



QUATERNARY POLYMERIC THERMODYNAMIC SYSTEM AND MEMBRANE FORMATION MATHEMATICAL MODEL

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ABSTRACT

A thermodynamic model of quaternary polymeric solution was developed for membrane formation. It incorporates two mixed solvents *N*-methyl-2-pyrrolidone (NMP) and tetrahydrofuran (THF), and two high molecular weight polymers cellulose acetate (CA) and polyvinyl chloride (PVC). Also, another polymeric solution was modeled by replacing (CA) with polyvinylpyrrolidone (PVP). The developed model depends on the extended modified Flory-Huggins model. Gibbs free energy was studied in the range of -200 J/mol at 313K to -450 J/mol at 363K. The polymer blend solution was homogenous in the studied range. In addition, the diffusion model of immersion precipitation process was investigated. The results indicate that the ratio of $\phi_{CA} / \phi_{solvents}$ increases with coagulation time due to removal almost all the solvents from the polymeric solution, while the thickness of polymer membrane decreases due to the coagulation process. The prepared membranes were tested by scan electron microscope and the test results have validated the model results.

Keywords: cellulose acetate, polyvinyl chloride, modelling, quaternary system, immersion precipitation, membrane preparation.

1. INTRODUCTION

Polymers blending to synthesise membranes have been widely researched for production of various membranes types for different applications. The blending process allows production of membranes with tailored performance due to mixed polymer matrix and cross-linking, [1-5]. Blended membranes are mostly prepared using phase inversion technique. The fabrication process is divided into three steps; mixing step, casting step and coagulation step. In mixing step polymers, solvent and non-solvent are mixed together for a certain period. In casting step, the polymeric solution is casted on a glass plate to form a thin film. Finally, in coagulation or immersion precipitation step, the casted polymeric film is immersed in a coagulation bath. Diffusion of solvent from casting solution into the coagulation bath leads to membrane formation [1-4].

Immersion precipitation is the most popular coagulation technique, where the prepared polymeric film is immersed in a coagulation bath. In this technique the diffusion process between solvent in prepared polymeric film and non-solvent in coagulation bath will lead to membrane formation [1-7].

The Flory-Huggins theory describes the polymeric systems behaviour in coagulation bath. The Flory-Huggins mathematical model accounts for combinatorial entropy of mixing, in molecular scale, in polymeric mixtures. Flory-Huggins model can be expressed as a function of the Gibbs free energy for polymers mixing. The main parameter in Flory-Huggins model is the dimensionless interaction parameter (χ), where the positive values of (χ) indicates immiscibility of polymers in the mixture, which is due to high molecular weight. A negative (χ) indicates miscible polymers mixture due to high interaction between segments of polymers in the polymeric mixture [7-10].

In the high molecular weight polymeric mixtures, the entropy of mixture is small and the miscibility of the polymeric mixture depends on the interaction parameter (χ). If χ is negative, the polymeric solution will remain homogeneous for long time, due to decrease of Gibbs free energy, which minimizes phase separation [11-16].

The objective of this work is to develop a thermodynamic model of polymeric solution miscibility for quaternary systems. The model predicts characteristics of membrane film formation based on diffusion theory. To validate the model, a set of experiments were carried out and the prepared membranes were characterized using SEM. The model would lead to a better understanding of membrane formation process.

2. MODEL DESCRIPTION

2.1 Model equations and assumptions

The modified Flory-Huggins theory [1, 2] is selected as the base for the quaternary polymeric system thermodynamic model. The model equations were encoded into MATLAB® software (The Math works, Release 2009b).

The Gibbs free energy of mixing of two polymers and two solvents are calculated using the following equations:

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

Where

ΔG_m = Gibbs free energy, J/mol

ΔH_m = Change in enthalpy during the mixing process, J/mol

T = Temperature, K



ΔS_m = Change in entropy during the mixing process,
J/mol/K

$$X_{ij} = \frac{V_r(\delta_i - \delta_j)^2}{RT} \quad (2)$$

Where;

The change in Gibbs free energy was evaluated in the temperature range 313-363K. For a spontaneous mixing process the Gibbs free energy must be negative.

During phase separation of aquaternary system, the critical value of interaction parameters to study the spinodal decomposition is calculated from Equation (2):

δ_i = Solubility parameter of component i
 V_r = Reference volume, chosen to be 100 cm³/mol
 R = Universal gas constant, J/mol/K

The main equation of the Flory-Huggins model for quaternary polymeric solutions is written as:

$$\Delta G_m = RT \left[\sum_{i=1,2,3,4} n_i \ln \phi_i + n_1 \phi_2 X_{12} + n_1 \sum_{i=1,2,3} \phi_i \sum_{j=2,3,4} X_{ij} + n_2 \sum_{i=3,4} \phi_i \sum_{j=3,4} X_{ij} + n_3 \sum_{i=4} \phi_i \sum_{j=3} X_{ij} \right] \quad (3)$$

Where;

n_i = Number of moles of component i, mole

ϕ_i = Volume fraction of component i

$$w_i = \frac{\phi_i}{\phi_i + \phi_3} \quad (6)$$

The pseudo-binary compositions are calculated using the following equations:

Chemical potentials, of components: 1-polymer (1), 2-polymer (2), 3-solvent (1), and 4-solvent (2), were employed to develop the quaternary coexistence curve. Chemical potentials were calculated using the first derivative of the Gibbs free energy of mixing equation with respect to the mole fraction of each component, Equations 7-10.

$$u_i = \frac{\phi_i}{\phi_i + \phi_1} \quad (4)$$

$$v_i = \frac{\phi_i}{\phi_i + \phi_2} \quad (5)$$

$$\frac{\Delta \mu_1}{RT} = a + b(1 - \phi_1) - c - \phi_2 u_2(1 - u_2) \left[\frac{\partial X_{12}}{\partial u_2} \right] - \phi_3 u_3(1 - u_3) \left[\frac{\partial X_{23}}{\partial u_3} \right] - \phi_4 u_4(1 - u_4) \left[\frac{\partial X_{24}}{\partial u_4} \right] \quad (7)$$

$$\frac{s \Delta \mu_2}{RT} = d + e(1 - \phi_2) - f - \phi_1 u_2(1 - u_2) \left[\frac{\partial X_{12}}{\partial u_2} \right] - s \phi_3 v_3(1 - v_3) \left[\frac{\partial X_{23}}{\partial v_3} \right] - s \phi_4 v_4(1 - v_4) \left[\frac{\partial X_{24}}{\partial v_4} \right] \quad (8)$$

$$\frac{r \Delta \mu_3}{RT} = g + h(1 - \phi_3) - k + \phi_1 u_3(1 - u_3) \left[\frac{\partial X_{13}}{\partial u_3} \right] + s \phi_2 v_3(1 - v_3) \left[\frac{\partial X_{23}}{\partial v_3} \right] + r \phi_4 w_4(1 - w_4) \left[\frac{\partial X_{34}}{\partial w_4} \right] \quad (9)$$

$$\frac{t \Delta \mu_4}{RT} = l + m(1 - \phi_4) - q + \phi_1 u_4(1 - u_4) \left[\frac{\partial X_{14}}{\partial u_4} \right] + s \phi_2 v_4(1 - v_4) \left[\frac{\partial X_{24}}{\partial v_4} \right] + r \phi_3 w_4(1 - w_4) \left[\frac{\partial X_{34}}{\partial w_4} \right] \quad (10)$$

The ratio between molar volumes of different components (V_i) is a function of s, r and t, Equations 11-13. In addition, variables a, b, c, d, e, f, g, h, k, l, m and q are used to simplify the appearance of the formula as shown in Table-1.

$$s = \frac{V_1}{V_2} \quad (11)$$

$$r = \frac{V_1}{V_3} \quad (12)$$

$$t = \frac{V_1}{V_4} \quad (13)$$

**Table-1.** Simplified variables list.

Variables	related equation
a	$\ln\phi_1 - s\phi_2 - r\phi_3 - t\phi_4$
b	$1 + X_{12}\phi_2 + X_{13}\phi_3 + X_{14}\phi_4$
c	$sX_{23}\phi_2\phi_3 + sX_{24}\phi_2\phi_4 + rX_{34}\phi_3\phi_4$
d	$\ln\phi_2 - \phi_1 - r\phi_3 - t\phi_4$
e	$s + X_{12}\phi_1 + sX_{23}\phi_3 + sX_{24}\phi_4$
f	$X_{13}\phi_1\phi_3 + X_{14}\phi_1\phi_4 + rX_{34}\phi_3\phi_4$
g	$\ln\phi_3 - \phi_1 - s\phi_2 - t\phi_4$
h	$r + X_{13}\phi_1 + sX_{23}\phi_2 + rX_{34}\phi_4$
k	$X_{12}\phi_1\phi_2 + X_{14}\phi_1\phi_4 + rX_{24}\phi_2\phi_4$
l	$\ln\phi_4 - \phi_1 - s\phi_2 - r\phi_3$
m	$t + X_{14}\phi_1 + sX_{24}\phi_2 + rX_{34}\phi_3$
q	$X_{12}\phi_1\phi_2 + X_{13}\phi_1\phi_3 + sX_{23}\phi_2\phi_3$

The solubility parameters and molecular interactions depend on the following three specific interactions, namely: non-polar interaction, hydrogen bonding and polar cohesive forces. Hildebrand solubility parameter (δ_t) can be calculated by dividing the cohesive energy by the molar volume. δ_t is used to evaluate the Hansen (δ_D), polar (δ_P), and hydrogen bonding dispersions (δ_H) components as shown by Equation 14. Solubility parameters of polymer solution components were evaluated using Equation 14 and the results are presented in Table-2.

$$\delta_t^2 = \delta_D^2 + \delta_P^2 + \delta_H^2 \quad (14)$$

Table-2. Solubility parameters of polymer solution components.

Component	δ_d	δ_p	δ_h	$\Delta\delta$
PVC	18.2	7.5	8.3	21.36
CA	7.9	3.5	6.3	10.7
PVP	19.4	17.4	11.3	28.4
NMP	18	12.3	7.2	22.95
THF	16.8	5.7	8	19.4

2.2 Diffusion model of immersion precipitation

2.2.1 Diffusion model assumptions

Preparation of membrane by immersion precipitation was studied in several articles considering models for diffusion process during membrane formation in the coagulation bath [1-7]. In our study, the following assumptions were considered during model development:

- The reference system is selected centered on the interface between casting membrane and the coagulation bath.
- The casting membrane interface in the coagulation bath initially has a composition like the original coagulation bath.
- The membrane polymer film is considered as a matrix; accordingly, the components with low molecular weight diffuse to the coagulation bath.
- The volume of the polymeric solution is not constant.
- Polymer film is considered a one phase system until the spinodal is reached.
- The spinodal takes place due to solvent diffusion to the coagulation bath.
- The fluxes of components in diffusion process are independent of the film thickness.

The model is governed by the diffusion taking place at polymer film and coagulation bath interface. The formula, describes diffusion in the polymer solution, is displayed in Equation (15), where, component (i) refers to polymer components (PVC, PVP and CA).

$$\frac{d(\frac{\phi_i}{\phi_n})}{dt} = \bar{v}_i \frac{\partial}{\partial m} \left\{ \sum_{j=1:n-1} \phi_n L_{ij} \frac{\partial \mu_j}{\partial m} \right\} \quad (15)$$

A coordinate transformation is carried out to avoid the change of polymer volume consequences. The Cartesian coordinate (x) in polymer solution is transformed in a polymer fixed reference system (m) and a reference system originating from interface between the



polymer solution and the coagulation bath (y). The transformation is given by Equations (16) and (17):

$$m = \int_0^L \phi_i dx \quad (16)$$

$$y = x - \Delta x \quad (17)$$

Where;

L: Total film thickness, m

The solvent diffusion during the immersion process in coagulation bath is shown in Equation (18), where component (j) represents solvent.

$$\frac{d\phi_i}{dt} = \bar{v}_i \frac{\partial}{\partial y} \left\{ \sum_{j=1:n-1} L'_{ij} \frac{\partial \mu_j}{\partial y} \right\} - \frac{\partial \phi_i}{\partial y} \sum_{k=1:n-1} J_k \quad (18)$$

Where:

$i = 1:n - 1$

t = Time, s

\bar{v}_i = Molar volume of component i, m³/mol

J_k = Flux of species k into the coagulation bath at the interface between polymer solution and coagulation bath at (y=0)

L'_{ij} and L''_{ij} = The matrix elements of the phenomenological coefficient matrix L and L' respectively.

L and L' = The inverse of the friction coefficient matrix R and R' respectively.

R and R' = friction coefficient matrix, calculated according to the following equations:

$$R_{ii} = - \left(\sum_{k \neq i} c_k R_{ik} \frac{RT\bar{v}_i}{M_i D_{ik}} + c_n \frac{RT\bar{v}_i}{M_i D_{in}} \right) \quad (19)$$

$$R'_{ii} = - \sum_{k \neq i} c_k \frac{RT\bar{v}_i}{M_i D_{ik}} \quad (20)$$

$$R_{ij} = c_j \frac{RT\bar{v}_i}{M_i D_{ij}} \text{ for } i \neq j \quad (21)$$

$$R'_{ij} = c_j \frac{RT\bar{v}_i}{M_i D_{ij}} \text{ for } i \neq j \quad (22)$$

Where

D_{ij} = Binary diffusion coefficient between i and j, m²/s

R = Universal gas constant, J/mol/K

T = Temperature, K

M_i = Molecular weight of component i, kg/kmole

Initial conditions

The initial conditions for polymeric solutions and coagulation bath are shown below, respectively:

$$\begin{aligned} \phi_i(m, t = 0) &= \phi_{i, \text{Polymersolution}}^0 \text{ for } i = 1:n - 1 \\ \phi_i(y, t = 0) &= \phi_{i, \text{Coagulationbath}}^0 \text{ for } i = 1:n - 1 \end{aligned}$$

Boundary conditions

The boundary conditions for polymeric solutions and coagulation bath are given below, respectively:

$$\begin{aligned} \frac{d(\phi_i)}{dt} &= 0 & \text{for } m &= \infty \\ \frac{d(\phi_i)}{dt} &= 0 & \text{for } y &= \infty \end{aligned}$$

Additional assumption considers equal fluxes and chemical potentials of different components around both sides of the interface:

$$\begin{aligned} \Delta\mu(m = 0) &= \Delta\mu(y = 0) \text{ for } i = 1:n - 1 \\ J_i(m = 0) &= J_i(y = 0) \text{ for } i = 1:n - 1 \end{aligned}$$

3. RESULTS AND DISCUSSIONS

The model was developed to investigate the effect of membrane preparation conditions on its formation and morphology. The study focused on two different membranes, PVC/CA blend membrane and PVC with PVP as pore former additive.

3.1 Model verification

3.1.1 Effect of polymer blend composition

Two different membranes were prepared, first membrane was prepared using PVC, CA, THF and NMP. Different compositions of CA polymer in range of 0.02 to 0.12 volume fraction were examined at different temperatures during polymersolution mixing. Figure-1 indicates that the Gibbs free energy is approximately constant in volume fraction range of 0.02 to 0.12. The Gibbs free energy ranged from -200 J/mol at 313K to -450 J/mol at 363K. Negative value of free energy of mixing, $\Delta G_m \approx \Delta H_m \leq 0$ within the phase stability condition ($\Delta G_m / \Delta H_m > 0$) indicates homogeneity of the polymeric solution, which depends on the macromolecular dimension and the domain size.

Straight lines Gibbs free energy in Figure-1 indicate that there is no limitation of miscibility between low compositions of the polymers. Also, the horizontal ΔG lines in Figure-1 indicate that the phase separation cannot occur under tested compositions [24] during mixing of the two polymers (PVC/CA). Figure-2 indicates that during mixing the chemical potential of CA at various temperatures decrease by increasing the ratio of CA, leading to inefficient blending of the two polymers when CA ratio of 0.12 is reached.

The second membrane was prepared using PVC, PVP, THF and NMP. The volume fraction of PVC was varied from 0.09 to 0.14. Figure-3 indicates that the Gibbs free energy varies slightly in this volume fraction range. Accordingly, the polymer and the additive has no limitation of miscibility and the solution was homogenous. Figure-4 shows decrease of chemical potential with the increase of PVC ratio at various temperatures of polymer



solution, which indicates complete mixing PVP additive (NMP). and PVC polymer in the two solvents mixture (THF and

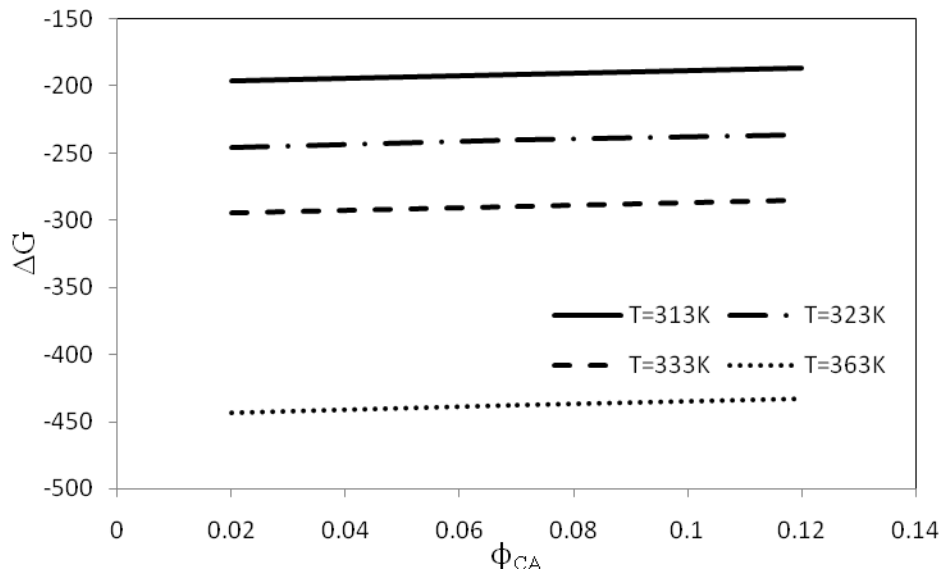


Figure-1. ΔG as a function of ϕ_{CA} at different temperatures.

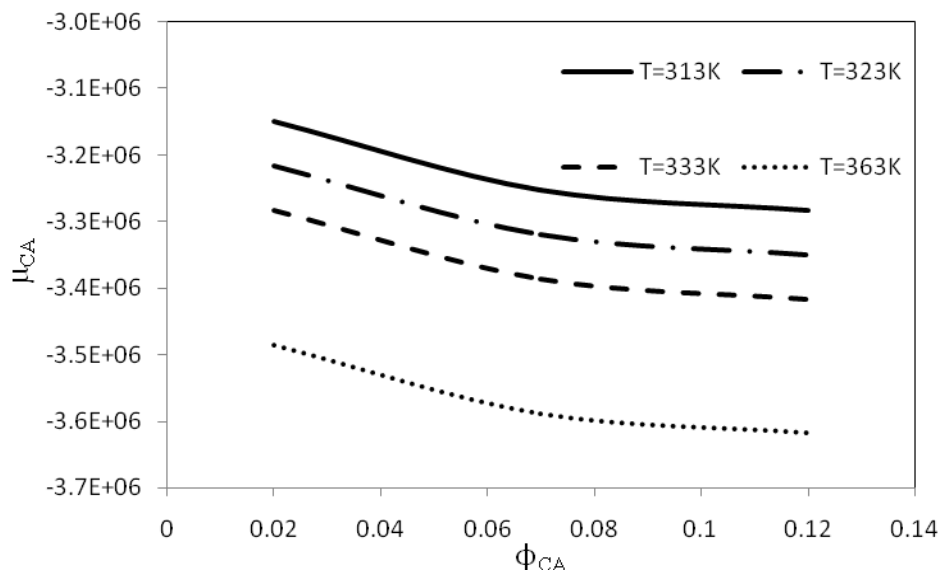


Figure-2. μ_{CA} as a function of ϕ_{CA} at different temperatures.

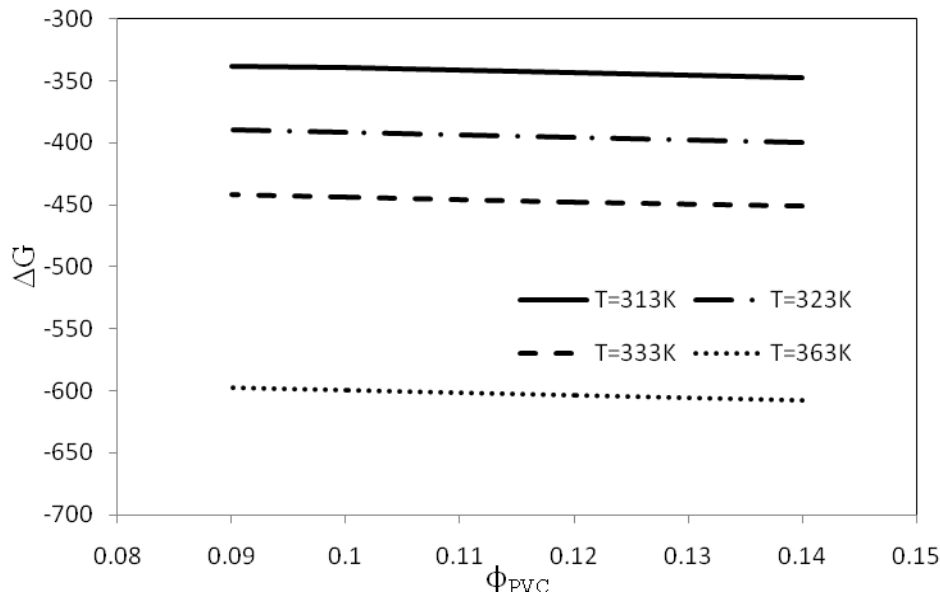


Figure-3. ΔG as a function of ϕ_{PVC} at different temperatures.

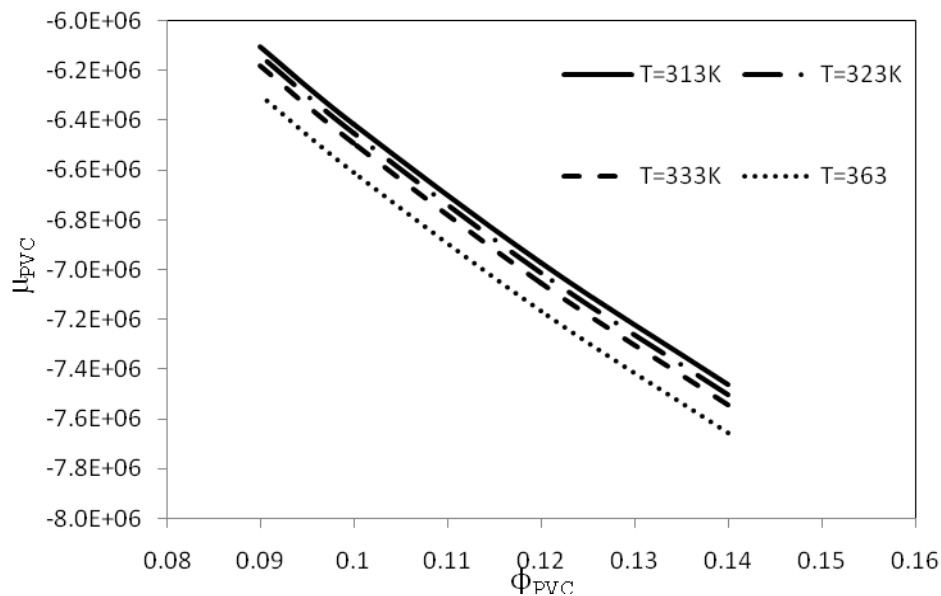


Figure-4. μ_{PVC} as a function of ϕ_{PVC} at different temperatures.

3.2 Verification of diffusion model for immersion precipitation

Two cases were studied to investigate the coagulation process parameters effect on the quaternary polymeric membrane formation. The immersion precipitation process model is described by Equations 17, 18, and 19. The model evaluates the immersion precipitation time effect on the diffusion process by removal of solvents from cast polymer solution to the coagulation bath. The solvent concentration increase in the coagulation bath (water) point to phase separation process proceeding. The polymeric blend membrane is formed after the polymers blend is concentrated as a result of solvent diffusion to coagulation bath [17-27].

The first case study of the model considered preparation of quaternary blend membrane of PVC, CA, THF and NMP. Figure-5 illustrates the effect of time on the membrane formation during the coagulation process. In this case, equal volume fractions of PVC and CA were used (0.07), while the volume fractions of solvents were $\phi_{NMP}=0.15$ and $\phi_{THF}=0.71$. The model results indicated that the ratio of $\phi_{CA}/\phi_{solvents}$ increased with coagulation time due to diffusion of solvents from the polymeric solution to the coagulation bath. Also, the thickness of polymer solution film on the glassplate decreased with time due to solvent removal, forming a concentrated polymer film. Figure-6 shows the variation of $\phi_{PVC}/$



ϕ_{solvents} ratio with time. Figure-5 and Figure-6 indicate that PVC and CA coagulation rates get closer to each other with time. Accordingly, the blend membrane can be formed. Figure-7 and Figure-8 show the increase of NMP and THF concentrations in coagulation bath with time due to diffusion of solvents from the casted polymer to the coagulation bath. Figures 7 and 8 showed a gradual decrease of NMP and THF concentration from 0-200 minutes followed by a slower decrease in solvents concentrations.

Figure-9 shows the formed membrane structure after 500 minutes in the coagulation bath. The figure illustrates that the upper selective layer was formed from CA and the middle and bottom layers were formed from PVC. The formed membrane thickness was 284 μm . By comparing the predicted composition with experimental work, a similar shape of membrane cross section was produced, where the dense top layer was CA and the bottom layer was PVC as shown in Figure-10.

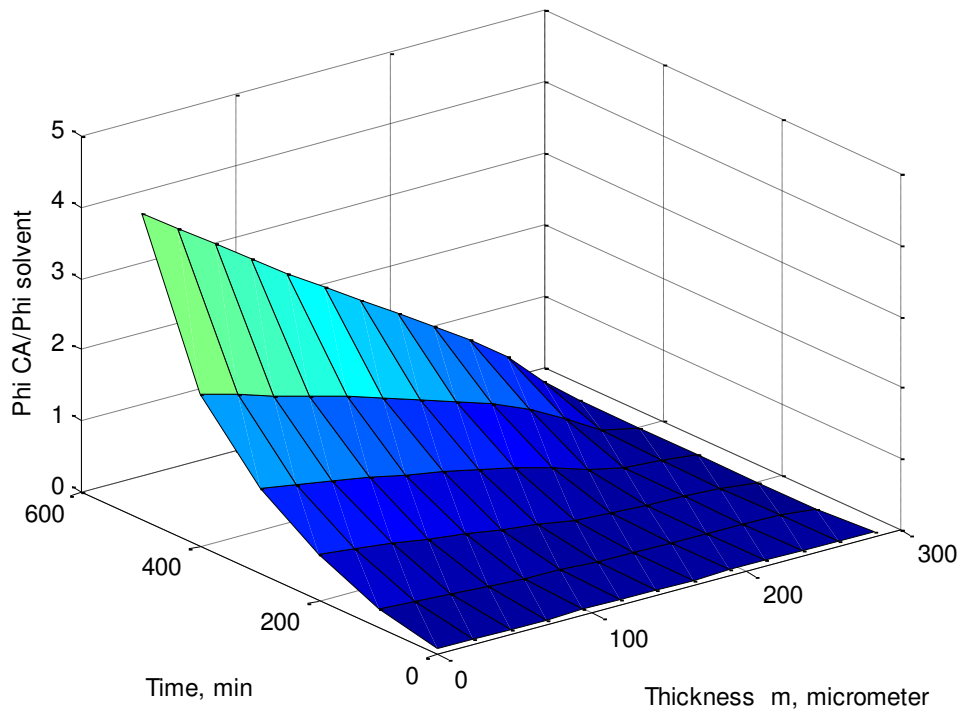


Figure-5. $\phi_{\text{CA}}/\phi_{\text{solvent}}$ as a function of time and thickness of membrane at $T=298\text{K}$,
 Initially; $\phi_{\text{CA}}=0.07$, $\phi_{\text{PVC}}=0.07$, $\phi_{\text{NMP}}=0.15$, $\phi_{\text{THF}}=0.71$.

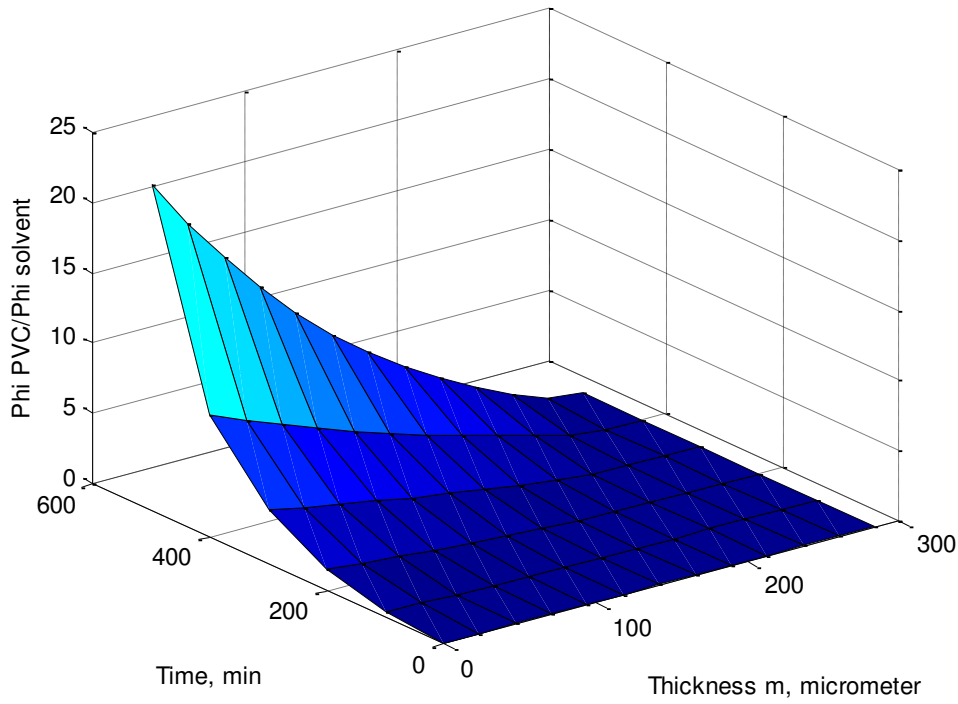


Figure-6. $\phi_{PVC}/\phi_{solvent}$ as a function of time and thickness of membrane at T=298K, Initially; $\phi_{CA}=0.07$, $\phi_{PVC}=0.07$, $\phi_{NMP}=0.15$, $\phi_{THF}=0.71$.

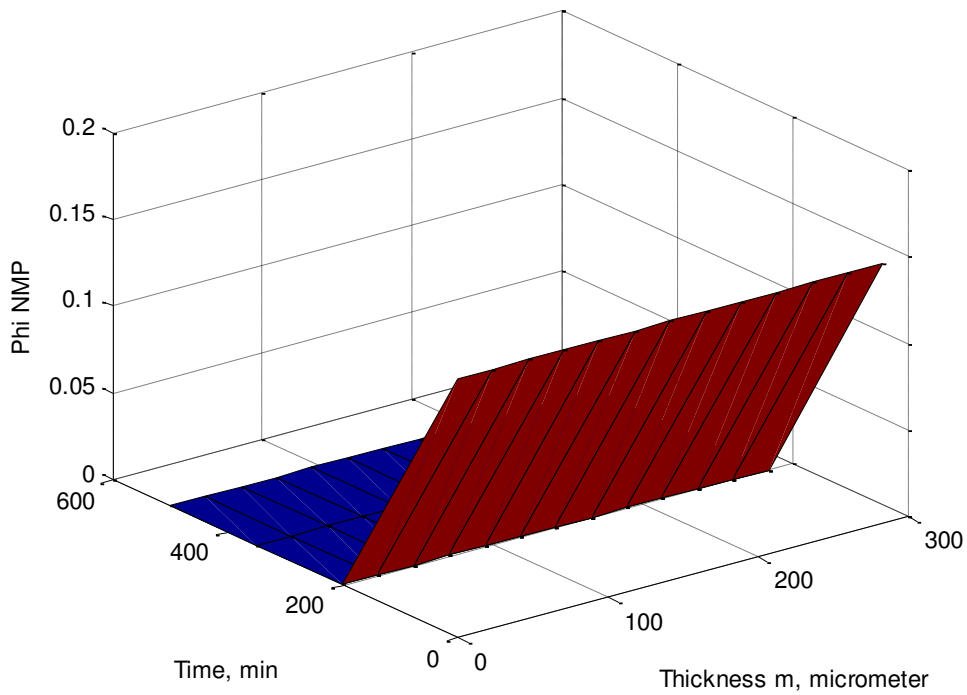


Figure-7. ϕ_{NMP} as a function of time and thickness of membrane at T=298K, Initially; $\phi_{CA}=0.07$, $\phi_{PVC}=0.07$, $\phi_{NMP}=0.15$, $\phi_{THF}=0.71$.

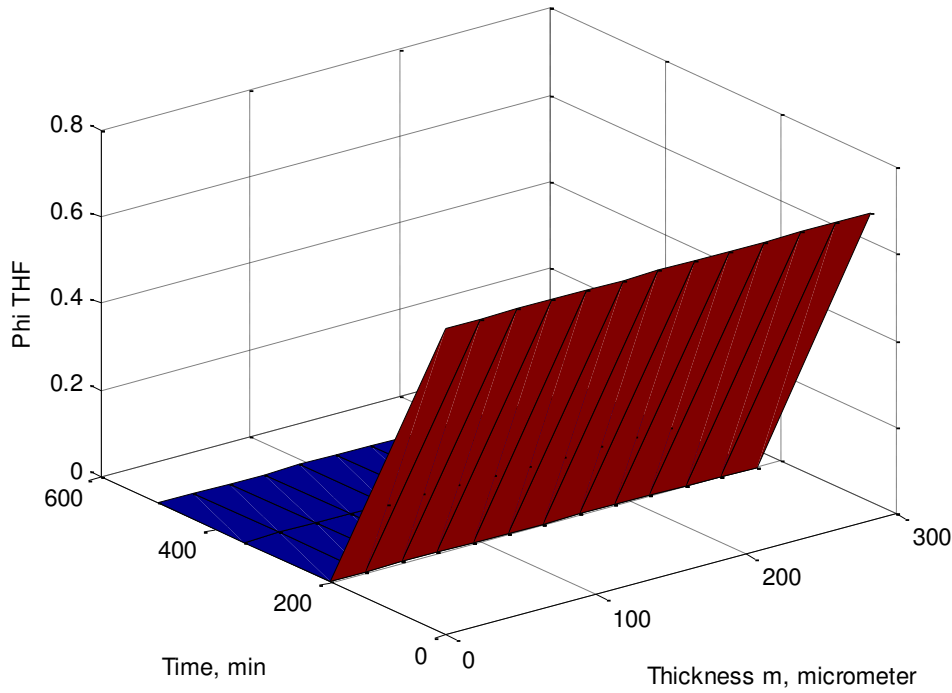
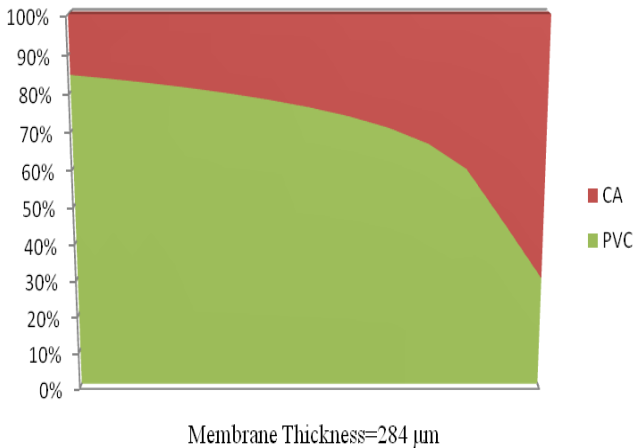


Figure-8. ϕ_{THF} as a function of time and thickness of membrane at $T=298K$, Initially;
 $\phi_{CA}= 0.07, \phi_{PVC}= 0.07, \phi_{NMP}=0.15, \phi_{THF}=0.71$.



Membrane Thickness=284 μ m

Figure-9. Representation of membrane constituents after 500 min of coagulation.

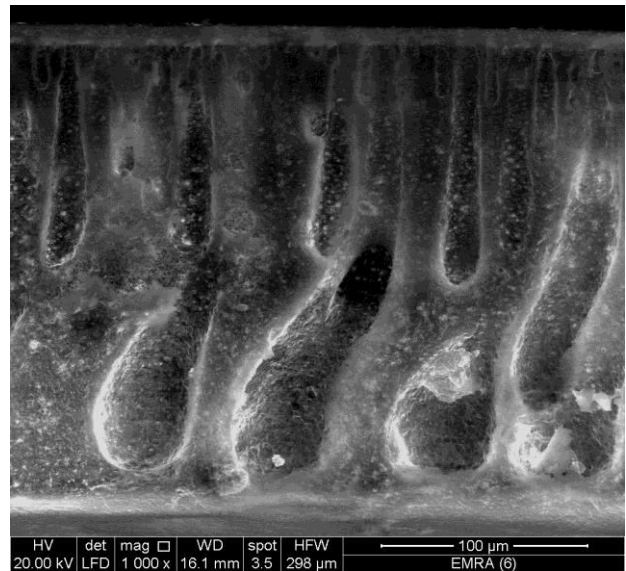


Figure-10. Electron scan of blend membrane PVC/CA.

The second case study considered preparation of quaternary blend membrane of PVC, PVP, THF and NMP. Figure-11 shows the effect of time on membrane formation during the coagulation process. Under such conditions, volume fractions of PVC and PVP were 0.14 and 0.04 respectively. The volume fractions of solvents ϕ_{NMP} and ϕ_{THF} were 0.15 and 0.67 respectively. The results indicate that the ratio of $\phi_{PVC} / \phi_{solvents}$ increased with coagulation time. The solvents diffusion and the thickness of polymer solution on the plate decreased with



time. Figure-12 shows the variation of $\phi_{PVP}/\phi_{solvents}$ ratio with time. The model results indicated that polymer (PVP) solution thickness decreases with time due to solvent removal. Figure-13 and Figure-14 illustrate that the solvents NMP and THF concentrations increased gradually in the coagulation bath with time, due to diffusion of solvents from the polymeric solution to the bath [17-27].

Figure-15 shows the formed membrane structure after 500 min in the coagulation bath, showing that the upper layer was formed mostly from PVC and that the middle and bottom layers were formed from PVC and PVP. The formed membrane thickness was 268 μm . By comparing the predicted structure Figure-16 with experimental work, similar porous shape of membrane cross section were evident. The results of the two case studies showed that the model can reproduce the experimental work. Accordingly, the model is validated.

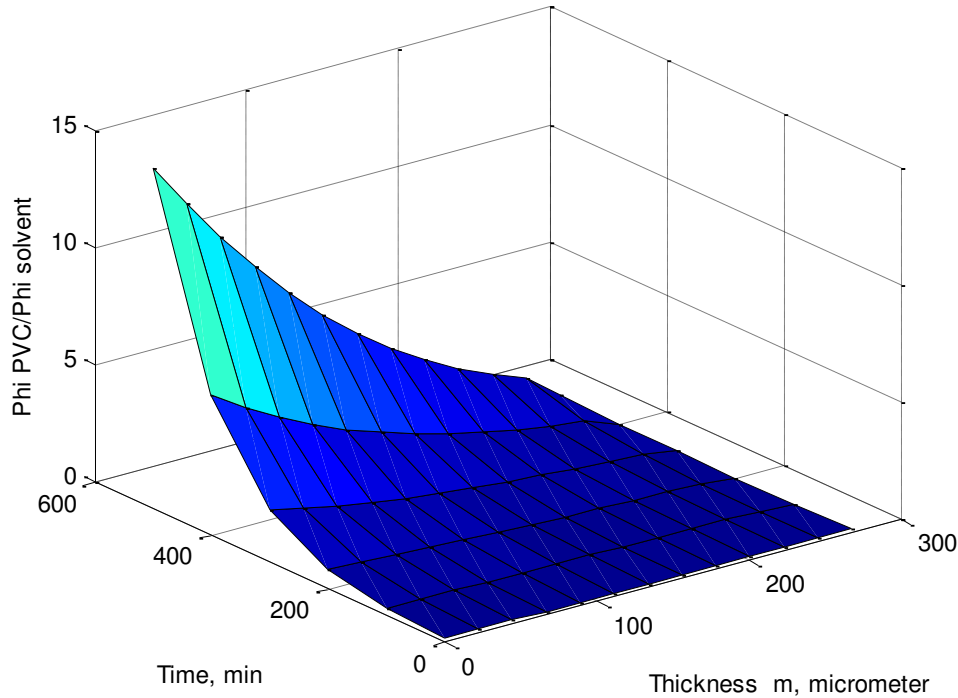


Figure-11. $\phi_{PVC}/\phi_{solvent}$ as a function of time and thickness of membrane at $T=298\text{K}$,
 Initially; $\phi_{PVC}=0.14$, $\phi_{PVP}=0.04$, $\phi_{NMP}=0.15$, $\phi_{THF}=0.67$

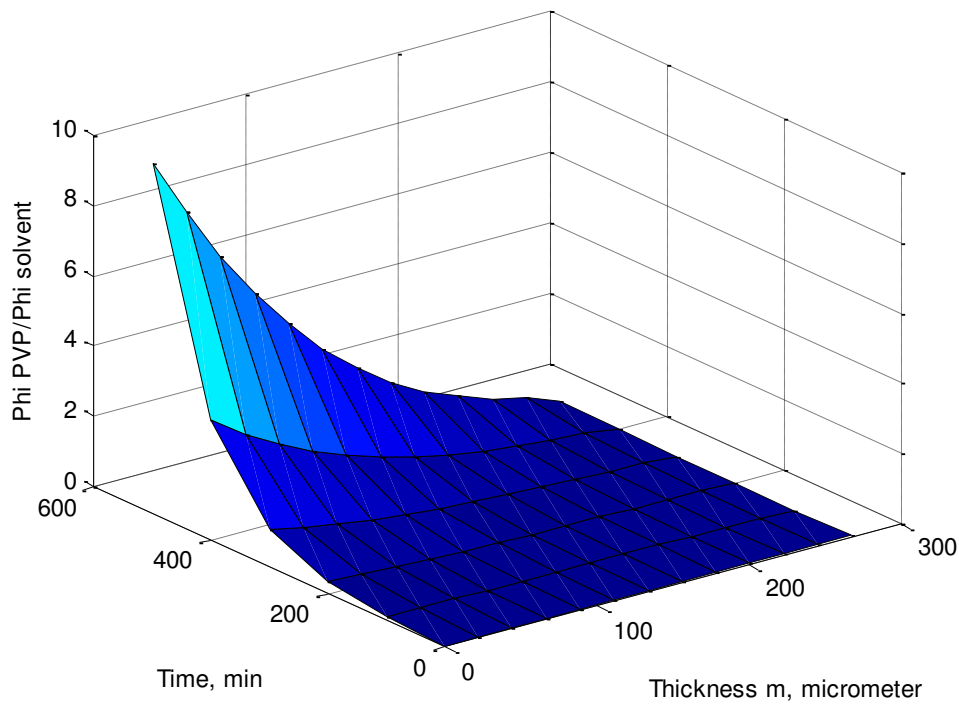


Figure-12. $\Phi_{PVP}/\Phi_{solvent}$ as a function of time and thickness of membrane at $T=298K$,
 Initially; $\Phi_{PVC}=0.14$, $\Phi_{PVP}=0.04$, $\Phi_{NMP}=0.15$, $\Phi_{THF}=0.67$

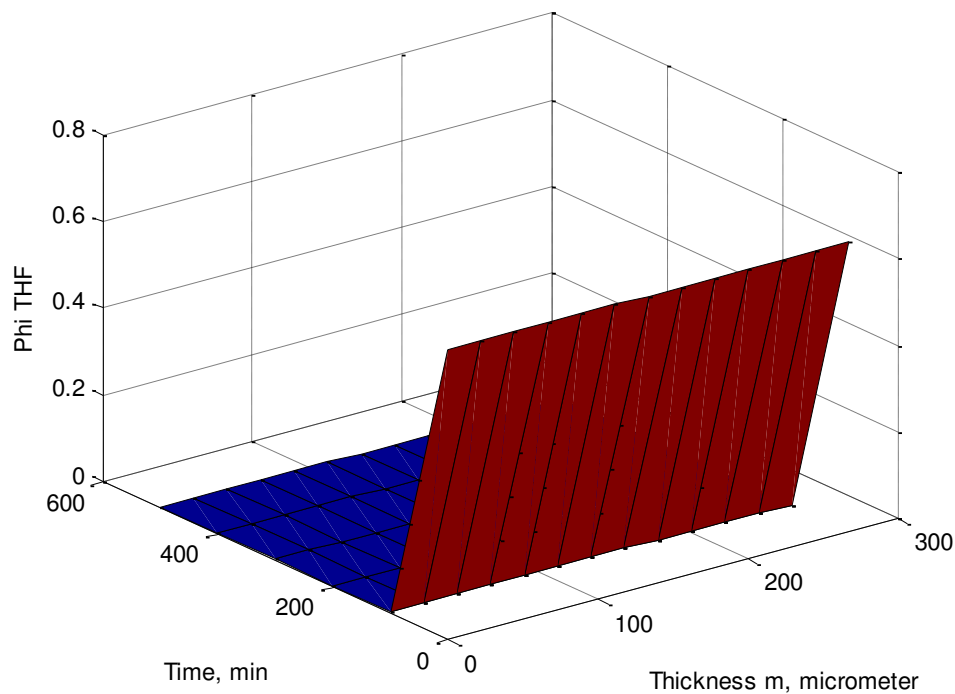


Figure-13. Φ_{THF} as a function of time and thickness of membrane at $T=298K$, Initially;
 $\Phi_{PVC}=0.14$, $\Phi_{PVP}=0.04$, $\Phi_{NMP}=0.15$, $\Phi_{THF}=0.67$

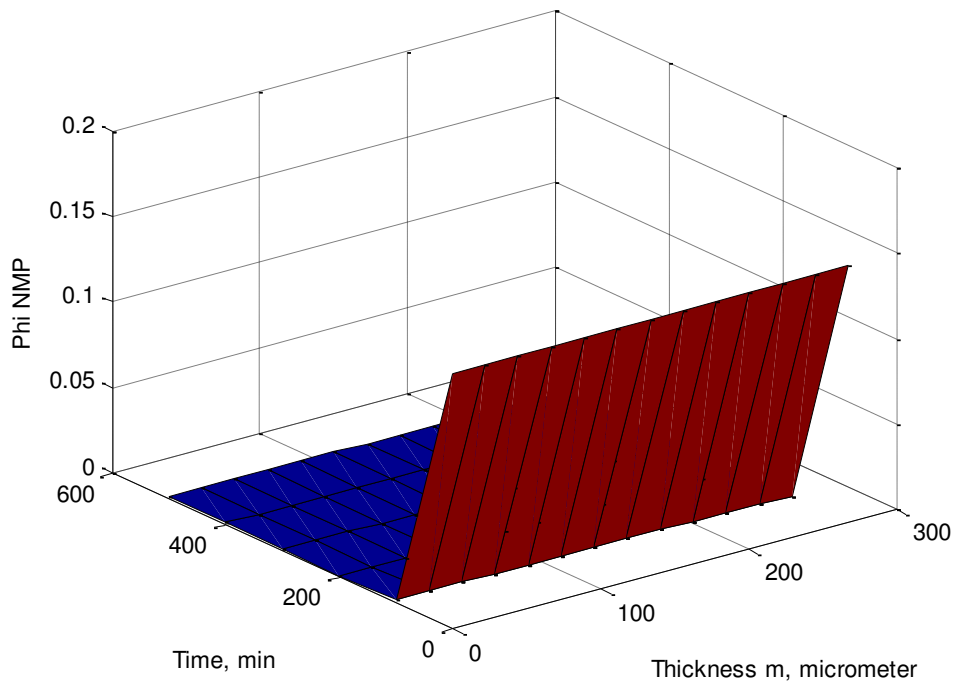


Figure-14. ϕ_{NMP} as a function of time and thickness of membrane at $T=298K$, Initially;
 $\phi_{PVC} = 0.14$, $\phi_{PVP} = 0.04$, $\phi_{NMP} = 0.15$, $\phi_{THF} = 0.67$

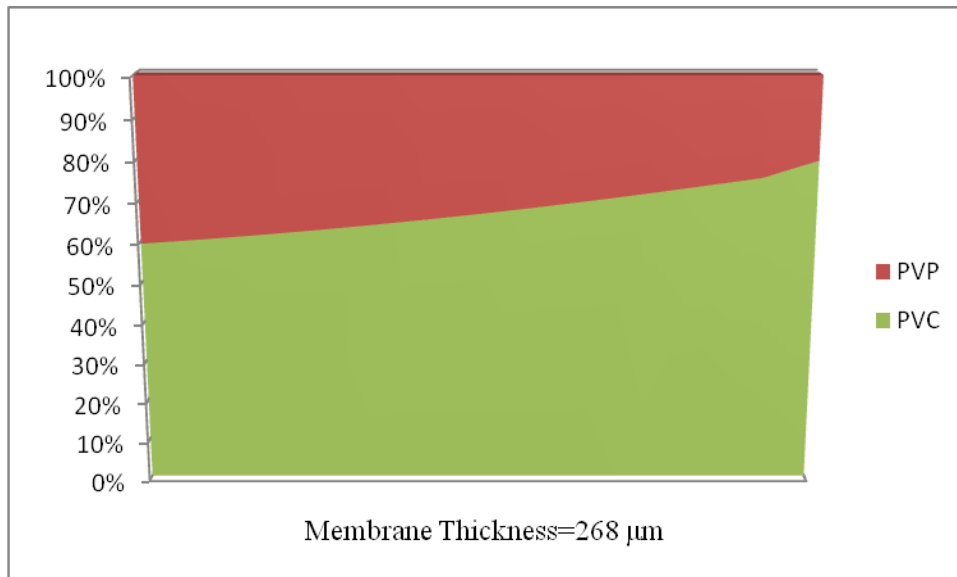


Figure-15. Representation of membrane constituents after 500 min of coagulation.

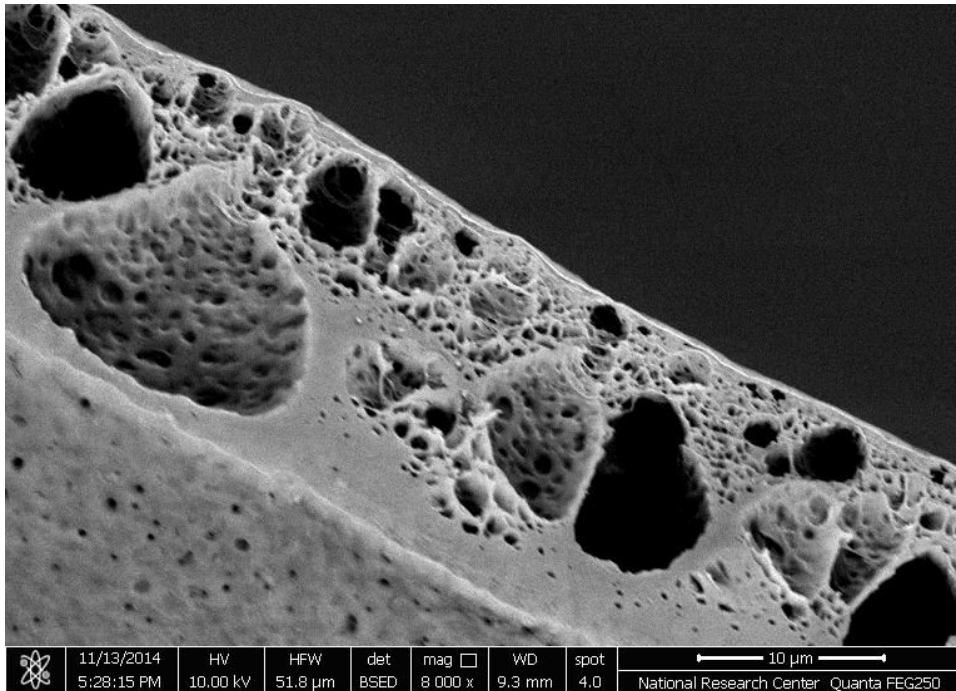


Figure-16. Electron scan of porous membrane PVC/PVP.

4. CONCLUSIONS

A mathematical model for investigating quaternary polymeric system was developed to study the coagulation process and thermodynamics of polymers mixing. Two cases studies of polymeric membrane preparation by phase inversion process were carried out, using both the model and experimental work. The mathematical model was validated using the experimental results. The following conclusions can be provided from the current study:

- The mixing of polymers and solvents was stable for all the polymers compositions at different solution temperatures in the two studied cases (PVC/CA blend and PVC/ PVPblend). This was indicated by a negative change of Gibbs free energy.
- According to the developed model, diffusion of the solvents from polymeric solution to the coagulation bath takes place during gelation time. During membrane formation the volume fraction of solvents in the bath increases and polymeric solution volume decreases for both studied cases.
- The results of the two case studies showed that the model can reproduce the shape and morphology of the experimental casted membrane.

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Nomenclature

D_{ij}	= Binary diffusion coefficient between i and j, m^2/s
ΔG	= Gibbs free energy of mixing, J/mol
J_k	= Flux of species k into the coagulation bath at the interface between polymer solution and coagulation bath at ($y=0$)
L	= Total film thickness, m
M_i	= Molecular weight of component i, $kg/kmol$
R	= Universal gas constant, $J/mol/K$
T	= Temperature, K
t	= Time, s
$\frac{t}{v_i}$	= Molar volume of component i, m^3/mol

Greek symbols

$\Delta\mu_i$	= Change in chemical potential of component I, J/mol
ϕ_i	= Volume fraction of component i
n_i	= Number of moles of component I, mole
δ_i	= Solubility parameter, $\frac{kJ^{\frac{1}{2}}}{m^{\frac{3}{2}}}$

Subscripts

PVC	= Polyvinyl chloride
CA	= Cellulose acetate
NMP	= <i>N</i> -methyl-2-pyrrolidone
THF	= Tetrahydrofuran



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