

Ionic Liquids for High-Temperature Separation of Methanol and Water

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The conversion of CO₂ into methanol is a crucial step in developing sustainable, decentralized energy storage systems. However, conventional methanol synthesis is limited by thermodynamic equilibrium, requiring high pressures and energy-intensive condensation steps for product separation. This study proposes a breakthrough approach by employing ionic liquid (IL)-based in situ sorption to selectively remove methanol and water from the reaction environment, thereby shifting equilibrium and enhancing conversion efficiency. In this study, we identify and validate ILs capable of operating in a trickle-bed reactor at 483–513 K, offering a robust and energy-efficient alternative to conventional separation methods¹. Through COSMO-RS modeling, a comprehensive screening of over 15,000 ILs was performed to evaluate their affinity for methanol and water at the reactor's operational temperature (Figure 1). Infinite dilution activity coefficients were used to assess ILs interaction with solutes. Similar trends were found at 298K and 513K, and strong dependency was found for ILs' anions with high punctual charged sites. The thermal stability of the best candidates was evaluated by *ai4solvents* software² to assure these ILs could operate at the reacting temperature. The best ion candidates were chloride, and phosphinated anions, and piperidinium and Lithium cations. The proposed IL-based separation process could enable methanol production at a higher yield by shifting chemical equilibrium within the trickle bed reactor.

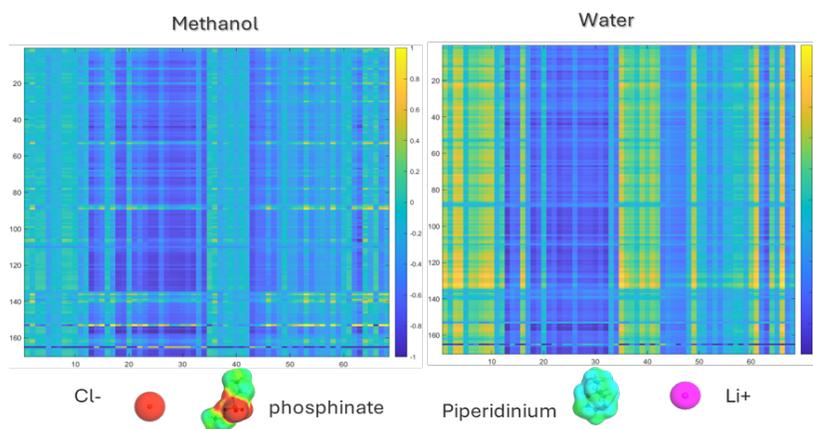


Figure 1: COSMO-RS screening for methanol and water solubility at 513 K, and best ion candidates

References

1. Reichert, J. et al. *Sustain Energy Fuels* **2019**, 3, 3399–3405.
2. Song, Z., Chen, J., Cheng, J., Chen, G. & Qi, Z. *Chem Rev* **2024**, 124, 248–317.



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