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# Mathematic modeling of purification of biodiesel with PES polymeric membrane

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## ABSTRACT

One of the new separation methods for purifying biodiesel used in recent years is the membrane separation process. In the current research, purification of produced biodiesel was carried out using Polymeric Poly Ether Sulfone(PES) based membrane. The prepared PVP membranes was containing 1, 1.5, 2 and 3 wt.% of PVP concentration with 16 wt.% PES. as additive. Reported experimental determining the membrane flux and separation efficiency (glycerol rejection) membrane was modeled by Maxwell Model. The result, including penetration rate, theory graph and experimental data comparison for biodiesel and glycerin, and error graphs have been explained. Results showed that the experimental data's have Compatibility with the model and, membrane with 2 percent PVP has provided more acceptable results.

***Keywords*:** Mathematic model, Maxwell Model, Biodiesel, PES, PVP.

## 1. Introduction

Biodiesel is produced from renewable sources such as vegetable oils or animal fats [1-6]. Biodiesel is produced through different techniques such as microemulsion, pyrolysis and transesterification[3,5]. However, the most notable way to produce biodiesel fuel is through

transesterification reaction.Transesterification is the reaction of triglycerides and low molecular weight alcohols such as methanol and ethanol in the presence of catalyst. Non-purified biodiesel will contain impurities such as glycerol, unreacted methanol, residual catalyst, bound glycerol (i.e., unreacted triglyceride (TG), diglyceride (DG) and monoglyceride (MG), and perhaps small amounts of soap and water. it is necessary to remove these impurities, because they will strongly affect engine performance [1].

The reported works showed that, the membrane separation process is a suitable alternative for biodiesel purification. In the present article, polymeric membranes were prepared for the separation of free glycerol dispersed in crude biodiesel. The polymeric membranes developed via phase inversion by immersion precipitation technique. In order to improve the properties and performance of the asymmetric poly ether sulfone (PES) membrane as the vital factors to purify the raw FAME by membrane processes [7], different contents of pvp polymer were added to the casting solution. It was attempted to understand the effects of different concentrations of pvp polymer on the structure and morphology of the pes membrane with the aim of glycerol removal from biodiesel. In this study we modeled experimental data from published experimental last works [12] by Maxwell model and comparing ability of permeation matrix membrane. Schematic diagram of an ideal MMM showed in Fig1.

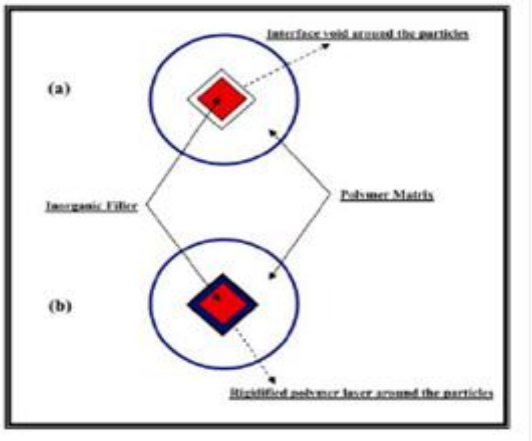


**Fig 1**.schematic diagram of an ideal MMM [8]

## 2. Experimental

### *Materials and Method*

Poly ether sulfone (PES Ultrason E6020P with MW=58,000 g/mol) and dimethyl acetamide (DMAC) as the solvent, polyvinyl pyrrolidone (PVP) with25, 000 g/mol as the pore former. Waste cooking oils, methanol (99.9% purity) and sodium hydroxide (NaOH) for biodiesel production.

### *Preparation of membranes*

Blend PES membrane with PVP polymer were prepared as method reported in last work [12] by using phase inversion induced by immersion precipitation technique. Casting solutions consisting of PES (16wt. %), DMAC and different concentration of PVP polymer (1, 1.5, 2 and 3 wt.%) as an additive and pore former were prepared by mechanical stirrer at 200-400 rpm and room temperature (25℃). After formation of homogeneous solution, the films were cast by a casting knife with 250 μm thickness. The prepared films were immersed in non-solvent bath for precipitation. The immersion process was carried out at room temperature. The non-solvent was only water. The prepared membranes were washed and stored in water for at least 1 day to completely leach out the residual solvents and additives. As the final stage, the membranes were dried by placing between two sheets of filter paper for 24 h at room temperature.

### *Maxwell's Model Method*

Maxwell's model is the most famous equation to predict the permeability and electrical conductivity in composite materials [10]. Maxwell presented this equation in 1873 heterogeneous media [8].Development of proper model(s) for prediction of MMMs different properties, especially those of separation performance, is essential for approaching this goal. On the other hand, having of this model(s) potentially can reduce necessity of the

experimental measurements' time and money for preparation and evaluation of different MMMs.Many theoretical and empirical predictive models have been adapted or developed for prediction of MMMs separation performance. the penetrates permeation through MMMs as follows:

$$P_r = P_c[\frac{P_d + 2P_c - 2\varphi_d(P_c - P_d)}{P_d + 2P_c + \varphi_d(P_c - P_d)}] \quad (3)$$

$$\varphi = \frac{V_{fil}}{V_{fil} + V_{pol}} \quad (4)$$

Where Pr is the ratio of MMM permeability (PMMM) to that of continuous polymer phase (Pc) as (PMMM/Pc), Pd is the incorporated dispersed filler particles, and ϕd is the volumetric filler particles loading. Even though many other models have been proposed for predicting the permeability of mixed matrix membranes but Maxwell model has been accepted most widely in the literature[10,11].In the case of MMMs containing impermeable filler particles (Pd= 0), this model is reduced to the following equation [10]:

$$P_r = P_c[\frac{1 - \varphi_d}{1 + 0.5\varphi_d}] \quad (5)$$

In the present study, 4 PES membranes separation ability were comparison. In addition, in order to enhance the separation performance of the prepared membranes, different amounts of PVP polymer effect on this separation, were incorporated into the membrane matrices. It is reasonably a novel work to examine the separation properties of PES membranes for the biodiesel purification. Then we predicted performance of membrane with Maxwell model and calculated AARE%.

**Table 1**. Experimental data and Theoretical data of the Maxwell model

| AARE (%) The Maxwell model | | Teorical $P_r$ | | Experimental $P_r$ | | sample |
|---|---|---|---|---|---|---|
| $P_{gly}$ | $P_{bio}$ | $P_{gly}$ | $P_{bio}$ | $P_{gly}$ | $P_{bio}$ | |
| 66.66 | 44.23 | 0.09 | 0.58 | *0.27* | *1.04* | 18%PES+1%PVP |
| 52.17 | 44.03 | 0.11 | 0.61 | *0.23* | *1.09* | 18%PES+1.5%PVP |
| 29.41 | 39.63 | 0.12 | 0.67 | *0.17* | *1.11* | 18%PES+2%PVP |
| 58.33 | 40.74 | 0.1 | 0.64 | *0.24* | *1.08* | 18%PES+3%PVP |

## 3. Results and discussion

The results of permeability for the biodiesel and glycerol in PES/PVP blend membranes are given in Table 1 at 25°C and 1 bar. As it is observed that PES/PVP introduced the high permeability.

However, several researchers were reported some increment in permeability of MMMs with incorporated impermeable filler particles. They concluded that increasing in the resultant MMMs' permeability may be due to disrupting the polymer chain packing density by adding filler and increment of the matrix polymer's free volume, especially in the vicinity of the filler particles. But According to the Maxwell model for impermeable filler particles, MMMs' permeability's are decreased as filler particles loadings increases (Fig. 3). It seems there is a better explanation for the case and that is the surface flux on the external surface of the incorporated filler particles [8]. The optimization criteria of prediction accuracy of the current developed model is absolute average relative error percentage (AARE %) of predicted MMMs' permeability's by the following equation [8]:

$$AARE\% = \frac{100}{N}\sum_{i=0}^{N}\left|\frac{P_i^{cal} - P_i^{exp}}{P_i^{exp}}\right| \qquad (6)$$

Fig 2 and 3 shows the comparison between Pr experimental data and Pr computational data of the glycerin and biodiesel component. However it is commonly that there is a difference between theoretical and experimental data. In this clearly, if the difference between theoretical and experimental data is less, it's better. So sample No.3 represents the smallest difference among all samples, it is the best sample.

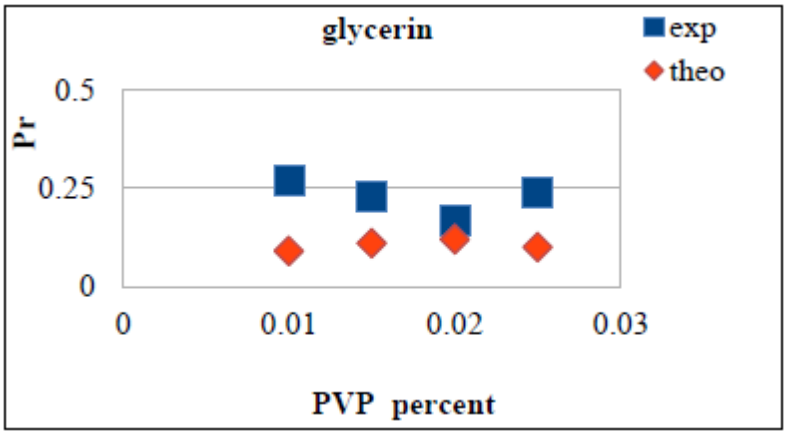


**Fig. 2**.Comparison of theoretical and experimental data for glycerin

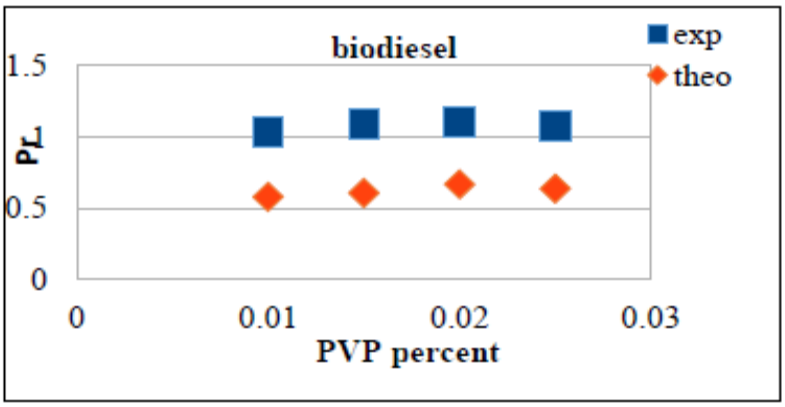


**Fig. 3**. Comparison of theoretical and experimental data for Biodiesel

The computational error rate between observed data and computational Maxwell modeldata is shown in Fig 4. The lower the error rate explained the less the difference between the empirical data and the theory, and the predicted model could well cover the experimental data. As it is seen, the membrane No.3 has the most matching.

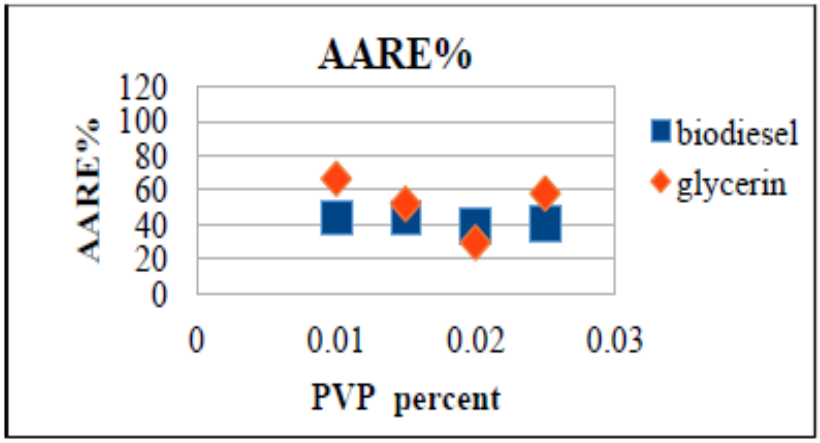


**Fig. 4**.error rate between theoretical and experimental data

## 4. Conclusions

PES/PVP blend membranes were successfully prepared with different PVP contents to investigate their behavior in biodiesel/glycerol separation. The results demonstrated that Due to the data obtained in the laboratory and the modelling performed by the software and as it is shown in diagrams, the model and experimental data has excellent accordance together. As the purpose of this study was to isolate glycerin from biodiesel, the amount of glycerin penetration in the outflow of membranes was minimal. In the case of experimental data and Pr theory, in both cases glycerin and biodiesel of the 2% PVP membrane showed more suitable values. The error rate of this sample was lowest.

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