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Journal of Systematic Innovation

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The works must be unpublished and refer to topics of electromagnetism, electrical distribution, sources innovation in electrical, engineering signal, amplification electrical, motor design science, materials in electrical power, plants management and distribution of electrical energies and other topics related to Engineering and Technology.

Presentation of the content

In the first article we present, *Removal of Oil Pollution in water using hydrophobic silica*, by SALAZAR-HERNÁNDEZ, Carmen, SALAZAR-HERNÁNDEZ, Mercedes, HERNÁNDEZ-ARIAS, Lizeth Jocelyn and MENDOZA-MIRANDA, Juan Manuel, with adscription in the Instituto Politécnico Nacional and Universidad de Guanajuato, in the next article we present, *Graphene oxide and graphite oxide used as reinforcement in composites synthesized from cellulose acetate and polyacrylic acid*, by SÁNCHEZ-MÁRQUEZ, Juan, FUENTES-RAMÍREZ, Rosalba and RUIZ-CAMACHO, Beatriz, with adscription in the Universidad de Guanajuato, in the next article we present, *Parametric design applied to die cutting machine*, by JARA-RUIZ, Ricardo, DE LA CRUZ, Jesús, RODRÍGUEZ-FRANCO, Martín Eduardo and DELGADO-GUERRERO, Sergio Humberto, with adscription in the Universidad Tecnológica del Norte de Aguascalientes, in the next article we present, *Methodology for the design of a multilayer polymeric membrane system with potential use in hemofiltration*, by NUÑEZ-HERNÁNDEZ Lourdes Nohemi, KANTUN-UICAB María Cristina, PÉREZ-CASTAÑEDA Laura Maryela, and TÉLLEZ-MARTÍNEZ Jorge Sergio, with adscription in the Universidad Politécnica de Juventino Rosas and Universidad Tecnológica de Tamaulipas Norte.

Content

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Removal of Oil Pollution in water using hydrophobic silica

Remoción de aceite en agua usando sílice hidrofóbica

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Abstract

Nowadays the contamination in waters by oily substances turns out to be a problem of world-wide scope and although some methods of removal of oils in water exist; these present some limitations; therefore, this project proposes the use of hydrophobic silicas as absorbent materials for oily substances. Modified silicas (R-SiO_2) were synthesized using the Stöber method, modifying the surface by co-condensation. Tetraethyl-orthosilicate (TEOS) and two surface modifiers were used as silica former: Methyl-trimethoxysilane (MeTEOS) and n-octyl-triethoxysilane (nOctyl-TEOS). The R-SiO_2 were characterized by infrared spectroscopy identifying the modifying groups and their hydrophobicity was qualitatively evaluated according to the change in solubility in water. Finally, the removability of an automotive motor oil was evaluated by determining the amount of oil removed per gram of modified silica.

R-SiO_2, Hydrophobicity, Oil removal

Resumen

Hoy en día la contaminación en aguas por sustancias oleosas resultan ser un problema de ámbito mundial y aunque existen algunos métodos de remoción de aceites en agua; éstos presentan algunas limitantes por lo que, en este proyecto se propone el uso de sílices hidrofóbicas como materiales absorbentes para las sustancias oleosas. Las sílices modificadas (R-SiO_2) se sintetizaron empleando el método de Stöber realizando la modificación de la superficie por co-condensación. Se utilizó como formador de sílice el Tetraetil-ortosilicato (TEOS) y dos modificadores de superficie: Metil-trimetoxisilano (MeTMOS) y el n-octil-trietoxisilano (nOctil-TEtOS). Las R-SiO_2 se caracterizaron por espectroscopia de infrarrojo identificando los grupos modificadores y su hidrofobicidad se evalúo cualitativamente de acuerdo con el cambio de solubilidad en agua observada. Finalmente, se evalúo la capacidad de remoción de un aceite de motor automotriz determinando la cantidad de aceite removido por gramo de sílice modificada.

R-SiO_2, Hidrofobicidad, Remoción de aceite

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Introduction

wastewater containing pollutant oil is commonly produced in a wide range of industries, such as oil extraction, petrochemical production, machinery manufacturing, and food production, causing groundwater to be directly affected by polluting oils (Escobar J, 2002), thus, the selective oil removal from water becomes an important issue for science and environmental engineering (García Pérez A, 2021). Current methods to removal waste oil from water can be divided into three methods as: 1) collecting oil from water surface, 2) mixing the wastewater with dispersing agents to promote the natural degradation of pollutant oil and 3) in situ polluting oils burning (Kumar Gupta R, 2017). However, these methods have different limitations, among them, the complete elimination of the pollutant oil. On the other hand, mesoporous silica has been explored as a removal system for different pollutants in water, for example, to remove heavy metals (Gutierrez-Valtierra M, 2019), pesticides (Moliner-Martínez, 2014), chlorinated compounds (Rodríguez D, 2013), colorants (Sienkiewicz A, 2019) among others. Thus, the aim of this paper is to evaluate modified silica with organic groups as a removal media for pollutant oils such as internal combustion engine oil.

Methodology

Synthesis of Silica Nanoparticles using Stöber's Method

100 mL of EtOH and 10 mL of water were placed in a vessel with stirring system and then 3 mL of NH3OH was added as a catalyst; taking care that the pH of the solution is lying between 9 and 10. Later, 10 g of TEOS (99.9% purity, Aldrich) were added and the solution was stirring for an hour and subsequently 12 h for aging. The solid obtained is filtered and washed using ethanol and dried for 6 h at 80ºC.

Silica Modification: Synthesis of R-SiO_2

The silica modification was carried out by Co-condensation; as shown in Figure 1; the polymerization of TEOS in an alkaline medium (pH 9-10) is carried out with the modifying agents; which were Methyl-trimethoxysilane (MeTMOS; 98% purity, Aldrich) and n-octyl-triethoxysilane (nOctyl-TEtOS; 97% purity, Aldrich).

The modifying agent was added to the TEOS solution in ethanol / water after 15 min of adding the TEOS. Table 1 shows the ratio of TEOS: modifying agent employed. The mixture is stirring for one hour and subsequently aged for 12 h, the solid obtained is filtered and washed with ethanol to dry at 80 ° C for 6 h.

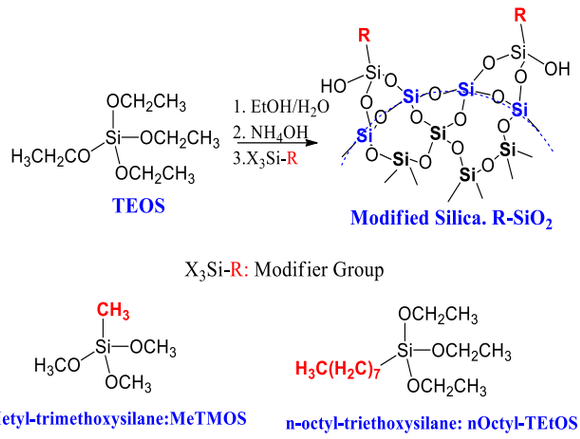

Figure 1 R-SiO_2 synthesis method

	TEOS	Modifier Group
MeTMOS	10 g	4.27 g
nOctyl-TEtOS	10 g	6.63 g

Table 1 TEOS / Modifying group used in the synthesis of R-SiO_2

R-SiO_2 Characterization

The chemical structure of silica and the addition of the modifier agent was studied by reflectance attenuation infrared spectroscopy (ATR-FT) using a Nicolet-iS10 Thermoscientific equipment, obtaining an average of 16 scans, with a 4 cm^{-1} resolution, and spectral window from 4000 to 600 cm^{-1}.

Oil Removal Capacity Measurement

One gram of combustion engine oil was poured into a beaker and modified silica nanoparticles were subsequently added. After the oil gelled, the mixture of silica and oil nanoparticles was placed on top of a mesh, and the measurement of the removal was carried out dividing the oil mass by the minimum mass of hydrophobic silica nanoparticles required for oil removal.

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Results

Infrared spectroscopic characterization of R-SiO_2

Figure 2 shows the silica and the modifying agents infrared spectra that were used; Table 2 shows the of the main peaks assignment; Furthermore, the modifying groups that will give the silica its hydrophobic properties are highlighted with a red circle. For methyl trimethoxysilane the hydrophobic characteristic is due by the methyl group ($–CH_3$); and in n-octyl-triethoxysilane the hydrophobic characteristic is due by group n-octyl ($–CH_2(CH_2)_6CH_3$).

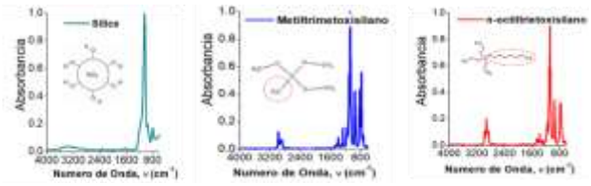

Figure 2 FT-IR reference spectrum for silica and modifying agents' materials

	Functional Group	Wavenumber (cm^{-1})
Silica	Si-O-Si	1150;570
	Free Si-OH	945
	hydrogen bridge Si-OH	3490-1600
MeTMOS	-CH3	2900-3100
		1400
	-Si-O	1100
	-Si-C	1200
nOctil-TEtOS	$-CH_2$ y CH_3	2900-3100
		1400
	-Si-O	1100
	-Si-C	1200

Table 2 IR-TF vibrational modes for silica and modifying groups

Figure 3 shows the modified silica spectra, the modifier group is highlighted in a circle. All silicas retain moisture on the surface in the form of free silanols as a thin shoulder present at 945 cm^{-1}; furthermore, the broad band at 3450 cm^{-1} indicates the presence of physisorbed water. Moreover, the siloxane base structure (Si-O-Si) is identified with the intense and wide peak observed around 1100 cm^{-1} and with the peak of moderate intensity at 600 cm^{-1}. Finally, the Si-C group (1200 cm^{-1}) of the modifier was observed with low intensity in SiO_2–Me and SiO_2–octyl.

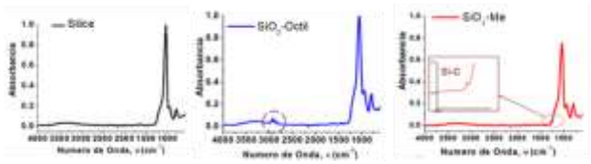

Figure 3 FT-IR spectrum of silica and modified silica (R–SiO_2)

Hydrophobic Behavior of R-SiO_2

Hydrophobicity was determined observing the change in solubility of silica in water; Thus, 0.3 g of silica and R-SiO_2 were added to 100 ml of distilled water, as shown in Figure 4. The silica precipitates towards to the bottom of the glass due to its poor solubility in water (Figure 4a). However, when the modifying groups are added, hydrophobic silicas were obtained that tend to float on the water surface (Figure 4b and c). According to these results, the degree of hydrophobicity has the following behavior: SiO_2 <SiO_2–Me <SiO_2–octyl.

Figure 4 Hydrophobicity test for silica and R–SiO_2

Evaluation of Oil Removal Capacity using R-SiO_2

Table 3 shows the qualitatively results of the adsorption of two grams of oil on the silicas. It is observed that the unmodified silica does not have the ability to remove oil, thus, the silica precipitates and the oil remains on the water. On the other hand, the modified silicas remove the oil efficiently, precipitating the silica and the trapped oil into the modified silica.

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Sample	Amount of Silica required for absorption (g)	
SiO_2	Sin absorción	
SiO_2-MeTMOS	0.742	
SiO_2-nOcilTEtOS	0.752	

Table 3 Results of the amount of silica required to carry out the oil absorption at 25 ° C

The adsorption capacity of the silicas was determined according to Equation 1. Thus, table 4 summarizes the adsorption capacity of modified silicas, the highest removal was observed with the modified silica containing PDMS followed by the modified silica containg the methyl group and the lowest removal capacity was for the modified silica containing the octyl groups.

Figure 5 shows the ratio of the required mass of modified silica nanoparticles for the removal different amounts of oil. For example, according to the removal capacity of silicas, to remove 100g of oil, 35 g of SiO2-Me and 37g of SiO2-octyl are required;

Therefore, the removal capacity (C.R) was calculated as expressed in Equation 1 for the silicas studied and its values are indicated in Table 4. Thus, similar removal capacity was quantified for both methyl and octil modifier groups. On the other hand, it is observed that the unmodified silica does not have oil removal capacity, this due to its hydrophilic properties.

$$C.R = \frac{oil\ mass}{silica\ nanoparticle\ mass} \quad (1)$$

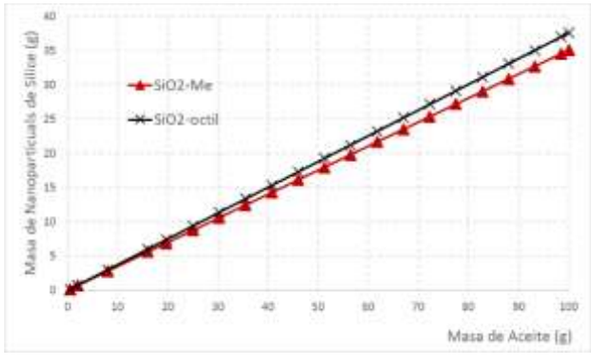

Figure 5 Amount of silica nanoparticles modified to remove oil

	Removal capacity ($g_{oil}/g_{silica\ nanoparticles}$)
SiO_2	---
SiO_2-Me	2.85
SiO_2-Octyl	2.66

Table 4 Oil removal capacity for R-SiO_2

Conclusions

Nanoparticles of mesoporous silica were modified coupling on the surface methyl (methyl-trimethoxysilane with the methyl group -CH_3) and octyl (n-octyl-triethoxysilane with the n-octyl group -CH_2 (CH_2) $_6CH_3$) groups. The modified silicas show high hydrophobicity with the following behavior: SiO_2 <SiO_2–Me <SiO_2–octyl. The modified silica was characterized and contrasted with its precursors for its development, results shows that the modified silicas have a base structure of siloxanes (Si–O–Si) as well as the Si–C group for its modifiers with hydrophobic properties coupled in their structure. According to the results obtained, both modified silicas presented similar removal capacity, being slightly higher for SiO_2-Me.

Acknowledgements

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Article **Journal of Systematic Innovation**
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Graphene oxide and graphite oxide used as reinforcement in composites synthesized from cellulose acetate and polyacrylic acid

Óxido de grafeno y óxido de grafito empleados como refuerzo en compositos sintetizados a partir de acetato de celulosa y ácido poliacrílico

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Abstract

This work focused on the synthesis and characterization of composites, obtained based on polyacrylic acid and cellulose acetate, which incorporated graphite oxide and graphene oxide as structural reinforcement. The composites were obtained using the phase inversion method and the incorporation of the reinforcement, during the synthesis process, was carried out in proportions of 1% by weight. The characterization of the composites was carried out using IR, Raman, BET, SEM spectroscopy techniques and methods for determining acidic and basic sites. The results obtained showed that it is possible to synthesize composites that present a network configuration, made up of layers that give the material the effect of depth. Furthermore, it was possible to observe that both graphite oxide and graphene oxide were deposited on the outer edge of the hexagonal pores present in the material. Finally, the concentration values of acidic and basic sites were obtained. The presence of these sites could be associated with carboxylic groups inserted during the oxidation of graphitic materials and with non-reactive sites present in cellulose.

Graphene oxide, Cellulose Acetate, Polyacrylic Acid

Resumen

Este trabajo se enfocó en la síntesis y caracterización de compositos, obtenidos a base de ácido poliacrílico y acetato de celulosa, los cuáles incorporaron óxido de grafito y óxido de grafeno como refuerzo estructural. Los compositos fueron obtenidos empleando el método de inversión de fases y la incorporación del refuerzo, durante el proceso de síntesis, se llevó a cabo en proporciones del 1% en peso. La caracterización de los compositos se realizó empleando técnicas de Espectroscopía IR, Raman, BET, SEM y métodos de determinación de sitios ácidos y básicos. Los resultados obtenidos mostraron que es posible sintetizar compositos que presenten una configuración en red, constituida por capas que den al material el efecto de profundidad. Además, fue posible observar que tanto el óxido de grafito como el óxido de grafeno se depositaron en el borde exterior de los poros hexagonales presentes en el material. Finalmente, los valores de concentración de sitios ácidos y básicos fueron obtenidos. La presencia de estos sitios pudo ser asociada con grupos carboxílicos insertados durante la oxidación de los materiales grafíticos y con sitios no reactivos presentes en la celulosa.

Óxido de Grafeno, Acetado de Celulosa, Ácido Poliacrílico

Citation: SÁNCHEZ-MÁRQUEZ, Juan, FUENTES-RAMÍREZ, Rosalba and RUIZ-CAMACHO, Beatriz. Graphene oxide and graphite oxide used as reinforcement in composites synthesized from cellulose acetate and polyacrylic acid. Journal of Systematic Innovation. 2021. 5-16: 6-13

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Introduction

It is important to point that cellulose acetate is one of the most used materials in the manufacture of porous materials. (Kutowy 1975,1449). From this material we can produce membranes with low binding and adequate porosity (Park 1968, 277). Furthermore, cellulose acetate is cheap, with adequate biocompatibility and good resistance to soiling. In relation to the disadvantages of this material we can say that this material has a poor mechanical strength and low thermal and chemical resistance (Sivakumar 1999, 1647) and (Sivakumar 2000, 215). On the other hand, polyacrylic acid is a high molecular weight polymer with an outstanding ability to absorb and retain water, as well as to swell and increase many times its original volume (hydrogel). Polyacrylic acid is commonly used in the manufacture of adhesives and as a dispersing or thickening agent in paint, drug, and cosmetic manufacturing processes. This project has worked on the synthesis of composites made from polyacrylic acid and cellulose acetate that can be used as a support for graphitic materials.

Previous studies have shown that it is possible to control the porosity of materials obtained from the crosslinking reaction of cellulose acetate and polyacrylic acid, just by varying the time of immersion in hot water. The pore diameter ranges from 3 to 100 microns in these materials, and it shows a nonlinear behaviour as a function of the temperature of the immersion medium (Estrada 2010, 3). The possibility of controlling the pore through an external factor, such as the variation of water temperature immersion, enhances the possible applications of these materials.

Graphene is one of the most important carbon nanostructures due to its outstanding physical and chemical properties. Graphene has a unique two-dimensional structure of superimposed layers that makes it attractive for multiple applications (Rao 2009, 7752), (Geim 2007, 183) and (Kovtyukhova 1992, 566). The mass production of graphene oxide (GO) has been possible from chemical methods (Hummers' Method) that include oxidation and the subsequent reduction of this compound to produce reduced graphene oxide (RGO). These procedures have favoured the search for applications for these materials (Sreeprasad 2011, 921).

However, it is important to note that to take advantage of the outstanding properties of graphene, we must consider that these materials need to be supported on other materials to obtain attractive composite structures with a better performance than the performance showed by pure initial components.

Thus, the addition of fillers in polymers is an attractive method to obtain materials with novel properties. The use of polymers provides support to graphene oxide and permits its use in continuous processes and new applications such as the adsorption of heavy metals (Gadupudi 2007, 224), (Tuzen 2007, 219) and (Hu 2009, 1542).

Methodology

Graphene oxide synthesis (OG)

Graphene oxide was obtained from crystalline graphite (Electron Microscope Science, No. 70230). The graphite was oxidized using the improved method of Hummers (Bin 2011, 31). This method allows obtaining graphite oxide using a mixture of graphite, sulfuric acid (Jalmek, purity: 95-98 %, MW = 98.08 g mol^{-1}) and potassium permanganate (JT Baker). The oxidation reaction was conducted at 35 °C, with a range of +/-3 °C, for 2 h, with a constant medium agitation. Then, the flask was removed from the heat and 92 mL of distilled water was slowly added to the flask.

The solution was kept under magnetic stirring for 15 min. Next, a mixture of 270 mL of distilled water and 10 mL of hydrogen peroxide (J. T Baker, 30% weight) was added. The final solution was washed with distilled water and the material obtained was dried at 65 °C (+/-2 °C) for 12 h. Graphene oxide was obtained from a sample of graphite oxide. The sample of graphite oxide was mixed with distilled water. This mixture was placed in an ultrasonic bath (Branson, Model 1510R-MTH) for 3 h at a frequency of 50-60 Hz. After this time, the solution was filtered and dried for later use.

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Synthesis of composite from cellulose acetate and polyacrylic acid

For the synthesis of the composites, the following chemical reagents were used: cellulose acetate (Sigma Aldrich) with a molecular weight of 50,000 by Gel permeation chromatography (GPC) and a degree of acetylation of 39.7% weight, and polyacrylic acid in aqueous solution (Sigma Aldrich) with a molecular weight of 30 000 g mol^{-1} and a percentage of 35% weight. All commercial reagents were used without any further purification step. Composite was prepared according to a procedure previously reported (Estrada 2010, 3). Initially, a solution was prepared dissolving 8 g of cellulose acetate in 100 mL of glacial acetic acid at room temperature.

Then, when the cellulose acetate had been completely dissolved, 10 mL of polyacrylic acid was added slowly with a constant medium agitation; this solution was heated at 60 °C under agitation for 30 min, allowing the crosslinking reaction between the cellulose acetate and the polyacrylic acid to take place. The final solution was cooled down to room temperature and stored for 3 days before use. To obtain the composites, several samples were poured into flat glad molds of 10 cm in diameter, leaving the molds with the solution floating on iced water at 4 °C, allowing the solution to reach the same temperature of iced water.

Thereafter, the mold with the polymer solution was completely immersed carefully into the cold water until the composites formed and subsequently permitted to rest for 15 min to allow the solidification of polymer solution. Once the composites were formed, they were withdrawn from the iced water and immediately placed into a bath of hot water at 60 °C. This procedure was applied to composites both with and without graphene oxide using concentrations of 1% by weight.

Surface Characterization

The characterization of polymer and graphene oxide was made by Fourier Transform Infrared spectroscopy with attenuated total reflectance (FTIR-ATR Vertex Model 70) in pressed KBr pellets (100mg KBr and 1 mg of sample) of graphitic materials.

For FTIR spectroscopy, the samples were dried at 333K for 24 h. The characterization by FTIR was complemented with a Raman analysis (Renishaw Raman Microscope Invia Reflex, Wotton-under-Edge, UK). Raman spectroscopy is a technique that offers numerous advantages in the chemical and structural analysis of the molecular networks of any material. This methodology relates values obtained from Raman spectra with structural characteristics of the material, based on bibliographic references (Bagheri 2021, 33).

The morphology of crosslinked polymer was investigated with the aid of the scanning electron microscope (Jeol JSM-6610LV) operated in the high vacuum mode at an acceleration voltage of 20 kV and a pressure of 20 Pa, the materials were previously coated with gold. The SEM images to the rest of materials were determined with an environmental scanning electron microscope (MEBA, PHILIPS: Model XL30) operated in the high vacuum mode too. The effective surface area and pore size distribution of the graphite materials were determined using N2-BET (ASAP 2010 V5.03). Finally, the surface charge and point of zero charge of the materials were evaluated using a potentiometric titration method proposed by Loskutov and Kuzin and the concentrations of acidic and basic sites were calculated using the equations proposed by Böehm.

Results

Infrared spectroscopy (FTIR-ATR)

The IR spectra of the mineral graphite and graphite oxide are compared in Graphic 1. The spectrum for mineral graphite shows peaks at 1300 and 1100 cm^{-1} associated with stretching vibrations of C-C bond and a peak at 1670 cm^{-1} associated with stretching vibrations of C=C bond. After the oxidation reaction, the spectrum for graphite oxide shows a peak at 3348 cm^{-1} associated with the stretching vibration of the OH bond in the water molecules present between the layers of graphite oxide. In addition, the peak at 1720 cm^{-1} is associated with the stretching of the carbonyl group (C=O) and the signal at 1589 cm-1 is attributed to the stretching of double bonds (C=C) of the graphite ring. Finally, the characteristic signals of the epoxy group (C-O-C) were observed at 1224 and 804 cm^{-1} and the stretching vibrations of the C-OH bond was observed at 1053 cm^{-1}.

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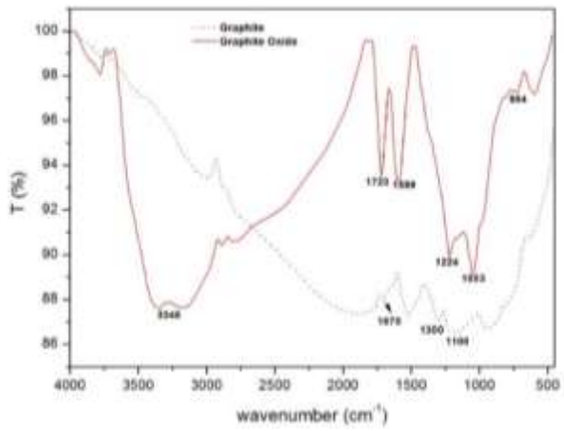
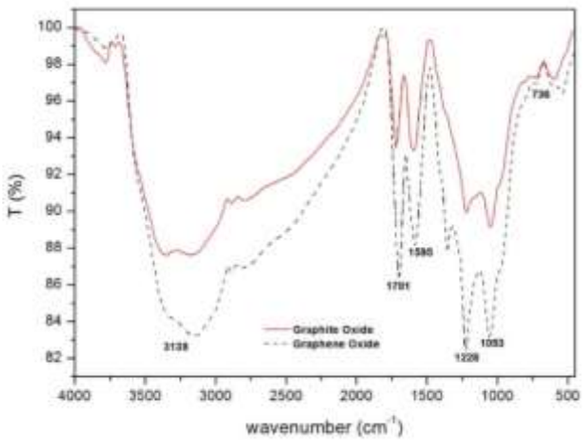


Graphic 1 Infrared spectra of graphite and graphite oxide

The IR spectra of graphite oxide and graphene oxide show functional groups with presence of oxygen. However, the graphene oxide shows more definite signs due to the reduced number of layers of material, Graphic 2.



Graphic 2 Infrared spectra of graphite oxide and graphene oxide

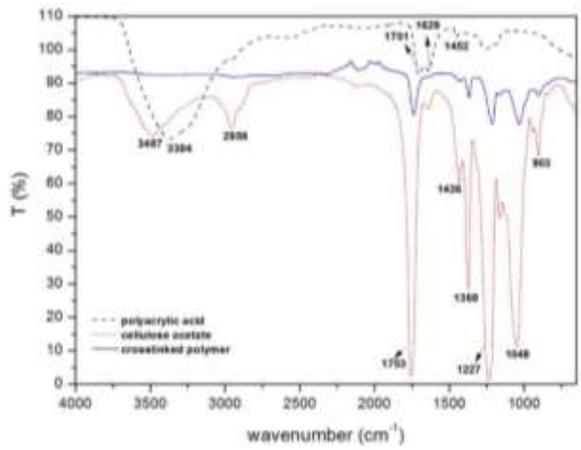
Crosslinked Polymer

Molecular interactions between materials were studied by obtaining their FTIR spectra. The IR spectra of cellulose acetate, polyacrylic acid and the crosslinked polymer are shown in Graphic 3. The spectrum for polyacrylic acid shows the typical bands for carboxylic acids, with the stretching absorption associated with the hydroxyl groups (O-H) in 3384 cm^{-1}, while the carbon-oxygen (C=O) absorption peak characteristic of carbonyl was observed at 1701 cm^{-1}. In addition, peaks for C=C and C-C stretching were observed at 1629 and 1234 cm^{-1}. Finally, the band in 1452 cm^{-1} can be assigned to the in-plane bending of the hydroxyl group.

The spectrum for cellulose acetate also showed an absorption band associated to the –OH stretching region in 3487 cm^{-1}, while the carbon–oxygen (C=O) absorption peak characteristic of carbonyl was observed at 1756 cm^{-1}. Peaks observed at 2958 cm^{-1} could be attributed to symmetric and asymmetric stretching vibrations while the signals placed at 1436 and 1368 cm^{-1} can be attributed to symmetric and asymmetric bending vibrations of the carbon-hydrogen bonds present in the methyl group.

Peaks observed between 1227 and 1048 cm^{-1} are characteristic of materials based on cellulose and they can be associated with the carboxylate group, the link between rings C-O-C and the pyranose ring, respectively. Finally, the band in 903 cm^{-1} cans be assigned to the out-plane bending of hydroxyl group. When the cellulose acetate and polyacrylic acid reacted, the bands associated with the carboxylic groups (C=O and OH) of the polyacrylic acid and the hydroxyl and acetyl groups of the cellulose acetate decrease significantly.

This proves that the crosslinking reaction between the polyacrylic acid and the cellulose acetate has occurred. Different graphitic materials were added to the crosslinked polymer. The IR spectra of polymer with materials made from graphite are shown in Graphic 4. These spectra show the characteristic peaks of the polymer crosslinked. In addition, it is not possible to observe interactions between the polymer and graphite materials from IR spectra.



Graphic 3 Infrared spectra of synthesized composite

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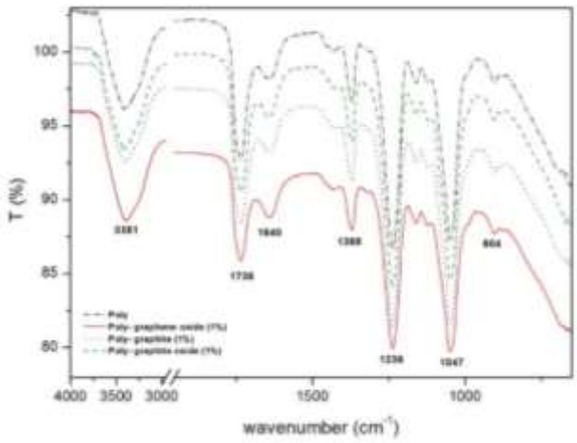
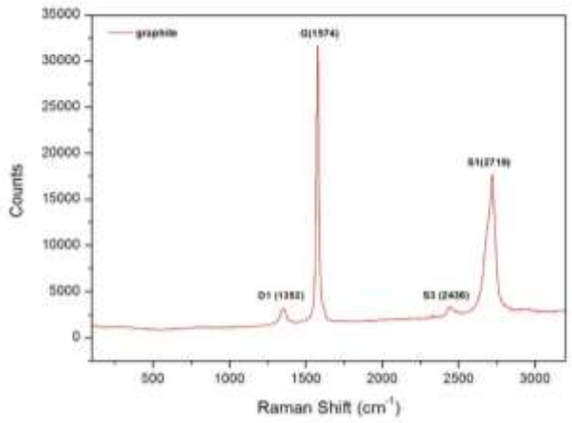


Graphic 4 Infrared spectra of the crosslinked polymer with graphite, graphite oxide and graphene oxide



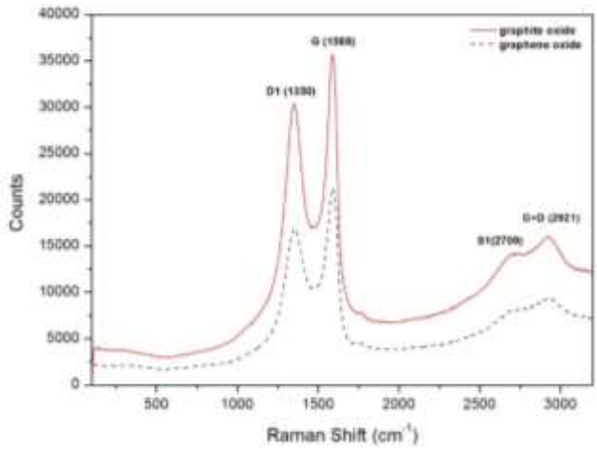
Graphic 5 Raman spectra of the mineral graphite

Raman spectroscopy

The most intense peaks observed for mineral graphite can be seen in Graphic 5. The peak at 1352 cm^{-1} (D1 band) is very small. It can be attributed to the graphite does not present many structural defects or impurities. In addition, the G band (1573 cm^{-1}) can be associated with the stretching vibration in hybridized carbon bond (C-C, sp2). This peak is the band that characterizes the mineral graphite. Finally, the peaks at 2719 cm^{-1} and 2436 cm^{-1} are known as S1 and S3, respectively.

The S1 band is considered an overtone associated with D1 band while S3 band is generated from transverse vibrations to the plane of graphite crystal and stretching vibrations in hybridized carbon bond. After chemical modification we can see a decrease in the order band (G band) and an increased in the disorder band (D band) with respect to that observed in graphite, Graphic 6.

The decrease in crystallinity may be due to the progressive incorporation of oxygen molecules between the graphene layers which make up the crystalline structure of graphite. Both graphite oxide to graphene oxide, an increase in the disorder causes second order bands (S1 and G+D band) begin to expand and lose intensity.



Graphic 6 Raman spectra of the graphite oxide and graphene oxide

Crosslinked Polymer Synthesis

When the crosslinking reaction takes place, the spectrum obtained shows primarily the characteristic Raman signals for the cellulose acetate while polyacrylic acid has remained undetected because their bands partially over-lapped those of cellulose acetate, Graphic 7.

The characteristic Raman signals for crosslinked polymer were present at 2939 and 1121 cm^{-1}, which are attributed to C-H stretching and asymmetric stretching vibration of the C-O-C glycosidic linkage, respectively. In addition, we observed the pyranose ring signal at 1081 cm^{-1} and the characteristic Raman signals for the acetyl group in 1731 corresponding to vibration of the carbonyl group (C=O) and asymmetric and symmetric vibrations of the C-H bond present in the acetyl groups, in 1431 and 1368 cm^{-1} respectively. Finally, the signals observed at 978, 906,834 and 659 can be associated with C-O, C-H, and O-H and C-OH bonds, respectively.

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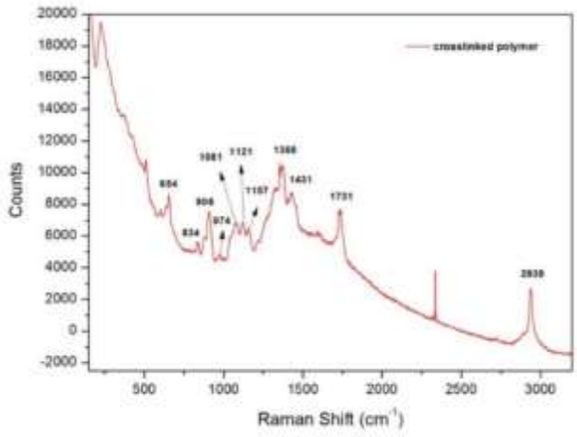
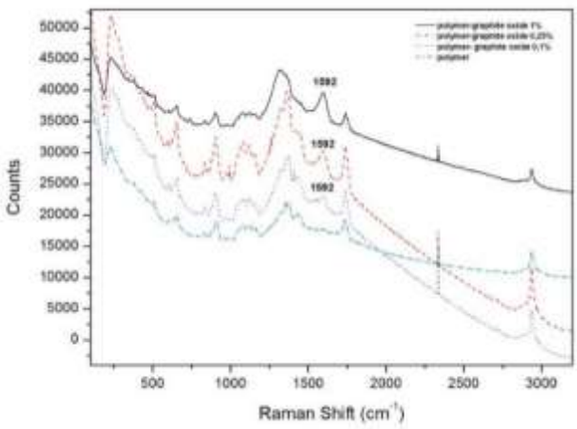
For crosslinked polymer we cannot observed the band associated with the C-OH bonds present in the glycosidic rings at 1265 cm-1 and we cannot see the characteristic Raman signals at 3444 and 1678 cm^{-1} corresponding with the oxygen-hydrogen bond vibration and carbonyl group (C=O) vibration present in the polyacrylic acid neither.

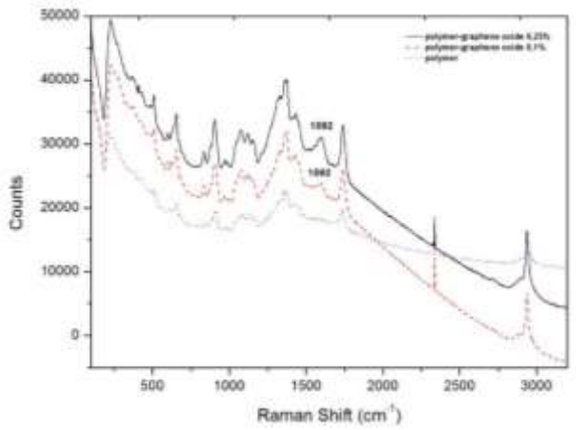


Graphic 7 Raman spectrum for the crosslinked polymer

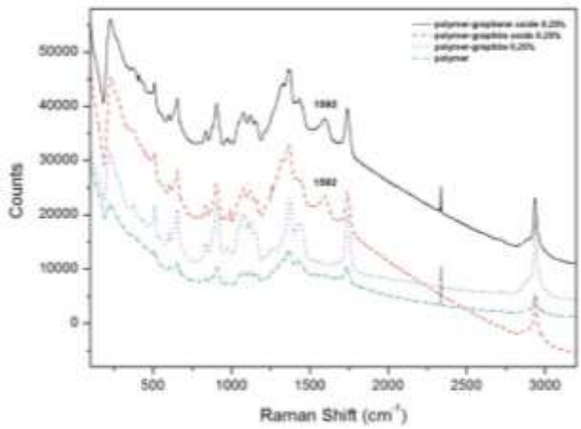
For polymer crosslinked with different concentrations of graphite we cannot observe signals associated with graphitic materials. When we added graphite oxide or graphene oxide to the crosslinked polymer, we can observe a signal at 1592 cm^{-1} associated with the order band (G band). The signal strength is stronger when the concentration increases, Graphic 8-10.



Graphic 8 Raman spectrum for the crosslinked polymer with graphite oxide



Graphic 9 Raman spectrum for the crosslinked polymer with graphene oxide



Graphic 10 Raman spectrum for the crosslinked polymer with graphite, graphite oxide and graphene oxide (0.25 % wt)

Scanning Electron Microscopy

The images obtained from electron microscopy are shown in Graphic 11. The figures correspond to the different kind of membranes synthetized. In accordance with the results obtained from the microscopic characterization, we can say that the polymeric membranes have pores of variable size. In some membranes, the pores are formed in layers, giving the effect of forming a deep network, 11a-11b. For the materials obtained from graphite we can observed that the graphitic material is deposited on the walls of the pores within the polymer structure, Figure 11c and 11f, respectively. Both graphite oxide as graphene oxide cover the walls of the material and they improve the structure polymer.

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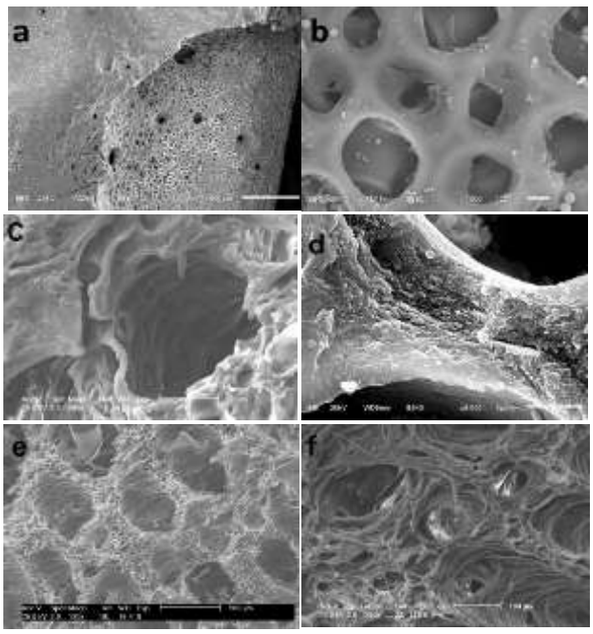
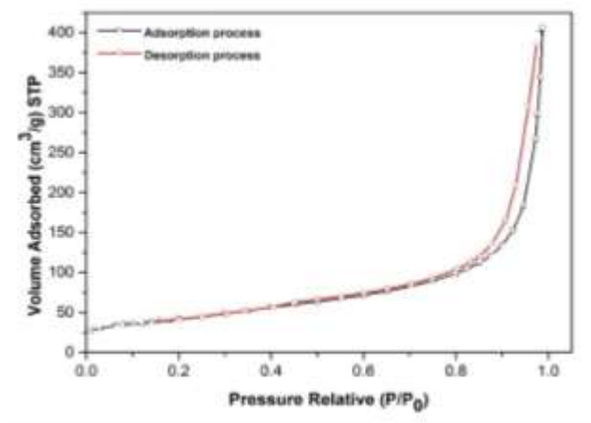


Graphic 11 Sequence of scanning electron microscope images for different polymeric materials. (a), (c) and (e) Graphite oxide, (b), (d) and (f) Graphene oxide

Determination of the surface area and pore size distribution in the graphene oxide

The BET analysis was applied to graphene oxide to determine the effective surface area and the pore size distribution of the material. The effective surface area of graphite (7.73 m^2/g), graphite oxide (2.85 m^2/g) and graphene oxide (20.86 m^2/g) were calculated with the same method. The average pore size for samples of graphite (9.4 nm), graphite oxide (8.9 nm) and graphene oxide (10 nm) showed small variations. In the case of graphene oxide, the adsorption-desorption isotherms obtained by BET analysis, Graphic 12, showed a characteristic behaviour of the isotherm of type 3 proposed by Brunauer, which shows that the adsorption occurs by a physical mechanism.



Graphic 12 Adsorption-desorption isotherm of graphene oxide

From adsorption-desorption isotherms obtained we can see that the analysed samples have a hexagonal tubular capillary.

Concentration of acidic sites and basic sites

Both, acidic and basic sites were calculated in graphene oxide and polymeric materials using a method proposed by Böehm based in an acid-base titration. For the graphite oxide and graphene oxide, concentration values for only the acid sites were obtained. The graphene oxide (2.28 meq/g) showed a higher concentration of acid sites than graphite oxide (1.45 meq/g). Both, acidic and basic sites on the membranes without graphitic material were calculated using the method proposed by Böehm. The concentration of acidic sites in the polymeric material (4.9 meq/g) is 1.25 times higher than the concentration of base sites (3.9 meq/g). The basic sites in the polymeric material may be associated with unreacted sites on the cellulose; while the acid sites can be ascribed to sites vacated in the polyacrylic acid during the synthesis process of the copolymer. For the membranes with graphitic materials, significant changes in the concentration values of the sites were not observed.

Conclusions

The results obtained show that it is possible to design polymeric composites with graphitic materials whose pores are formed in layers, giving the effect of depth forming a network. The graphitic material is deposited on the outside of the polymeric material. The adsorption-desorption isotherms obtained by BET analysis showed that the adsorption occurs by a physical mechanism and that the analysed samples have a hexagonal tubular capillary. Besides, the isotherms of adsorption / desorption obtained for graphite, graphite oxide and graphene oxide showed characteristics like the carbon nanotubes or graphite.

For the graphite, graphite oxide and graphene oxide, concentration values for only the acid sites were obtained. These acid sites can be associated with the presence of carboxylic groups inserted during oxidation of the graphitic materials. The basic sites in the polymeric material may be associated with unreacted sites on the cellulose; while the acid sites can be ascribed to sites vacated in the polyacrylic acid during the synthesis process of the copolymer.

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For the composites with graphitic materials, no significant changes were observed in the concentration values of the sites.

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Parametric design applied to die cutting machine

Diseño paramétrico aplicado a una máquina Suajadora

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Abstract

In this paper, the particularities of applying parameterization in industrial machines corresponding to the manufacturing area are exposed and analyzed. For its development, the parameterized design of a die cutting machine is proposed as an object of study, which is formulated from the main elements considered of importance in the principle of operation, being necessary to carry out a prior investigation to analyze it and how the parameterization process influences. Parameterization is a quality of the components to adapt flexibly to the needs of the industry or sector, facilitating the redesign and manufacturing process, allowing the desired dimensional update or adjustment to be carried out only to the central component and the others are automatically adapted. Attending to the current needs and trends of the fourth industrial revolution, as well as establishing the benefits of this type of flexible design processes to expand their implementation to different industrial machines such as robot configurations.

Parameterization, Die cutting machine, Flexible manufacturing

Resumen

En el presente trabajo se expone y se analizan las particularidades de aplicar la parametrización en máquinas industriales correspondientes al área de manufactura. Para su desarrollo se plantea el diseño parametrizado de una máquina suajadora como objeto de estudio, el cual se formula a partir de elementos principales y considerados de importancia en el principio de funcionamiento siendo necesario realizar una investigación previa para analizar dicho principio y cómo influye el proceso de parametrización. El parametrizado es una cualidad de los componentes para adaptarse de forma flexible a las necesidades de la industria o sector, facilitando el proceso de rediseño y fabricación al permitir realizar la actualización dimensional o ajuste deseado únicamente al componente central y el resto de los elementos se adaptan de manera automática. Lo anterior atendiendo a las necesidades y tendencias actuales de la cuarta revolución industrial, así como el establecer los beneficios de este tipo de procesos de diseño flexibles para ampliar la implementación de los mismo a diferentes máquinas industriales como los son las configuraciones de robot.

Parametrización, Máquina suajadora, Manufactura flexible

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I. Introduction

At present it is quite common to find applications in the industry where there is a need to make some improvements to the mechanisms in order to make adjustments, correct errors, increase production, etc .; For this reason it is necessary to expand or reduce the dimensions of the machine in general, that is where the concept of parametric design comes in, which allows a joint update considering the dimension and position of each of the components.

Creating parametric designs in 3D allows you to enter a series of variables or parameters, such as spatial limits or volumes to manipulate them through algorithms and thus obtain geometric designs in which everything is related to each other; The objective of parametric design is the automation of the process where it is sought to reduce or eliminate errors when editing the design.

For example, in a large assembly when having the need to modify the dimensions, it would have to be edited piece by piece, taking a great amount of time to edit, in addition to the risk of generating errors in the assembly, on the other hand, if the design has the parameterization, it would only be enough to change the dimension of one of its components and all the others would be adapted automatically.

The priority of this research being to facilitate the redesign process in existing models, taking into account the new trends in Industry 4.0.

Industry 4.0

The Industry 4.0 concept is associated with a new way of organizing production systems, from the conception of the product, the needs to optimize processes and the intensive use of new technologies, with the use of quality tools, as well as optimization of the processes allowing to achieve an increase in efficiency and competitiveness and adjusting to the personalized needs of the consumer (GARCÍA, 2017).

Design

Engineering design has been defined as "the process of applying the various techniques and scientific principles with the purpose of defining a device, a process or a system with sufficient details that allow its realization" (Norton., 2009).

Parametric design

Parametric CAD is responsible for assigning non-linear rules between the proportions of a design, through equations of any type, and at the same time establishing geometric relationships, seeking the functionality of the model or its aesthetics. When performing the parameterization of a CAD, it is possible to change each of the measures that make up the design so that they can later be edited (BERNAL & SALOMÓN, 2017).

SolidWorks

SOLIDWORKS® CAD software is a mechanical design automation application that enables designers to quickly sketch ideas, experiment with features and dimensions, and produce detailed models and drawings (Corporation, 1995-2015).

Manufacture

It is the process of converting raw materials into products. It also includes activities in which the manufactured product itself is used to make other products (Schmid, 2008).

CAD systems

Graphical analysis is performed using traditional drawing procedures or a CAD system, as is normally done in industry. For mechanism analysis, it is possible to use any of the various commercially available CAD systems. The most common 2D CAD system is AutoCAD. Although the commands differ from one system to another, all CAD systems have the ability to draw lines with designated lengths and angles with high precision. This is exactly the characteristic required by graphical mechanism analysis. In addition to increased accuracy, another advantage of CAD is that lines do not need to be scaled to fit on a piece of drawing paper. In the computer, the lines are drawn on an infinite size "virtual" paper.

Also, the restricted drawing mode in three-dimensional modeling systems, such as Inventor, SolidWorks, and ProEngineer, are often extremely useful in plane kinematic analysis. Geometric constraints, such as length, perpendicularity, and parallelism, must be met when performing kinematic analysis. Such constraints are automatically executed in 3D modeling drawing mode (Myszka, 2012).

Mechanism

It is a device that transforms movement into a desirable pattern, and generally develops very low forces and transmits little power (Norton., 2009).

Machine

It is defined as a combination of resistant bodies arranged to make the mechanical forces of nature perform work accompanied by determined movements (Norton., 2009).

Clamping process

The die, or also called suaje, consists of a tool manufactured with a steel plate to bend, cut or mark materials such as fabric, paper, leather, etc. In reality, the cutting plates are metal strips sharpened on one side, and the bending plates are dull (Industriales, 2021).

II. Methodology

Problem Statement

Currently, there is a need for flexible designs that adapt to the needs and specifications of the user with the sole purpose of allowing optimization of the redesign process, reducing time and errors when some adjustment or dimensional update is required.

General objective

Implement a parametric design to a die-cutting machine that allows it to be flexibly adapted to the user's own needs, optimizing the process, reducing time and minimizing redesign errors.

Particular objectives

- Generate a previous diagnostic study.
- Develop a design based on the previously diagnosed study.
- Analyze areas for improvement.
- Redesign implementing improvements and parameterization.
- Present results.

Diagnosis

As part of a previous study of the problem, it is decided to use a SWOT analysis as a tool to identify important points to consider for the planning and development of the proposal.

SWOT analysis.

Strengths.

- Reduction of times and costs in the design process of machines or mechanisms.
- Reduction of times and costs in the process of modifying already established designs.
- Identification of possible improvements.
- Identification of possible failures in the mechanisms.
- Modification of dimensions avoiding inconsistencies in the assembly document.
- Prevention of future errors when machining or assembling the design.

Weaknesses

- Design time of the first assembly.
- Need to have the knowledge about parameterization in SolidWorks.
- Necessary mathematical equations.
- Greater complexity when designing.

Threats

- Default design customs in the industry.
- Standardization of dimensions in industrial machinery.
- Lack of training in industrial design upgrades and updates.
- Editing restrictions of some machines according to patents.
- Lack of training in industrial design upgrades and updates.

Opportunities.

- New updates in the industry.
- Industry 4.0 implementation.
- Micro-enterprises that have the need to adapt to the market.
- Companies dedicated to design.

Development

A manual die cutting machine design is considered as a reference to establish the elements, mechanisms and dimensions used in the current market. Once this information is specified, the base design is generated using the specialized SolidWorks design software, considering an analysis of possible improvements to make the stamping process more productive.

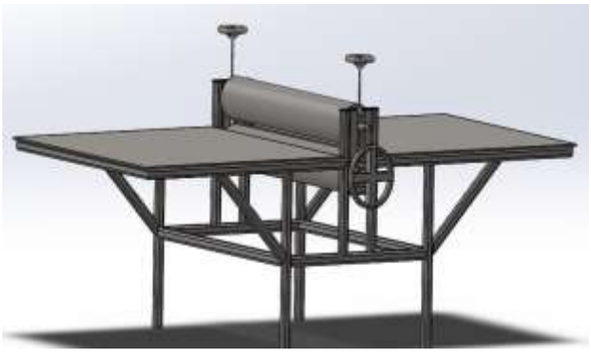

Figure 1 Manual die cutting machine design
Source: Own Elaboration [SolidWorks]

After the evaluation of the improvements derived from the analysis, they continue with the implementation of the same, being that it is chosen to automate the machine to make the process of smoothing the material faster, more efficient, precise and safe for the user.

The automation is applied directly to the roller mechanism that acts as a material feeder for processing according to the operating principle of the die-cutting machine, for which a motor, a transmission and control system are contemplated for the change of rotation of the same.

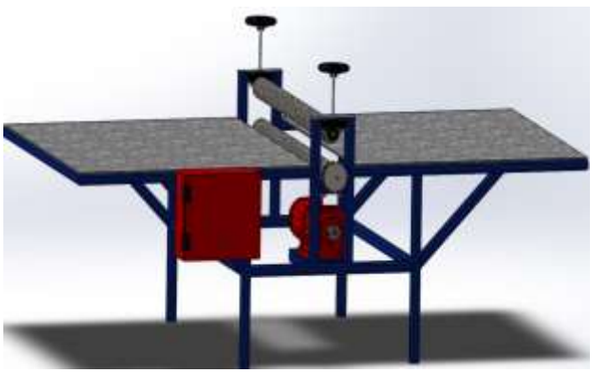

Figure 2 Automated die cutting machine
Source: Own Elaboration [SolidWorks]

Design parameterization

To generate the design parameterization, the general operation of the object of study is analyzed to decide which component will act as the central element and which parameter is taken as a reference, being that it is detected that the dimension of the rollers (Figure 3) allows to control the capacity and size of material to be processed.

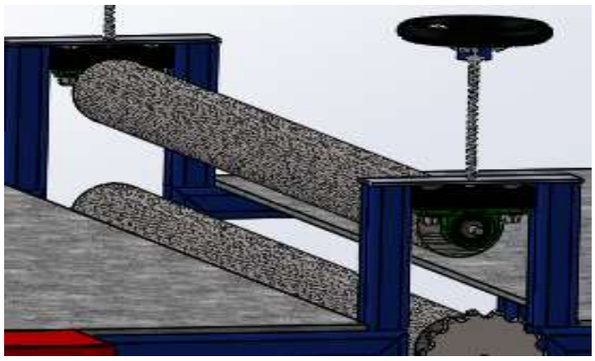

Figure 3 Die machine rollers
Source: Own Elaboration [SolidWorks]

For this, the parameterization is applied in the arrow that supports the rollers, contemplating it is adjusted independently to adapt to the position of the bearings, so a relationship of equation is used (Figure 4).

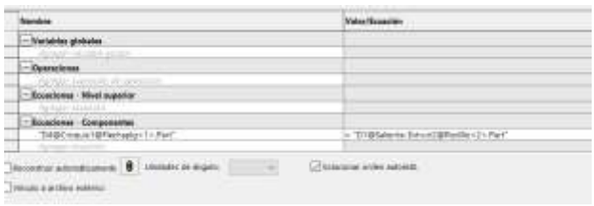

Figure 4 Arrow - Roller Parameterization.
Source: Own Elaboration [SolidWorks]

In the case of the general assembly, two equations were used, one of them was applied to the main structure in relation to the length of the rollers and one more to adapt the plates corresponding to the new size of the structure (Figure 5).

Figure 5 Roll parameterization - main structure
Source: Own Elaboration [SolidWorks]

Constraints are one of the elements that must be taken into account when creating a parameterized industrial design since, if they are omitted, the design could take a different form or lose the relationships previously established.

In the process used to add dimensions, the pieces are considered as an independent element, however, the reality when creating a parametric assembly the components must work as part of a coordinated set. The restrictions were established from the mechanical position relations used in the assembly of the reference die cutting machine. The relationships or constraints used to achieve the purpose are mainly concentricity, coincident, parallel and distance.

A concentric relationship is applied between the date and bearing elements (Figure 6) essential to maintain the position when carrying out an update in the dimension of the rollers.

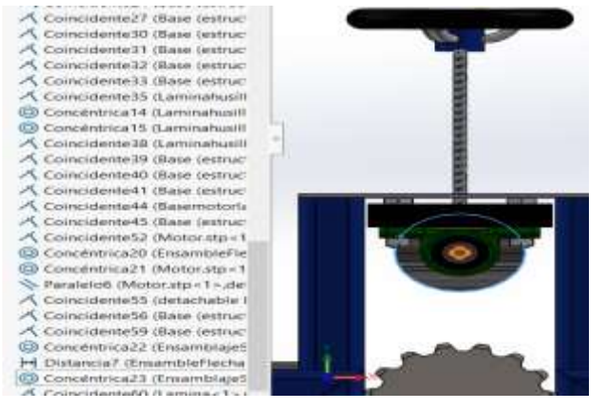

Figure 6 Concentric arrow-bearing relationship
Source: Own Elaboration [SolidWorks]

In addition, a distance relationship between the roller and the internal profile of the structure (Figure 7) is considered, restricting a safe distance to avoid friction and wear between both elements.

When applying the parameterization, the components are adapted to the desired dimension of the rollers, respecting the assigned relationship in size and position automatically without being necessary to individually edit each element such as the structure, the plates, the ½ inch arrow, etc. . (Figure 8 and 9).

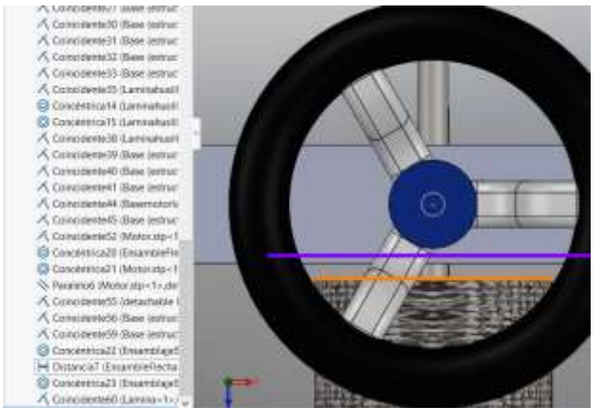

Figure 7 Relation between the end of the roller and the end of the profile
Source: Own Elaboration [SolidWorks]

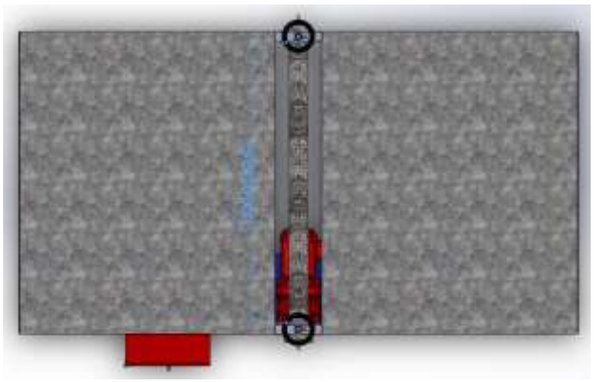

Figure 8 Parametric design of a 1.5 meter (1500mm) roller die cutting machine.
Source: Own Elaboration [SolidWorks]

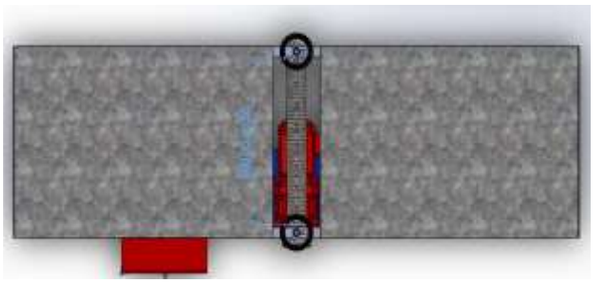

Figure 9 Parametric design of a 0.8 meter (800mm) roller die cutting machine
Source: Own Elaboration [SolidWorks]

All the restrictions and equations applied to the design have the sole purpose of establishing a hierarchy and dependency based on parameters established between the components, respecting their position and assigned dimension, in this way an adequate and optimal parameterized model is guaranteed that allows reducing time and costs of editing on industrial machines.

III. Results

With the implementation of the parameterization process in the design of the die cutting machine, it was possible to analyze the critical points and important areas for improvement to meet the objective of this project.

By concentrating all of the design editing in a single parameter corresponding to an element, it was possible to simplify the redesign process and reduce time between 30 and 40 percent compared to the conventional process.
In addition, a general standardization of the different commercial models of this type of industrial machines is established in a single design based on the dimensions and location of the components necessary for their manufacture according to the user's requirements.

By providing this type of design with this capacity, the market field for said machinery can be expanded to be used not only in printing presses, but also in industrial companies where stamping is used.

The scope of this research goes beyond the results obtained from the application of parametric design in a die cutting machine, and its future implication in the design of industrial machines and flexible manufacturing is analyzed, so it would be convenient to apply the parameterization to designs of industrial robot configurations.

IV. Conclusions

Industrial design knowledge plays an important role in generating a parameterized model, since a more extensive vision capable of identifying the components with the greatest influence on the design of any important machine is needed to establish the pertinent restrictions and the parameterization process.

The process of editing any design can become too complex, since an analysis would have to be carried out again to make the changes that you want to make, on the other hand, having a parameterized design of the machine reduces the process. to adjust the value of the key components, in this case the roller.

Parametric design is a scheme with great possibilities for industrial designs that provides different advantages when making modifications, either to obtain an improvement or by necessity, facilitating the redesign in any of its components without having to carry out an individual analysis again. of each mechanism or structure.

Studying the parameterization allowed detecting the need to update the stamping machines, since in recent years no improvements have been applied to commercially established designs, that is why the development of this project was carried out considering the applied methodologies in the industry and proving its innovation.

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Methodology for the design of a multilayer polymeric membrane system with potential use in hemofiltration

Metodología para el diseño de un sistema de membranas poliméricas multicapa con uso potencial en hemofiltración

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Abstract

Chronic kidney disease is generally complicated by poor care or by ignoring it. Among the causes that influence these conditions are obesity, diabetes, smoking, or genetic inheritance. Coordinated efforts are currently being made in multiple countries to control a strong case rate. The clinical techniques of treatment rely on the efficiency of blood purification (function that´s done by kidneys in organisms). Therefore, there is great interest in the development of devices that accomplish this function. Hemofiltration through porous membranes is an efficient process, but the flow conditions in a microchannel system can be complex. Analysis of blood flow in a parameterized conduit arrangement shows streams with desired trajectories, others are held back (stagnant), and others return to the stream from which it´s separated. In addition, the friction conditions and the reduction of the area drastically reduce the movement of the fluid, promoting clogging and consequently the inhibition of filtering. Based on these simulation results, it was proposed that the membrane coupling system could be modified to eliminate extensive flow in conduits generating a new concept of separation through a threshold.

Hemofiltration, Porous membrane, **Flow simulation**

Resumen

Generalmente una enfermedad renal crónica se complica por atención deficiente o en algunos casos por ignorarla. Entre las causas principales que influyen en este padecimiento destacan: la obesidad, la diabetes, el tabaquismo o la herencia genética. Las técnicas clínicas de tratamiento recaen en la eficiencia de depuración de sangre (función que realizan los riñones en los organismos). Por lo tanto, existe un gran interés en el desarrollo de dispositivos que cumplan esta función. Se considera que el proceso de hemofiltración es eficiente pero las condiciones de flujo en conductos diminutos pueden ser complejas. El análisis del flujo de sangre en un arreglo de conductos parametrizado muestra que existen corrientes con trayectorias deseadas, otras son retenidas (estancamiento) y otras retornan a la corriente de donde se separó. Además, las condiciones de fricción y la reducción de área reducen drásticamente el movimiento del fluido promoviendo obstrucciones y en consecuencia la inhibición del filtrado. De acuerdo con estos resultados obtenidos por simulación, se propone que el sistema de acoplamiento de membranas puede modificarse para eliminar el flujo extenso en conductos generando un nuevo concepto de separación a través de un umbral.

Hemofiltración, Membrana porosa, Simulación de flujo

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Introduction

According to the reports presented at the World Congress of Nephrology (ISN, 2021), chronic kidney diseases are a global problem since 1 in 10 people in the world suffers from that. A blood and urine test are part of routine tests that look at glomerular filtration rate, which measures the kidneys' ability to filter blood. Also, the presence of protein in the urine is measured as a disease prevention parameter.

The term dialysis has been coined to define the procedure that replaces the function of a kidney. In the dialysis technique, a filtering process is developed through a porous membrane that allows the flow of small molecules of urea, water, creatinine, and glucose. Red blood cells, white blood cells, platelets, and most proteins in plasma are retained (Li Norman, Fane Anthony, Winston Ho, & Matsuura, 2008).

The term porous membrane refers to a solid or liquid material capable of separating two macroscopic phases, whether liquid, gas, solid, having a selective control of the transfer of mass and energy between them. The transport mechanisms of chemical species through membranes can be define as convective-diffusive. Depending on the physical characteristics of the membranes, some predominates. In this sense, research is currently being carried out to design an efficient blood flow purification device (Forni & Hilton, 1997) (Mott, et al., 2020) (Stamatialis, et al., 2008) (Mollahosseini, Abdelrasoul, & Shoker, 2020) (Lenshof & Laurel, 2009) (Yu, et al., 2017).

The development of biocompatible polymeric membrane manufacturing technologies has allowed researchers in the dialysis processes in any treatment modes: Hemodialysis, Hemofiltration or Hemodiafiltration to be optimized. Recent research has shown that membrane filtration analysis through simulation programs is validated with experimental measurements (R., S., S., P., & K., 2020) (Chandra, Pathiwada, & Chattopadhyay, 2019) (De Napoli, et al., 2014) (Eloot, 2004) (Filipovic, 2020) (Foughalia, Rosminazuin, Anis, & Noorjannah, 2015) (Restrepo-Flórez & Maldovan, 2018) (Tahvildari, Razavi, Tavakoli, Mashayekhi, & Golmohammadzadeh, 2015) (Yaqoob, Ahsan, Hussain, & Ahmad, 2020).

In this work, hemofiltration is of particular interest. Its nature of separation by a convective mechanism defines it as a fast procedure. A fundamental part of the hemofiltration technique are the membranes contained in the dialyzer (Göhl, Konstantin, & Gullberg, 1982). Blood is forced through the pores that are part of the internal structure of the membrane. It has been shown that up to 15 medium and large molecules are efficiently separated compared to hemodialysis, where there is a small amount of waste removed along with the already accumulated fluid. Therefore, the technological challenge is to design a multilayer membrane system that presents high permeability and selectivity of molecules without disregarding biocompatibility.

The recirculation flows in shared cells (coupled membranes) are studied using the Navier-Stokes and Brinkman equations to describe the transport of fluids in porous media. However, in this work, a parameterized model is presented that emulates a unit of the complex system of interconnected pores within a membrane.

Methodology

Multilayer membrane systems for blood purification have now been found to be of great interest. In these systems, it does an attempt to retain molecules by their size. The blood circulates through a material that contains interconnected pores resembling tunnels, but only molecules that have a size smaller than the pore circulates. The rest have been kept back on the surface of the membrane. The process can continue sequentially with subsequent membranes with fluid flow due to a pressure difference. These systems require a pumping device or a centrifugal mechanism.

It can be assume that the tunnels are of homogeneous size in a membrane. In this case, when coupling two membranes with different tunnel sizes, an interconnection with reduction is generated. The concept of tunnel link allows to proposal parametric system. Then, it shall be deemed two tunnels with bifurcations and a return connection for the flow of blood. Through this system, laminar flow simulations were performed to understand the flow pattern and the velocity field in nano-magnitude tunnels.

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Figure 1 shows this system drawn in COMSOL Multiphysics V5.2a software (COMSOL, COMSOL, 2020). The large duct measures 10 nm per edge and the small duct 6 nm per edge. This geometry allowed the generation of a structured mesh.

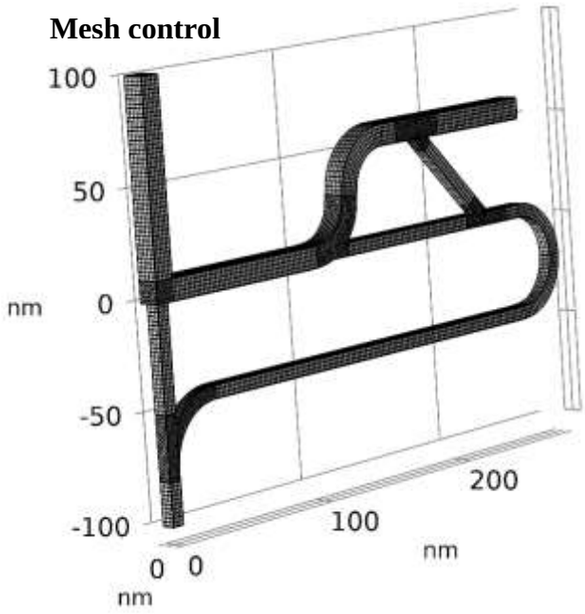

Figure 1 Parametric model of the duct link proposed for flow analysis in a membrane. *COMSOL Multyphysics V5.2a.*

The flow simulations were performed by solving the stationary Navier-Stokes equations and the continuity equation.

$$\rho(u \cdot \nabla)u = \nabla[-pI + K] + F$$
$$K = \mu\left(\nabla u + (\nabla u)^T\right) \quad (1)$$

$$\rho\nabla \cdot u = 0 \quad (2)$$

Gravitational effects or external pressure conditions do not influence the studied system such that equation (1) is simplified. Simulations started with a flow magnitude as a boundary condition reported in the investigation by (Mott, et al., 2020), which implied a high speed.

The results indicated necessary changes to the system that will help improve fluid separation. The calculation of the velocity profiles makes it possible to determine the characteristics of the rapid flow of the fluid in the ducts. A region where low speed is specified determines slow mobility and the tendency to stagnation, which happens on the duct walls. Another stagnant situation occurs when a portion of the fluid remains moving in a circuit (vortex).

An analysis of the velocity field can be obtained for the parametric model and subsequently include the presence of particles. It is possible to implement the presence of particles in the streams to evaluate the interaction: 1) fluid-particle, 2) particle-particle, and 3) particle-wall. With the results, it will expect to define design parameters to obtain the proposed objective.

In COMSOL software (COMSOL, COMSOL, 2020), the equation that governs the calculation of particle trajectories from a velocity field is define as:

$$\frac{d(m_p\mathbf{u})}{dt} = \mathbf{F}_t \quad (3)$$

Again, the system was simplified by analyze the behavior in a single bifurcation. With this change, the entrance speeds were specified between 0.2 to 20 ms^{-1}. The analysis of the flow separation in a bifurcation as a function of the entering velocity was conclusive. These showed the separation system design needs, and with them, a new proposal for a membrane system for the convective separation of molecules of blood is in the making.

Results

Studies carried out a flow of 20 ms^{-1} was considered entering the large duct, while in the locks, the flows are free. The results of the velocity field are show in Figure 2.

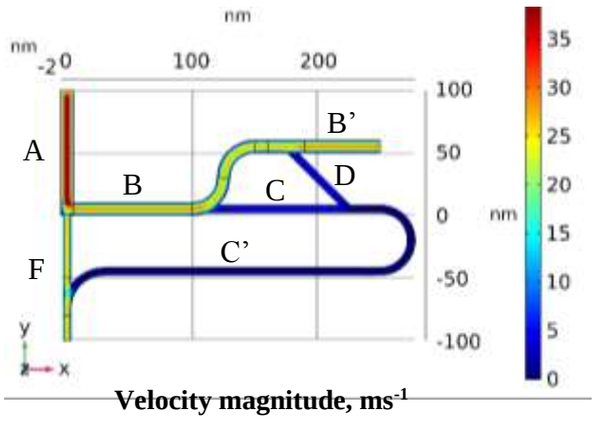

Figure 2 Velocity profile estimated in the parameterized system. *COMSOL Multyphysics V5.2a.*

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According to the color scale, it can observed that there is a fluid stagnation condition in the return duct because higher speed currents contribute to this stagnation. An analysis of the streamlines at branch C shows separate fluid returns at branch B' (See figure 3) through at branch D due to resistance imposed by stagnation fluid in C'.

In the calculations, 73.46% of the flow flows in the B stream. Therefore, the complementary percentage (26.54%) is associated with the E current. The 7.05% fraction of the flow in B flows through C. 99.3% of the flow in C returns to B 'through D, and only 0.7% circulates through branch C'. Concerning the initial flow, 5% of the fluid returns through stream D. This amount should be added to the branch E through C', and even stream D should increase it. Therefore, branch D should not exist.

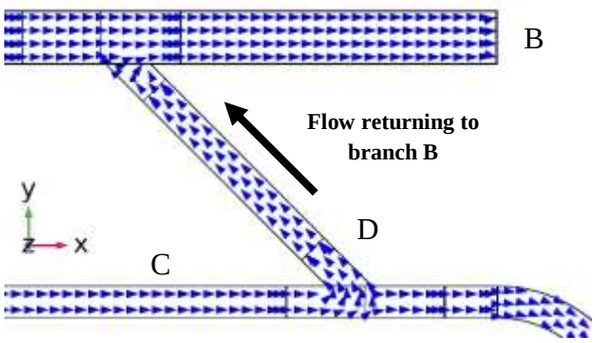


Figure 3 Normalized streamlines in arms B, C and D of the parametric system. *COMSOL Multyphysics V5.2a*

The elimination of branch D shows an improvement in separation flow in the return duct (branch C). However, the velocity continues to decrease dramatically, as shown by the particle trajectory profile on a cut plane in Figure 4. The accumulation of particles in the return duct indicates stagnation. The diameter of the particles for this analysis was 1.8 nm.

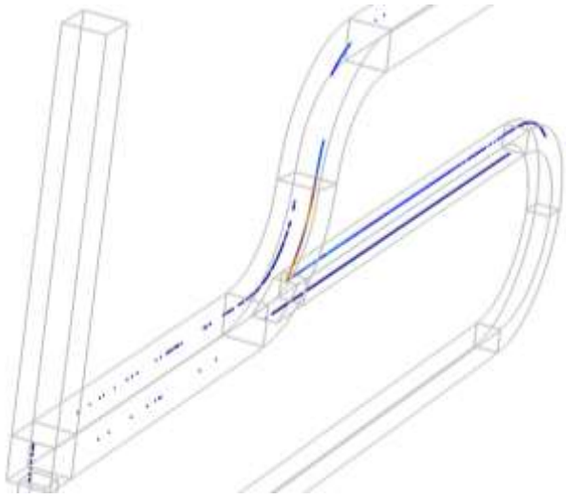
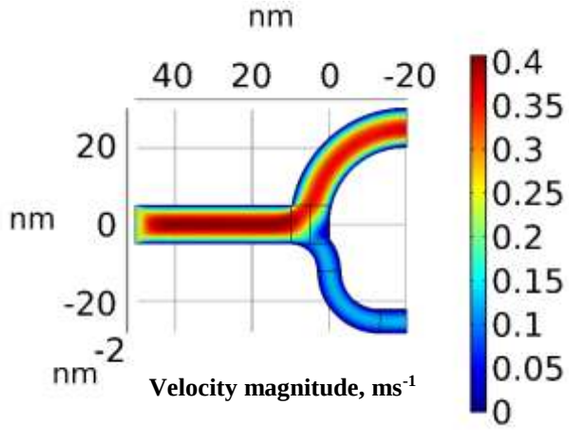


Figure 4 Particle flow in the fluid stream coinciding with the center shear plane. *COMSOL Multiphysics V5.2a.*

The results of this simplified model of linked pipelines indicate that there is a high possibility of unwanted returns and stagnation. In a membrane porous system, this process can multiply, and then the number of derivations, the transversal, and the length size of the conduits, should be kept to a minimum.

The bifurcation containing branches A, B, and E (see figure 2) is an example of the simplicity of separation without alternate connections. A similar model was created to evaluate the rate separation of the flow in branch A towards branches C and E. In this new system, the velocity field was calculated considering an input velocity of 0.2 ms^{-1}. The flow calculations determine approximately a relationship of 89% and 11% flow in the larger and the smaller ducts. Figures 5(a) and 5(b) show the velocity field in 2D and 3D perspectives. In the contour graph, it can be observed that the current with the highest relative velocity, is found in the center of the ducts and that it reaches twice the input value.



(a)

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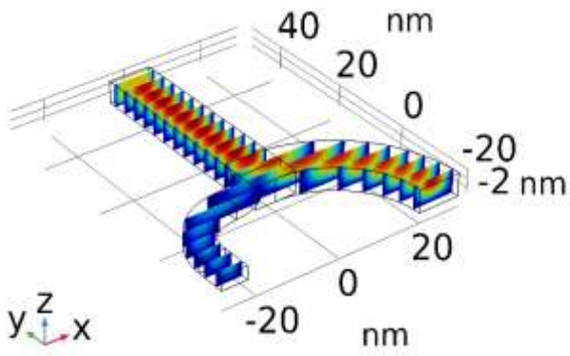
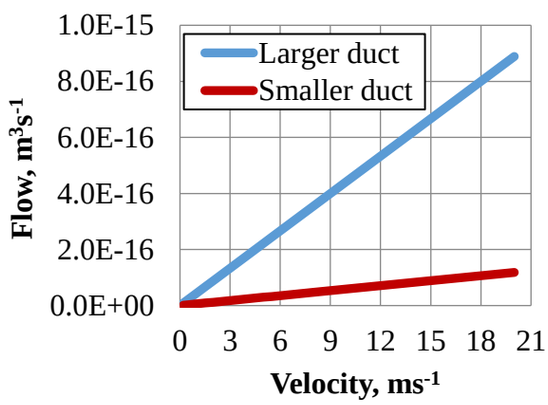


(b)

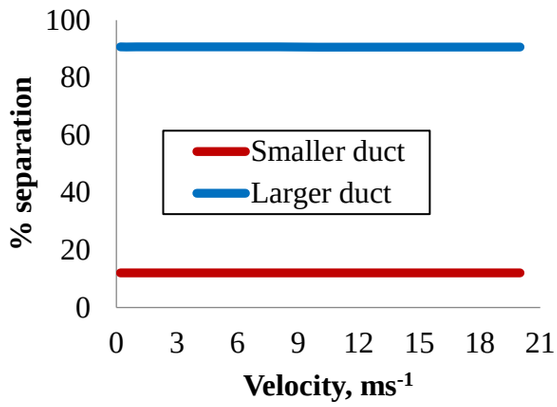
Figure 5 Velocity field in 2D and 3D perspectives at a bifurcation. *COMSOL Multiphysics V5.2a*

The figures show one of the sections of the system cut by symmetry. A smaller flow flows through the smaller duct due to the reduction in area and intrinsic viscous forces. The inertial forces can increase in the narrow duct region increasing the input velocity. Therefore, the velocity profiles were calculated at various input velocities between 0.2 and 20 ms^{-1}. The results show the same pattern obtained before. Figures 6(a) and 6(b) show the rate flow and % separation in the branches as a velocity function.

It can be observed that the percentage of separation is constant, and the flow in each branch is proportional to this. By analyzing the system, the bloodstream in the larger duct can be separated by implementing a new bifurcation. Several branches can be couple to obtain a consecutive separation. The process is attractive since it develops at higher rate than a diffusive process and doesn´t require great external forces. However, it´s not already as efficient for processing high volumes of blood. The problem of circulation through ducts where friction can lead to stagnation tendencies continues.



(a)



(b)

Figure 6 Relation between rate flow and separation % in the branches as a velocity function. *MS Excel 2013*

An alternative to the separation of molecules from the bloodstream is to channel them free up to a threshold where only molecules of selected size can cross. In this case, the molecules would be propelled from one room towards the transfer threshold to another room. The "threshold" can be describe as a "door" between two spacious rooms. This new system avoids most of the friction by contact between the blood and the wall ducts.

In this sense, a concentric container system will assume whose walls are separated by a distance that generates a collection volume. A centrifugation system to drive fluid from a central container will also be consider. Walls are compounds by two assemble membranes ablation grooved such that they set the threshold. The result of the blood flow pattern analysis of this concept is shown in Figure 7.

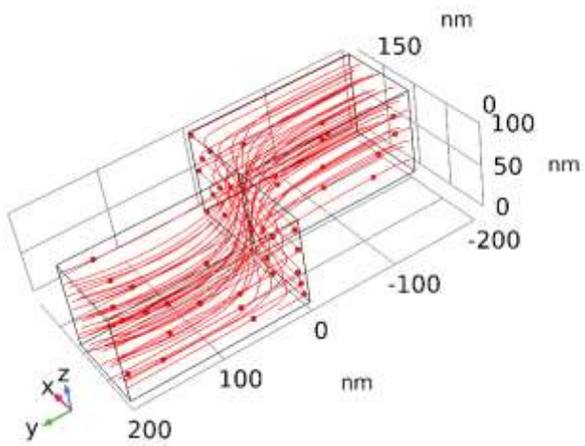


Figure 7 Streamline of blood flow through the membrane coupling system defining the separation by means of a threshold. *COMSOL Multiphysics V5.2a*

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The particular future work of hemofiltration in this investigation will be based on this approach derived from duct flow. The concept of flow through the threshold and turbulent flow patterns have been obtained in a system centrifuged at 500 rpm that generates velocities of 20 ms^{-1} on the inner wall of a cylindrical container. Figure 8 shows the velocity field calculated using the k-ϵ turbulence model. The color scale determines the speed profile reached in the system.

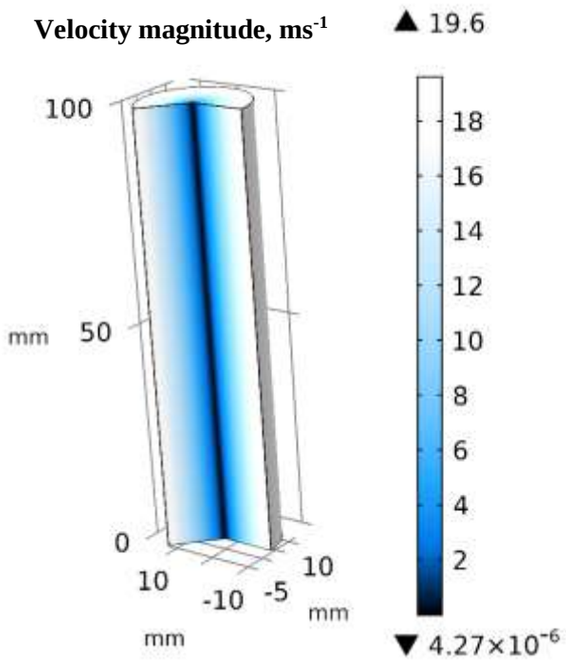

Figure 8 Velocity field of a blood fluid subjected to centrifugation. *COMSOL Multiphysics V5.2a*

The system was defined with a 4:1 ratio, height:diameter, to avoid the edge effect. From now on, the particle trajectory calculation will be implemented. The approach behavior of the blood molecules to the threshold and the crossing capacity will be analyze.

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Conclusions

In this work, it's mathematically supported by simulation that the hydrodynamic separation technique can be obtained by controlling the speed of flow, the geometry of the tiny channels, and the configuration of the outlets in porous membranes. The process is attractive since it develops at a high velocity compared to a diffusive process.

The simplification of a complex system of tunnels in a porous membrane led to creating conditions for the derivation of the flow of a pipeline in two branches to obtain sequential filtering of particles of different sizes taking advantage of convection in tiny channels. As a result of the analysis, it was demonstrated that the flow capacity at nanometric scales would be adapt to smaller fluid volume processing systems.

In a dialysis process, a significant amount of blood is required to be processed for cleaning. In this sense, although the filtering process imitating a natural procedure can be developed, it doesn´t apply to the necessary flow levels.

Essentially, it was shown that the change of flow to narrow passages is not a desirable condition. Therefore the path in the separation is believed to be reduced to the crossing of an interface (cross a threshold). According to the analysis, this kind of separation can be adapt to the most common blood cell separation technique, centrifugation, with the component of obtaining a high manipulation of the protein separation.

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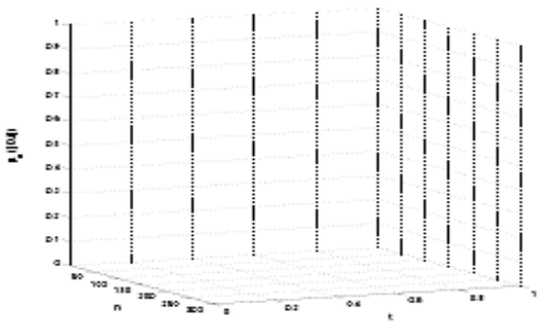

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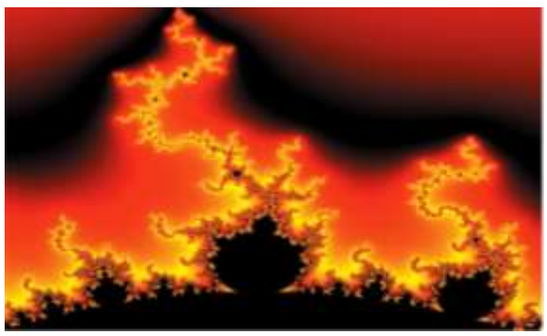

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