Multiscale computational modeling of organic compounds separation using microporous membranes

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Abstract

Computational modeling and numerical simulation of separation processes have been carried out in this work. A computational model is developed and numerically solved to calculate and obtain the concentration of a liquid solution in a pervaporation membrane process. The model considers basic conservation equations for the solution of water/alcohol in a membrane separation process. The governing equations are then solved and interpreted using computational fluid dynamics approach in order to optimize and design the process of interest. The results of computational simulations indicate that the model is well developed and can predict the performance of separation process with high accuracy.

Keywords: Computational modeling; Numerical simulation; Purification; Alcohol; Water