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Multiscale Modeling of Direct Contact Membrane Distillation: Macroscopic Modeling and Pore Scale Modeling

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Membrane distillation (MD) using porous hydrophobic membranes finds applications in various areas such as desalination of seawater, industrial wastewater treatment, and pharmaceutical separation of mixtures. In this study, a direct contact membrane distillation (DCMD) module with commercially available polytetrafluoroethylene (PTFE) membranes (GE-Osmonics/0.22 μ m and MS-3010/0.45 μ m) is investigated with a multiscale approach. A 2D macroscopic, multiphysics model considering the conservation of species, momentum, and energy has been developed in the present study to gain an understanding of the processes in such a DCMD system. Instead of empirical correlations, this study uses a microscopic model to determine the effective transport properties, including effective mass diffusivity and thermal conductivity. The flowchart of workflow, the graphical representation of the multiscale approach used in the present study, is shown in Fig. 1. As illustrated in Fig. 1, a stochastic numerical reconstruction method is first developed to generate virtual membranes based on the membrane's pore size, fiber orientation distributions and the structure data of membranes presented by the manufacturers. To compute the transport properties subsequently needed in the macroscopic model, a finite volume operator in AVIZO and a finite volume solver in OpenFOAM, are employed to perform pore-scale simulations on the reconstructed geometries.

For virtual reconstructed GE-Osmonics/0.22 μ m PTFE membrane, the effective thermal conductivity and the effective mass diffusivity in through-plane direction are determined 0.0582W/mK and 1.07e-5 m²/s, respectively, while these transport properties are calculated 0.0571W/mK and 1.13e-5 m²/s for virtual reconstructed MS-3010/0.45 μ m PTFE membrane. It shows a good agreement between the simulation results and published data as well as empirical relations.

Fig. 1. Workflow flowchart of the multiscale approach.

With the objective to understand the effect of transport properties computed by microscopic methods in macroscopic modeling, simulation results of the present study in relation to the experimental data with previous studies are compared and realized that the average error of flux of distillate water is reduced from 10.5% and 6% found in previous studies to 7.9% and 5.3% calculated in the present study for feed inlet temperatures of 333.15 and 313.15, respectively.

Fig. 2. Comparison of flux of distillate water for experimental and predicted responses by Hwang et al. and present model for different feed inlet temperatures and inlet velocities (permeate inlet temperature of 293 K, NaCl mass fraction of 1%, GE-Osmonics/0.22 μ m).

Furthermore, comparing two stochastically reconstructed membranes, GE-Osmonics/0.22 μ m and MS-3010/0.45 μ m, show that the average amount of produced freshwater in the DCMD module with MS-3010/0.45 μ m is 24% more than produced freshwater in the DCMD module with GE-Osmonics/0.22 μ m.

Fig. 3. Comparison of flux of distillate water for two stochastically reconstructed membranes, GE-Osmonics/0.22 μ m and MS-3010/0.45 μ m, for different inlet velocities (Feed inlet temperature of 333.15K permeate inlet temperature of 293K, NaCl mass fraction of 1%, Countercurrent flat sheet).

Time Block Preference

Time Block A (09:00-12:00 CET)

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