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Modeling desulfurization of organic compounds by use of polymer membranes with the help of COMSOL Multiphysics software

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Abstract

The authors in this study considered the amount Thiophene Alkane separation through the process of pervaporation by means of polymer membranes and with the help of COMSOL Multiphysics modeling. Pervaporation can be utilized for separation of many Organic mixed .The experimental data were compared and analyzed with the model data.
In this study, for the separation of Thiophene Alkane four polymer membranes was used and the error percentage of the actual value for flux were compared to the modeling values by the each membrane (PEG_PES, PDMS_PAN, PDMS, PEG). The error percentages in desulfurization by use of PEG-PES, PDMS_PAN, PDMS, PEG membranes were respectively calculated to be 0.013; 2.56; 2.90 and 0.69.

Keywords: Modeling, desulfurization, Organic compound, polymer membrane, COMSOL software

1. Introduction

Sulfur-containing compounds are one of the most important pollutants in petroleum products, and removing them is considered as a goal in the refinement process. The Desulfurization process emerged in 1933, and so far, a great number of researches have been conducted on this subject. Environmental regulations for sulfur content in fossil fuels are getting more and more rigid, and international regulation-making organizations has defined the permissible amount of sulfur content in petroleum products to be 15 ppm in order to limit and lower the amount of this dangerous substance. However, the amount of sulfur content in the petroleum products produced in Iranian refineries is about 500-1000 ppm, and this amount of sulfur content can seriously pollute the air and environment [1].
As reduction of sulfur content in the fuel is influential over the Diesel engine performance, automobile-makers are obliged to design and manufacture automobiles that are compatible with low-sulfur fuels [2]. Moreover, existence of poisoning expensive metal catalysts used in the refineries, and deactivation of these substance while getting in contact with these harmful compounds is another reason of necessity for fuel desulfurization. Regarding the rigid regulations on fuel desulfurization [3], the researchers are trying to find solutions for desulfurization of fuels in the recent years. One of the fuel desulfurization methods that have attracted attention of the researchers in the recent years is desulfurization by use of membrane processes. In this technology, a semi-permeable membrane is used for separation of different compounds. This method is much more economic than other common methods of desulfurization regarding the costs, consumed energy, and required equipment [4]. The pervaporation process is a notable progress in the field of solvent Desulfurization, Desulfurization of volatile organic compounds, water partial Desulfurization, and recently, Desulfurization of organic-organic solutions. Furthermore, it is approved that such method has a good efficiency in separation of sulfur impurities. Due to high overall efficiency and high energy efficiency, this method is getting more popularity in the industries right now. Selection of the proper membrane is one of the most important phases in the evaporation process. In most of the evaporation processes, the driving force is the pressure difference between the feed current and the permeated current, and, the vacuum pomp provides the required driving force for mass transfer of the compounds [5]. In this study, a membrane procedure will be simulated in COMSOL software. The produced feed from Sulfur and

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hydrocarbon compounds undergo the procedure, and will be analyzed under different conditions regarding temperature and pressure in separation efficiency. Moreover, other influential parameters on the evaporation process will be defined [6, 10].

2. Experimental

2.1 Multiphysics COMSOL software

Multiphysics COMSOL software is a modeling software that runs all the phases in the modeling process. Different modeling phases that COMSOL is capable of phase by phase modeling are drawing geometric structure of the model, meshing model, drawing the major physics of model, resolving the model, and graphical presentation of the modeling results. Due to usage of default physical structures in this software, modeling in this software is done very fast. It is possible to electromagnetically analyze a vast range of mechanical structures by this software. It is also possible to define the material characteristics, source parts, and the approximate border of objects as arbitrary functions of the independent variables.

2.2 Modeling Desulfurization of organic compounds by use of COMSOL Multiphysics software

Such organic compounds as acetone, butanol, ethanol, isopropanol, and methanol were selected for this study, and the COMSOL Multiphysics version 4.2.0.150 was used for modeling. The procedure description is as follows [11-15]:
After opening the software, select the 2D mode to enter the phase definition phase. In the phase definition section, select "Transport of Concentrated Species" (that is applicable for thick solutions) for the mass transfer mode. For the fluid mechanics issue, select the "laminar Flow" mode, and for the heat transfer mode, select "Heat Transfer Solids".
Select the study type to be "Type Dependent". This type is applicable for solving equations that depend on time. On the setting page, for length unit select mm, and for size unit select degrees.

$$\rho\frac{\partial\omega_t}{\partial t} + \nabla.j_j + \rho\,(u.\nabla)\,\omega_j = R_j$$

$$N_i = j_j + \rho u\omega_j$$

$$j_j = -\,(\rho\, D_j^F\, \nabla\omega_j + \rho\omega_j\, D_j^F \frac{\nabla M_n}{M_n} + D_j^T \frac{\nabla T}{T}$$

$$M_n = \left(\sum \frac{\omega_j}{M_j}\right)^{-1}$$

In this equation, ω, D, R, U and M are respectively concentration, penetration coefficient, reaction term, velocity and molecular mass.
Now, it is time for definition of geometry, draw the first rectangle as vertical, and the second rectangle as horizontal.
The next step will be selection of materials. As the name suggests, water and alcohols are needed for this study. Water enters the system from the top, and alcohol enters from the bottom, Then, the materials will be mixed, and exit from the right. So, the system will have two inputs and one output. Mesh is the starting point for Finite Element Method, and its mission is partitioning geometry into smaller units with simpler shapes.

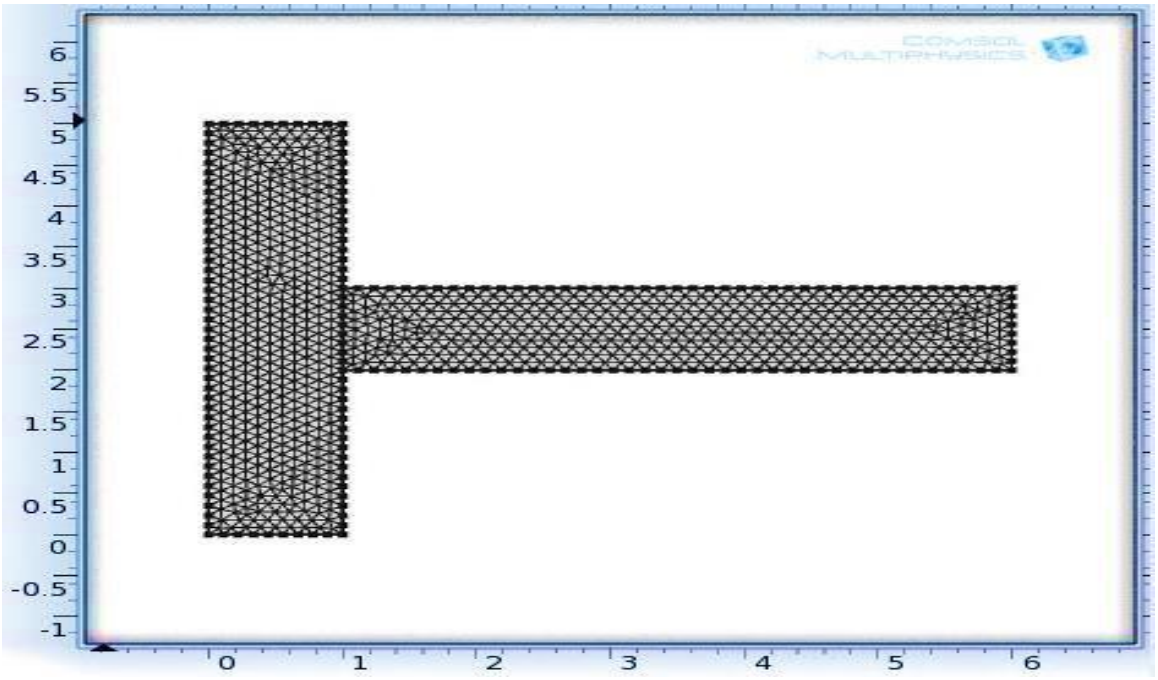

Figure 1. Meshing the membrane module in the Desulfurization process of Alcan- Thiophene by different membranes

Now, it is time to draw geometry. Right click on the "study", and click "Compute" option. On the "results" part, you see counters that display temperature, flux, velocity, and pressure. The results for the Polyethylene Glycol and Polyether Sulfone membrane are as follows [16-19]:
In the temperature graph, the input equals with the atmosphere temperature, and temperature gradually decreases along the membrane. The reason is that due to existence of vacuum in membrane output, condensation occurs, and accordingly, temperature in the membrane output decreases from thermodynamic point of view, and becomes cool.

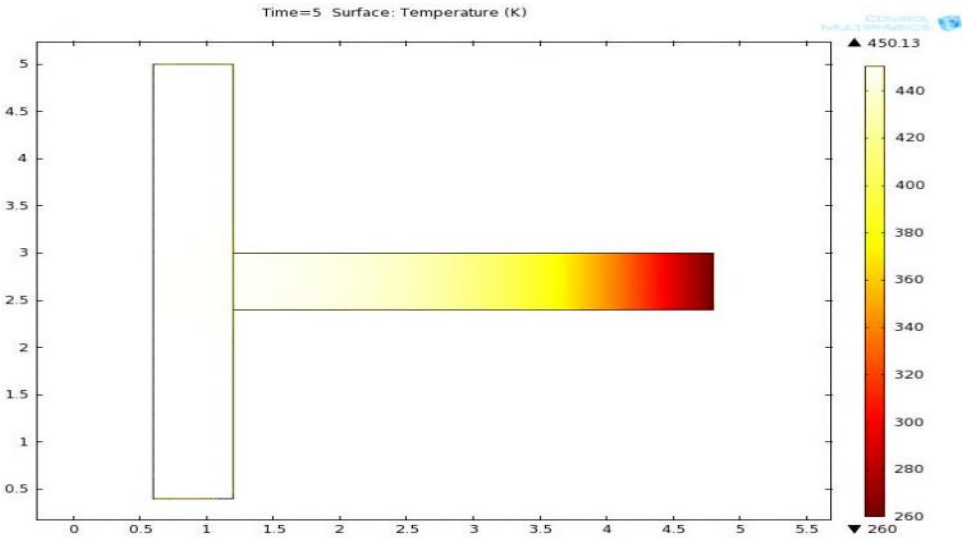

Figure 2. The temperature graph in Desulfurization process of Alcan-Thiophene by Polyethylene Glycol and Polyether Sulfone membrane

As there is feed in the input of the flux graph, the flux decrease is not so notable. The flux did not change in the membrane walls. However, due to increase of pressure within the membrane, flux increased. The error percentage for flux is 0.013.

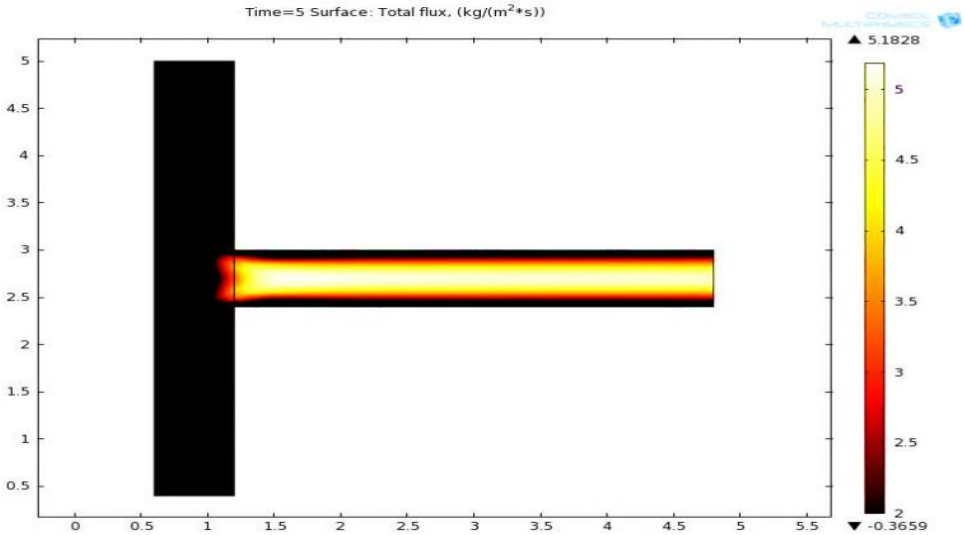

Figure 3. The flux graph in Desulfurization process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane

It is witnessed that in velocity graph, the current velocity in the input is low, and it decreased along the wall too. However, the velocity increased within the membrane as the temperature decreased along the membrane, and sulfur concentration increased.

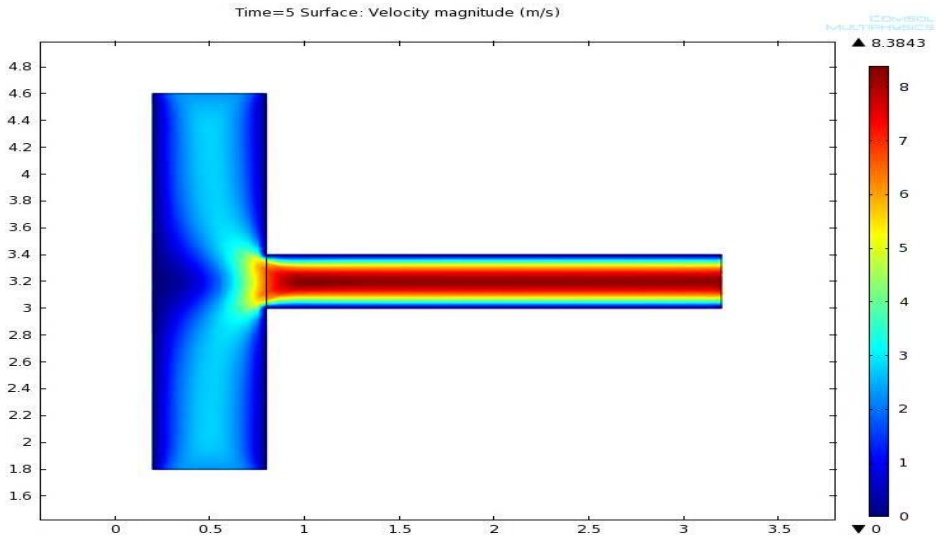

Figure 4. The velocity graph for Desulfurization process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane

In the pressure graph, the pressure is equal to atmosphere pressure at the input, and it decreased along the membrane. The reason can be increase of the driving force along the membrane.

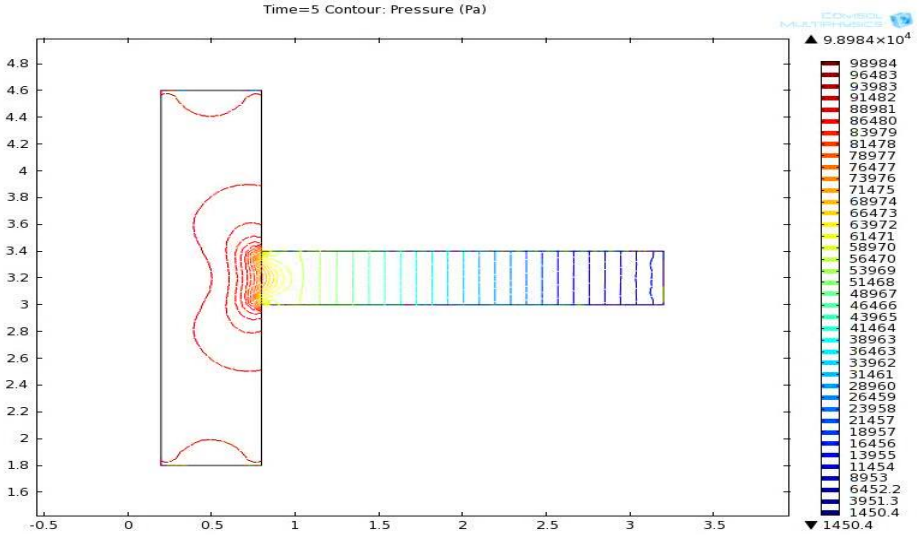

Figure 5. The pressure graph for for Desulfurization process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane

With regard to the error percentage, it can be concluded that modeling results was acceptable. As a result, COMSOL solves the problems in general.

Table 1: The percentage of COMSOL error compared to actual values for membranes

Flux obtained in membranes $kgm^{-2}h^{-1}$ / Modeling type	Membrane 1 PDMS_PAN [13]	Membrane 2 PDMS [14]	Membrane 3 PEG [15]
COMSOL	5.526	1.7116	3.0233
Actual values	5.384	1.72358	2.93548
Error percentage of COMSOL	2.56	0.69	2.90

3. Conclusion

The maximum amount of flux modeled by COMSOL, and the real amount of flux were compared in this study. The amount of error percentage in COMSOL was achieved to be 0.013 that was acceptable.
Desulfurization of organic compounds by means of evaporation was modeled in COMSOL too. It was concluded that Polyethylene Glycol- Polyether Sulfone Glycol membrane used for so doing is suitable for desulfurization of organic compounds. Moreover, the COMSOL could reflect the flux error very well in this study.

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