

Thermodynamic Screening of Solvents for Ternary Cellulose Acetate Blend Membranes Using Hansen Solubility Parameters

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Abstract

Solvent selection for phase inversion membranes still relies mostly on trial and error, even though the solvent governs how well a polymer blend forms into a stable, separation-capable structure. Few studies quantify that relationship before casting. This study calculates Hansen Solubility Parameters (HSP) for a ternary blend of Cellulose Acetate (CA), Polyethylene Glycol (PEG), and Polyvinyl Chloride (PVC) against six candidate organic solvents, with water as the nonsolvent, to test whether thermodynamic distance can predict membrane morphology ahead of fabrication. We calculated the interaction distances for all six solvents, then cast and visually examined membranes from three of them, dimethylacetamide (DMAc), dimethylformamide (DMF), and N-methyl-2-pyrrolidone (NMP), to check the calculations against real morphology. DMAc gave the smallest polymer-solvent distance ($\Delta p-s = 1.623$), ahead of DMF (2.394) and NMP (4.228), pointing to the strongest calculated affinity with the polymer blend among the six candidates. This ranking was consistent with the macroscopic appearance of the membranes: DMAc produced a smooth, glossy surface without visible defects, DMF a uniform matte surface without visible cracks, and NMP a wrinkled and deformed surface. Because morphology was assessed only by macroscopic photography, this agreement is qualitative and does not confirm skin-layer structure or selectivity. Nevertheless, the results suggest that HSP-based $\Delta p-s$ calculation has potential as a simple, non-empirical preliminary screening step for solvent selection ahead of experimental fabrication. Membranes prepared with low- $\Delta p-s$ solvents such as DMAc are hypothesized to show better separation performance, and salt-rejection testing and cross-sectional microscopy are proposed as future work.

Keywords Cellulose Acetate, Hansen Solubility Parameters, Phase Inversion, Predictive Solvent Selection

INTRODUCTION

Membranes made from blended polymers, such as Cellulose Acetate (CA), Polyethylene Glycol (PEG), and Polyvinyl Chloride (PVC), combine mechanical strength, thermal stability, and separation performance in ways that single-polymer membranes rarely achieve (Lam et al., 2018). Phase inversion, the most common method for fabricating these membranes, depends heavily on the thermodynamics and mass-transfer kinetics among the polymer, solvent, and nonsolvent (Lim et al., 2021). Once a multicomponent blend such as CA-PEG-PVC is paired with an organic solvent, for example dimethylacetamide (DMAc), dimethylformamide (DMF), or N-methyl-2-pyrrolidone (NMP), and a nonsolvent, the resulting thermodynamic interactions are difficult to anticipate from

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experience alone. Choosing a solvent by trial and error wastes material and time and explains little about why a given system worked or failed, or why it phase-separated as it did. A quantitative approach to evaluating component compatibility before casting would close that gap ([Ramadhani et al., 2021](#)).

HSP offers a way to quantify that compatibility mathematically, based on each component's solubility characteristics, before casting a single drop of dope solution. HSP alone cannot capture everything, since the final membrane structure depends on the phase inversion step itself and not only on the initial thermodynamic match between polymer and solvent, but it does give researchers a starting point for narrowing down candidate solvents on paper. Whether that starting point actually holds up against real membrane morphology, and for a ternary blend specifically, is a question the existing literature has not settled.

Predictive HSP screening for ternary polymer blends such as CA-PEG-PVC is still rare; most published work still selects solvents empirically ([Wang et al., 2026](#)), discovering a mismatch only after fabrication, once phase inversion has already fixed the membrane structure and the material is spent ([Cao et al., 2024](#)). This study addresses that gap by calculating the polymer-solvent ($\Delta p-s$), solvent-nonsolvent ($\Delta s-ns$), and polymer-nonsolvent ($\Delta p-ns$) interaction distances for the CA-PEG-PVC system across six candidate solvents, NMP, DMF, DMAc, DMSO, acetone, and THF, with water as the nonsolvent. Three of these solvents, DMAc, DMF, and NMP, were then used to fabricate membranes so the calculated distances could be checked against the morphology that actually formed. A full evaluation of separation performance through salt-rejection testing is left for a follow-up study built on the screening framework developed here.

LITERATURE REVIEW

Selecting an appropriate solvent is critical in fabricating phase inversion membranes because it determines polymer-solution homogeneity, the solvent-nonsolvent exchange rate during coagulation, and the resulting membrane morphology. A solvent system with high affinity for the polymer promotes the formation of a thermodynamically stable dope solution, leading to a more uniform membrane structure while minimizing premature phase separation prior to membrane casting ([Baker, 2012](#); [Reningtyas et al., 2025](#)). Therefore, evaluating compatibility among the polymer, solvent, and nonsolvent is essential before membrane synthesis.

One of the most widely adopted approaches for predicting such compatibility is the HSP. Unlike the Hildebrand solubility parameter, which considers only the total cohesive energy density, HSP divides the cohesive energy into three intermolecular interaction components: dispersion forces, polar forces, and hydrogen bonding. This approach provides a more accurate prediction of polymer dissolution behavior, particularly in multicomponent systems such as membrane-forming solutions ([Barton, 2017](#); [Hansen, 2007](#)).

In phase inversion membrane fabrication, HSP has been widely used as a preliminary tool to select solvents compatible with specific polymers ([Acarer, 2022](#); [Dehghan et al., 2024](#)). High compatibility between the polymer and solvent produces a more homogeneous dope solution, whereas the difference in solubility parameters between the solvent and nonsolvent influences the solvent-nonsolvent exchange during phase inversion. Consequently, these interactions can influence macrovoid formation, pore size, membrane porosity, and the transport properties of the resulting membrane ([Ruiz-García et al., 2023](#); [Wang et al., 2024](#)).

The kinetics of phase inversion, rather than HSP distance alone, mediate the link between thermodynamic compatibility and the resulting membrane structure. During immersion precipitation, the exchange rate of solvent and nonsolvent across the polymer-solvent-nonsolvent interface governs whether demixing proceeds instantaneously or is delayed ([Hui et al., 2022](#)). When the solvent-nonsolvent pair exhibits a large Hansen distance ($\Delta s-ns$), indicating strong

thermodynamic dissimilarity, nonsolvent influx into the dope solution is rapid, driving the system across the binodal boundary almost immediately after immersion. This instantaneous demixing typically produces an asymmetric structure with a thin, dense skin layer and finger-like macrovoids extending into the sublayer, reflecting the abrupt, localized precipitation front (Mulder, 1996). Conversely, a smaller Δs -ns slows the exchange rate, allowing the dope solution to remain in a metastable, homogeneous state for longer before crossing the binodal; this delayed demixing favors the formation of a denser, more sponge-like sublayer with fewer or no macrovoids, at the expense of a longer coagulation time (Huang et al., 2023; Xu et al., 2022).

The polymer-solvent interaction distance (Δp -s) governs this process earlier by setting the dope solution's initial thermodynamic quality. A small Δp -s corresponds to a well-solvated, thermodynamically stable polymer chain conformation and, typically, a higher dope viscosity; this greater resistance to solvent outflow further favors delayed demixing and additionally promotes the formation of a more uniform, defect-free skin layer, since polymer chain rearrangement at the precipitation front is less abrupt (Mousavi & Zadhoush, 2017). A poorly compatible solvent (large Δp -s), by contrast, yields a less viscous, less thermodynamically stable dope, which can lead to faster solvent outflow and less-controlled chain packing, resulting in surface irregularities and structural defects at the membrane surface.

These morphological features, in turn, directly determine separation performance. A thin, dense, defect-free skin layer acts as the primary selective barrier, favoring solute rejection at the cost of permeate flux, whereas a porous or macrovoid-laden structure raises flux but sacrifices selectivity and mechanical integrity (Korriem et al., 2023). HSP interaction distances therefore do not predict performance directly; they predict the thermodynamic driving forces governing demixing kinetics, which shape the morphology that controls performance. This causal chain, from Δp -s and Δs -ns through demixing kinetics and morphology to separation behavior, underpins the present screening approach.

Thermodynamically, the Flory-Huggins parameter χ , which scales with the square of the Hansen distance, governs the free energy of mixing and hence the binodal and spinodal positions in the ternary phase diagram (Hansen, 2007). A larger distance (higher χ) shifts the binodal toward the polymer-rich corner, narrowing the metastable region and shortening the time for controlled demixing, favoring instantaneous over delayed demixing.

In this study, HSP analysis was applied to the CA-PEG-PVC polymer blend against the same six solvents introduced earlier, NMP, DMF, DMAc, DMSO, acetone, and THF, with water as the nonsolvent. This analysis provides a theoretical basis for selecting a solvent system with high affinity for the CA-PEG-PVC polymer blend, promoting a stable membrane-forming solution before phase inversion.

The phase inversion process directly influences the final membrane surface and sublayer morphology (Nurkhamidah et al., 2019). A suitable combination of polymer-solvent affinity and solvent-nonsolvent interaction can promote the formation of a continuous, structurally stable membrane. Conversely, an unsuitable thermodynamic combination may contribute to structural irregularities that reduce separation performance. Therefore, evaluating HSP interactions provides a theoretical baseline for interpreting membrane morphology and predicting membrane separation performance (Hui et al., 2022).

According to Hansen (2007), the total solubility parameter is the sum of the contributions from three intermolecular interaction components, namely the dispersion force (δ_d), the polar force (δ_p), and the hydrogen-bonding force (δ_h), and is expressed as follows:

$$\delta_t^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \quad (1)$$

Table 1 presents the HSP of the components used in this study.

Table 1. Hansen solubility parameter values of the polymers, solvents, and nonsolvent

Polymer/Solvent/Nonsolvent	δ_d	δ_p	δ_h	δ_t
Cellulose Acetate (CA – Cellidora A)	18.2	12.4	10.8	24.4
PVC (Polyvinyl Chloride)	18.7	9.7	7.7	22.1
NMP (N-Methyl-2-Pyrrolidone)	18	12.3	7.2	23.3
DMF (Dimethylformamide)	17.4	13.7	11.3	24.8
DMAc (Dimethylacetamide)	16.8	11.5	10.2	23.1
DMSO (Dimethyl sulfoxide)	18.4	16.4	10.2	29.5
Acetone	15.5	10.4	7	19.7
THF (Tetrahydrofuran)	16.8	5.7	8	19.5
Water (H ₂ O)	15.5	16	42.3	46
PEG (Polyethylene Glycol)	17	7.3	13.5	22.8

For a system consisting of a multicomponent polymer blend, the effective Hansen solubility parameter components ($\delta_d, \delta_p, \delta_h$) are calculated using a mass-fraction-weighted average of the individual polymer components, as expressed by:

$$\delta_{(x,mix)} = \sum_i F_i \cdot \delta_{(x,i)} \quad (x = d, p, h) \quad (2)$$

where F_i is the mass fraction of polymer component i relative to the total polymer mass, and $\delta_{(x,i)}$ represents the corresponding individual Hansen solubility parameter component ($\delta_d, \delta_p, \delta_h$). This empirical linear mixing method provides a straightforward baseline to estimate the effective HSP values of polymer blends prior to evaluating their compatibility with candidate solvents (Hansen, 2007)

The compatibility between two materials is subsequently evaluated using the Hansen distance (R_a), which is calculated according to the following equation:

$$R_a = \sqrt{(\delta_{d1} - \delta_{d2})^2 + (\delta_{p1} - \delta_{p2})^2 + (\delta_{h1} - \delta_{h2})^2} \quad (3)$$

A smaller R_a value indicates a greater similarity in the intermolecular interaction characteristics of the two materials, resulting in better thermodynamic compatibility. Conversely, a larger R_a value indicates lower affinity between the materials and a greater tendency for phase separation to occur (Hansen, 2007; Barton, 2017). Based on Equations (2) and (3), the Hansen solubility parameter of the CA-PEG-PVC polymer blend and the Hansen distances for the polymer-solvent, solvent-nonsolvent, and polymer-nonsolvent pairs were calculated.

RESEARCH METHOD

Determination of Hansen Solubility Parameters

The calculation begins by determining the mass fraction (F_i) of each component in the CA-PEG-PVC polymer blend based on the mass of each component relative to the total mass of the blend. Subsequently, the HSP of the blend is calculated using the weighted average method based

on the mass fraction of each component, resulting in the effective dispersion (δ_d), polar (δ_p), and hydrogen bonding (δ_h) parameters of the CA-PEG-PVC blend. After obtaining the HSP values of the blend, the next step is to calculate the Hansen solubility distance (R_a) between the polymer blend and the solvent using the HSP equation to evaluate the degree of affinity and compatibility between the polymer and solvent components.

Membrane Fabrication

Figure 1 schematically illustrates the complete membrane fabrication procedure, including polymer dissolution, casting, and phase inversion.

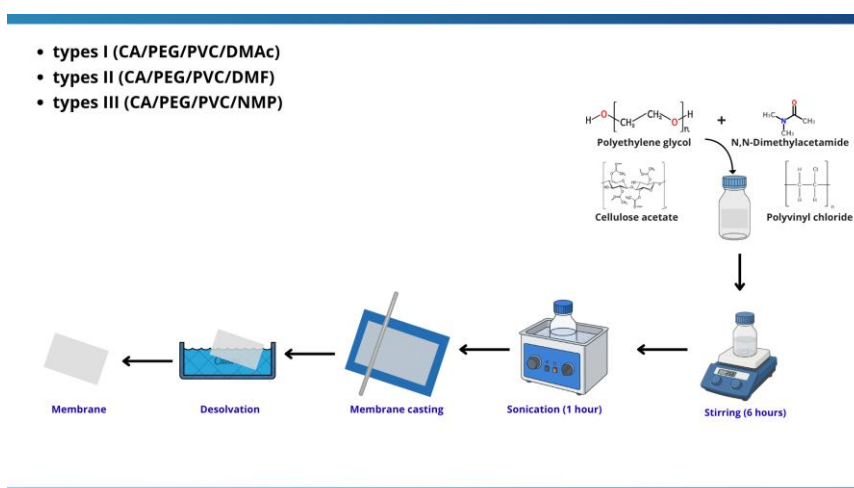


Figure 1. Schematic diagram of the membrane fabrication process using different solvents via the phase inversion method

The main materials evaluated in this study were cellulose acetate (CA, 2 g), polyethylene glycol (PEG, 0.5 g) as a pore-forming agent, and polyvinyl chloride (PVC, 0.01 g) as a secondary polymer additive. Various organic solvents, including dimethylacetamide (DMAc, 17 mL), N-methyl-2-pyrrolidone (NMP), dimethylformamide (DMF), and other prospective organic solvents, were systematically evaluated. Distilled water (H₂O) served as the nonsolvent in the coagulation bath. The main equipment utilized in the simulated and experimental process included an ultrasonic sonicator, magnetic stirrer, glass plate, and coagulation tank.

To investigate the effect of different solvent systems on the thermodynamic stability and phase separation kinetics of the CA-PEG-PVC blend, the procedure was formulated as follows:

1. **Solvent and Pore-Former Mixing:** A designated volume (17 mL) of the target solvent (e.g., DMAc, DMF, or NMP) and PEG (0.5 g) were mixed using a magnetic stirrer for 30 minutes, followed by ultrasonication for 1 hour to achieve initial uniform dispersion.
2. **Polymer Blend Dissolution:** Cellulose acetate (CA, 2 g) and polyvinyl chloride (PVC, 0.01 g) were added to the solvent-PEG mixture. The solution was stirred continuously for 6 hours until the polymer fully dissolved, then ultrasonicated for 2 hours to eliminate microbubbles and ensure dope homogeneity.

The homogeneous dope solution was cast onto a flat glass plate using a doctor blade set to a fixed thickness of 200 μm , then immediately immersed in a coagulation bath of distilled water at room temperature (28 $^{\circ}\text{C}$) to induce non-solvent-induced phase separation. Each membrane composition was fabricated in triplicate ($n = 3$) to account for run-to-run variability in the casting

and phase-inversion process. Membrane morphology was assessed qualitatively by digital photography after coagulation and drying [under consistent lighting, distance, and background]. Each membrane was evaluated based on four visual criteria: (i) surface texture (smooth or wrinkled), (ii) surface appearance (glossy or matte), (iii) presence of visible defects such as cracks, pinholes, or bubbles, and (iv) shape stability (flat or deformed). This assessment serves only as a preliminary qualitative comparison with the HSP predictions.

FINDINGS AND DISCUSSION

Results

The thermodynamic compatibility and solubility behavior of the polymer blend system were evaluated using the Hansen Solubility Parameter (HSP) approach. The system consisted of a ternary polymer blend of Cellulose Acetate (CA, 2 g), Polyethylene Glycol (PEG, 0.5 g), and Polyvinyl Chloride (PVC, 0.01 g), six candidate solvents (NMP, DMF, DMAc, DMSO, acetone, and THF), and water (H₂O) as the nonsolvent.

The mass fraction of each polymer component was first calculated relative to the total polymer mass ($\sum m = 2.51$ g), using the following equation:

$$F_i = \frac{m_i}{\sum m} \quad (4)$$

where F_i is the mass fraction of component i , m_i is the mass of component i , and $\sum m$ is the total mass of all polymer components. Applying this equation to each component yields:

$$F_{CA} = \frac{2}{2.51} = 0.796813$$

$$F_{PEG} = \frac{0.5}{2.51} = 0.199203$$

$$F_{PVC} = \frac{0.01}{2.51} = 0.003984$$

The individual HSP of the blend dispersion ($\delta_{d,mix}$), polar ($\delta_{p,mix}$), and hydrogen-bonding ($\delta_{h,mix}$) components were then determined using the mass-fraction-weighted average method:

$$\delta_{x,mix} = \sum F_i \cdot \delta_{x,i} \quad (5)$$

Substituting the mass fractions and the individual HSP values of CA, PEG, and PVC gives:

$$\delta_{d,mix} = (0.796813 \times 18.2) + (0.199203 \times 17) + (0.003984 \times 18.7) = 17.962948 \text{ MPa}^{1/2}$$

$$\delta_{p,mix} = (0.796813 \times 12.4) + (0.199203 \times 7.3) + (0.003984 \times 9.7) = 11.373307 \text{ MPa}^{1/2}$$

$$\delta_{h,mix} = (0.796813 \times 10.8) + (0.199203 \times 13.5) + (0.003984 \times 7.7) = 11.325498 \text{ MPa}^{1/2}$$

These three values define the effective Hansen solubility parameter of the CA-PEG-PVC blend, which serves as the reference point for evaluating its interaction with each candidate solvent and with the nonsolvent (water).

To evaluate polymer dissolution behavior and phase-separation dynamics, the interaction

distance (Δ or R_a) between two HSP points was calculated using the three-dimensional Hansen distance formula:

$$\Delta = \sqrt{(\delta_{d1} - \delta_{d2})^2 + (\delta_{p1} - \delta_{p2})^2 + (\delta_{h1} - \delta_{h2})^2} \quad (6)$$

A smaller value of R_a (or Δ) indicates better thermodynamic compatibility between the two components, while a larger value indicates weaker interaction or poorer solubility. This relationship assesses three interactions relevant to the membrane-formation system: polymer-solvent, solvent-nonsolvent, and polymer-nonsolvent.

As an example, the interaction distance between the polymer blend and DMAc ($\delta_d = 16.8$, $\delta_p = 11.5$, $\delta_h = 10.2$) was calculated as follows:

$$\Delta_{p-s} = \sqrt{(17.962948 - 16.8)^2 + (11.373307 - 11.5)^2 + (11.325498 - 10.2)^2}$$

$$\Delta_{p-s} = \sqrt{(1.162948)^2 + (-0.126693)^2 + (1.125498)^2}$$

$$\Delta_{p-s} = \sqrt{1.352449 + 0.016055 + 1.266749}$$

$$\Delta_{p-s} = \sqrt{2.635253} = 1.623 \text{ MPa}^{1/2}$$

The relatively small Δ_{p-s} value indicates good thermodynamic compatibility between the polymer blend and DMAc, suggesting that DMAc effectively dissolves the CA-PEG-PVC blend.

The interaction distance between DMAc and water ($\delta_d = 15.5$, $\delta_p = 16$, $\delta_h = 42.3$) was then calculated:

$$\Delta_{s-ns} = \sqrt{(16.8 - 15.5)^2 + (11.5 - 16)^2 + (10.2 - 42.3)^2}$$

$$\Delta_{s-ns} = \sqrt{(1.3)^2 + (-4.5)^2 + (-32.1)^2}$$

$$\Delta_{s-ns} = \sqrt{1.69 + 20.25 + 1030.41}$$

$$\Delta_{s-ns} = \sqrt{1052.35} = 32.440 \text{ MPa}^{1/2}$$

The large Δ_{s-ns} value reflects the strong dissimilarity between DMAc and water, particularly in the hydrogen-bonding component, which is consistent with DMAc's role as a solvent and water's role as a nonsolvent during phase inversion.

Finally, the interaction distance between the polymer blend and water was calculated:

$$\Delta_{p-ns} = \sqrt{(\delta_{d,mix} - \delta_{d,ns})^2 + (\delta_{p,mix} - \delta_{p,ns})^2 + (\delta_{h,mix} - \delta_{h,ns})^2} \quad (7)$$

$$\Delta_{p-ns} = \sqrt{(17.962948 - 15.5)^2 + (11.373307 - 16)^2 + (11.325498 - 42.3)^2}$$

$$\Delta_{p-ns} = \sqrt{(2.462948)^2 + (-4.626693)^2 + (-30.974502)^2}$$

$$\Delta_{p-ns} = \sqrt{6.066110 + 21.406290 + 959.419773}$$

$$\Delta_{p-ns} = \sqrt{986.892173} = 31.415 \text{ MPa}^{1/2}$$

The large Δ_{p-ns} value confirms that the polymer blend is poorly soluble in water, as expected and desired for a nonsolvent in the phase-inversion process: it allows the polymer to precipitate and form a solid membrane structure once water displaces the solvent. Table 2 presents the complete set of calculated interaction distances for all six solvents.

Table 2. Calculated Hansen interaction distances (Δ) for the CA-PEG-PVC membrane system

Polymer Blend	Solvent	Nonsolvent	Δ_{p-s} (MPa ^{1/2})	Δ_{s-ns} (MPa ^{1/2})	Δ_{p-ns} (MPa ^{1/2})
CA-PEG-PVC	NMP	Water	4.228	35.383	31.415
CA-PEG-PVC	DMF	Water	2.394	31.143	31.415
CA-PEG-PVC	DMAc	Water	1.623	32.440	31.415
CA-PEG-PVC	DMSO	Water	5.170	32.233	31.415
CA-PEG-PVC	Acetone	Water	5.072	35.741	31.415
CA-PEG-PVC	THF	Water	6.678	35.837	31.415

We applied the same calculation procedure to the remaining candidate solvents (NMP, DMF, DMSO, acetone, and THF) and their interactions with water. In each case, the resulting R_a (or Δ) values were compared: the smaller the value, the better the compatibility between the polymer blend and the solvent, while a larger value between the solvent and the nonsolvent indicates a more favorable driving force for phase separation during membrane formation.

Discussion

Polymer-Solvent Thermodynamic Affinity (Δ_{p-s})

The polymer-solvent interaction distance (Δ_{p-s}) is used as a predictive indicator of thermodynamic affinity. A smaller Δ_{p-s} means the HSP of the solvent is closer to that of the polymer blend, so the solvent is predicted to interact more favorably with it. As shown in Table 2, DMAc has the smallest Δ_{p-s} (1.623), followed by DMF (2.394) and NMP (4.228). Acetone (5.072), DMSO (5.170), and THF (6.678) have larger values and are therefore predicted to have lower affinity toward the CA-PEG-PVC blend.

Based on this HSP prediction, DMAc is the most compatible solvent for the CA-PEG-PVC blend, with DMF and NMP also showing relatively good compatibility. In contrast, THF, DMSO, and Acetone are predicted to be less favorable, with THF being the least compatible. These results are theoretical estimates derived from HSP calculations and do not directly represent actual dissolution or membrane performance. In addition, membrane formation during phase inversion also depends on the solvent-nonsolvent interaction.

Visual Correspondence with HSP Predictions

The physical macro-morphology of the fabricated CA-PEG-PVC flat-sheet membranes provides empirical information that can be compared with the calculated HSP interaction distances. The comparison focuses on the experimentally fabricated membranes cast from DMAc, DMF, and NMP, as shown in Figure 2.

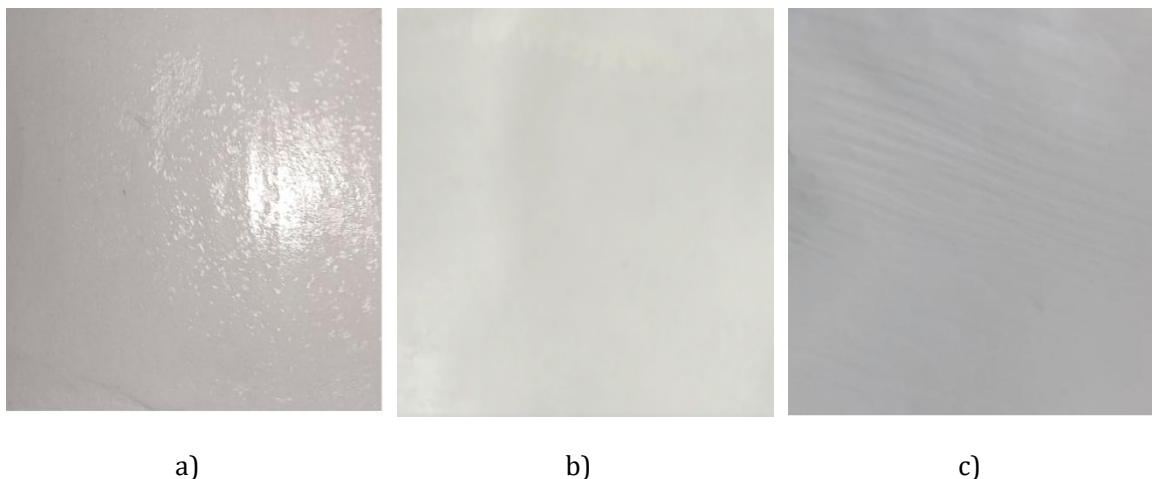


Figure 2. Displays the physical appearance of the synthesized membranes cast using a) DMAc; b) DMF; and c) NMP

As presented in Figure 2, the three fabricated membranes exhibit surface characteristics that vary systematically with their calculated polymer-solvent interaction distance. The DMAc-cast membrane ($\Delta p-s = 1.623$) displays a smooth, glossy surface; the DMF-cast membrane ($\Delta p-s = 2.394$) exhibits a uniform, matte finish; and the NMP-cast membrane ($\Delta p-s = 4.228$) shows visible wrinkling and surface deformation. This progression aligns with the HSP-based prediction that a lower $\Delta p-s$ indicates greater thermodynamic compatibility between the polymer blend and the casting solvent, and thus a more homogeneous membrane surface. Nevertheless, as these observations are derived solely from macroscopic photography, they should be interpreted as a preliminary, qualitative correspondence rather than definitive evidence of skin-layer integrity, pore architecture, or membrane selectivity; verification of these properties requires cross-sectional microstructural characterization.

HSP-Derived $\Delta p-s$ as a Predictive Indicator for Membrane Separation Performance

The $\Delta p-s$ values may also give an early indication of membrane separation performance. In phase inversion membranes, a uniform, regular surface generally indicates better selectivity, while wrinkling and structural irregularities tend to reduce separation efficiency (Koriam et al., 2023; Mousavi & Zadhoush, 2017). On this basis, the DMAc-based membrane, which showed the smallest $\Delta p-s$ and a smooth, glossy surface, may perform better than the NMP-based membrane, which showed visible wrinkling. However, this is only a qualitative expectation based on HSP calculations and visual observation, not a measured result. Separation performance testing and microstructural characterization (e.g., SEM) are needed in future work to confirm it. Within its current scope, this study demonstrates that HSP-based $\Delta p-s$ calculation can serve as a simple, non-empirical first-stage tool for screening solvents before experimental testing.

CONCLUSIONS

This study evaluated the thermodynamic interactions in the CA-PEG-PVC membrane

system using HSP by calculating interaction distances between the polymer blend, candidate solvents, and water. Among the six candidates, DMAc showed the highest predicted polymer solvent affinity, followed by DMF and NMP, with Δp -s values of 1.623, 2.394, and 4.228, respectively. This ranking was consistent with the macroscopic appearance of the fabricated membranes: the DMAc membrane had a smooth, glossy surface, the DMF membrane a uniform, crack-free matte surface, and the NMP membrane visible wrinkling and deformation. These results suggest that Δp -s could serve as a simple preliminary screening tool for solvent selection in multicomponent membrane systems. Whether a lower Δp -s leads to better separation performance remains a hypothesis to be tested.

These correlations, while consistent, are drawn from only three fabricated solvent systems and rely on literature-tabulated HSP values combined through a linear mass-fraction mixing rule rather than values measured directly for this specific blend. Establishing the generality of this predictive framework will require validation across a broader range of solvents, replicate fabrication runs, and, ideally, experimentally determined HSP values for the polymer blend itself.

LIMITATIONS & FURTHER RESEARCH

This study is not intended as a complete evaluation of membrane performance, but as the foundation for a predictive, HSP-based framework for solvent selection, validated at this stage through calculated interaction distances and qualitative membrane morphology. Building on this foundation, a follow-up study will focus specifically on quantitative performance testing, including salt-rejection measurements across all six evaluated solvent systems, particularly DMF, to confirm the predictions established here. This subsequent stage will also incorporate cross-sectional characterization using SEM or AFM to directly examine selective-layer thickness, pore structure, and sublayer macrovoid evolution, alongside systematic variation of the PEG and PVC contents to determine how composition affects the calculated HSP interactions, dope properties, membrane morphology, and filtration performance. Experimental measurements of solvent-nonsolvent exchange and phase-inversion behavior may also be conducted in future work to establish the quantitative relationship between HSP interaction distances and membrane performance.

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