

**Methanol-Toluene mixtures confined in a Polymer of Intrinsic Microporosity (PIM-1): Molecular simulation study**

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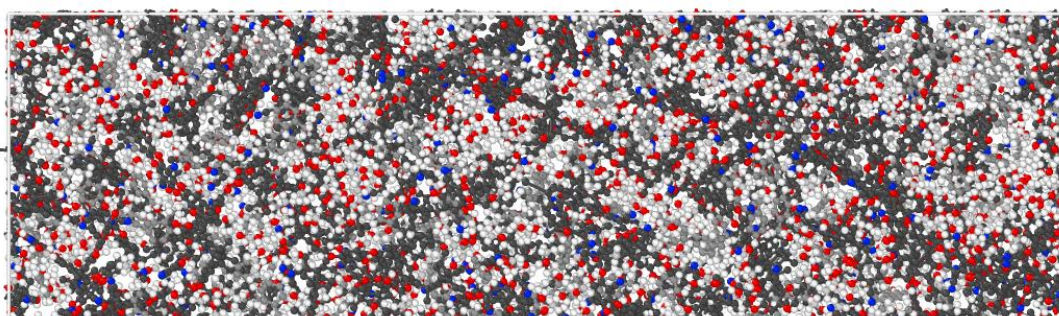
Separation is among the most energy-intensive processes in the chemical and pharmaceutical industry. It costs between 40 and 70% of energy consumption [1]. Membrane separation seems to be among the most promising solutions to reduce this energy cost. However, their use for organic fluids is relatively little studied compared to the purification of water and gas separation because of the difficulty of developing membrane materials that are both stable and scalable in organic media [2]. Organic Solvent Nanofiltration (OSN) is a separation process that started in the 2000s with the development of polymer membranes that had improved resistance to organic solvents. This technique has recently shown great potential, particularly in the petrochemical [3] and pharmaceutical industries [4]. Molecular simulations seem particularly well suited to investigate solvent-membrane interactions at the nanoscale and thus to elucidate the separation mechanisms involved in OSN. In this work, molecular dynamics simulations have been carried out to investigate methanol-toluene mixtures confined in a Polymer of Intrinsic Microporosity (PIM-1), paying special attention structural and dynamic properties of the confined fluids.

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[3] R.M. Gould, L.S. White, C.R. Wildemuth, *Environ. Prog.* 20 (2001) 12.

[4] S. Darvishmanesh, L. Firoozpour, J. Vanneste, P. Luis, J. Degève, B. van der Bruggen, *Green Chem.* 13 (2011) 3476.



**Figure 1** : .Methanol-Toluene mixture confined in a Polymer of Intrinsic Microporosity (PIM-1)