a temperature of 298.15. Initially, the values of the thermodynamic parameters were calculated using the relations 4-6 to 4-8, that results presented in tables 5 to 7.

$$\Delta H(298K) = \Sigma \Delta H_{prod}(298K) - \Sigma \Delta H_{reac}(298K) \quad (4\text{-}6)$$

$$\Delta G(298K) = \Sigma \Delta G_{prod}(298K) - \Sigma \Delta G_{reac}(298K) \quad (4\text{-}7)$$

$$\Delta G = \Delta H - T\Delta S \quad (4\text{-}8)$$

In evaluating DNA bases observed that Guanine base compared to other bases has less ΔH and less ΔG as well as higher ΔS than other bases, indicating that the guanine base is oxidized more readily than other bases and its irregularity increases.
In evaluating DNA nucleotides observed that guanosine nucleotide compared to other nucleotides has less ΔH and less ΔG than other bases, indicating that guanosine

nucleotide is relatively oxidized more easily than other bases and its irregularity increases.

In evaluating single-stranded DNA observed that the guanine-guanine base pair has less ΔH and less ΔG as well as higher ΔS than the other bases, indicating that guanosine nucleotide is relatively oxidized more easily than other bases and its irregularity increases.

Table 5: Difference of Thermodynamic Functions of DNA Bases and their oxide form

structure	ΔE Kcal/mol	ΔCV Cal/mol-kelvin	ΔS Cal/mol-kelvin	ΔH Cal/mol-kelvin	ΔG Kcal/mol
Adenine	-3.854	-1.676	-0.0006	96.7619	96.9502
Guanin	-3.77	-0.265	0.0018	92.8714	92.3066
Cytozin	-3.016	-0.73	-0.001	99.3347	99.6485
Thymin	-5.838	-3.148	-0.009	109.1239	111.8221

Table 6: Difference of Thermodynamic Functions of DNA Nucleotides and their oxide for

structure	ΔE Kcal/mol	ΔCV Cal/mol-kelvin	ΔS Cal/mol-kelvin	ΔH Cal/mol-kelvin	ΔG Kcal/mol
Adenosine monophosphate	4.427	0.603	-0.02	114.3322	120.0362
Guanosine monophosphate	4.301	-6.44	0.01	108.4612	105.0077
Cytidine monophosphate	4.197	-3.059	0.0032	148.9707	149.5355
Thymidine monophosphate	3.874	-2.392	0.0033	145.7077	144.9684

Table 7: Difference of Thermodynamic Functions of single-stranded DNA and their oxide form

structure	ΔE Kcal/mol	ΔCV Cal/mol-kelvin	ΔS Cal/mol-kelvin	ΔH Cal/mol-kelvin	ΔG Kcal/mol
Single-strand AA	-4.743	-7.867	-0.37	362.1984	298.0670
Single-strand GG	-8.382	-12.386	0.21	348.3305	359.5001
Single-strand CC	-14.708	-16.225	-0.36	356.1743	367.4068
Single-strand TT	-16.548	-23.659	-0.06	379.5804	397.4645
Single-strand GC	-7.797	-9.83	-0.05	383.5338	399.1473
Single-strand AT	-5.095	-7.244	-0.013	361.8847	365.8562

3.8. Comparing the results of this study with similar research methods

A comparision table 8 between the results of this study and other research methods is presented.

Table 8: compares the results of this study with other research methods.

Research group	Type of review	Research Methodology	Results
Forster& et al., 2018	Influence of oxygen on DNA Degradation	Monte Carlo	59/5% of Degradation in 19% eV
Baglion&et al., 2008	Examining the DNA structure containing 42 bases	Monte Carlo	Bottom 6-sided structure with a diameter of 7 nm
Kino& et al., 2012	Degradation and oxidation of guanine	Gossin	Sustainable Energy 19/9 kcal/mol for Sp2:G 16/3 kcal/mol for Oz:G
Current Research	Investigation of Physical and Chemical Properties Of nucleotides in DNA mutation and oxidation	Gossin	GG sequence with 0/45919 E_{Gap} in single-stranded and sequence of GC in double-stranded with the most-likely points of mutation and oxidation. And by examining the NMR spectrum and the spectrum differences in the cases of normal and abnormal, identified cancer DNA.

2,2,4-Triamino-5(2H)-oxazolone: guanine

Oz:G

Sp2:G spiro-imino-dihydantoin: guanine

Conclusion

The results of the DFT calculations and Gaussian and NBO software have very high accuracy and the results from the calculations with this software have shown good agreement with experimental results. The computational method of QM / MM is superior to that of taking all the forces of gravity and physical, chemical and electron repulsion between atoms and their links between them, in comparison with other methods. Also it can be seen by examining the chemical displacement spectra and

anisotropy of the latency tensor in the Double-stranded DNA with GC sequence, the oxygen atom of the phosphate group in the guanosine nucleotide of the abnormal form has the highest value than the natural form and oxygen atoms belonging to the phosphate group in the cytotine nucleotide changed with less intense than guanine in these parameters. Also it can be seen by examining the spectra of Double-stranded DNA with AT sequence that the oxygen atom of the phosphate group in the abnormal form of the adenine nucleotide has the highest value than the natural form of DNA. Also the oxygen atom of the phosphate group in the thymidine nucleotide changed with less intense than adenine in these parameters.

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