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Segmentation and Flow Characterization of Block Copolymer Ultrafiltration Membranes

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Ultrafiltration membranes have a wide range of applications from drug delivery to water purification and virus filtration (Dorin et al. 2014; Li et al. 2017). A class of ultrafiltration membranes that has received much attention is the past decade is block copolymer membranes synthesized by self-assembly and non-solvent induced phase separation (SNIPS). These polymer membranes often exhibit an asymmetric, hierarchical structure comprising a thin (50-150 nm) separation layer with ordered nano-scale pores, and a support layer with a nanoporous solid matrix and disordered micro-scale pores.

Although optimizing flow is critical to the performance of such ultrafiltration membranes, not much success has been reported on their numerical flow characterization. The main challenges have been reported as i) hierarchical pore structure delineation (Sundaramoorthi et al. 2016) and ii) lack of an image-based micro-scale modeling approach that is computationally efficient and that can capture such wide pore size distribution (Shi et al. 2015).

In this study, we address the challenge of hierarchical pore structure delineation of an ISV triblock terpolymer membrane by combining a ~100 nm resolution 3D image of the membrane with high-resolution (2-4 nm) 2D SEM images. The 3D image is segmented using an automatic segmentation method (continuous max-flow algorithm) to delineate the micro-scale pores of the support layer. To capture the sub-resolution nanopores in the separation layer and in the solid matrix of the support layer, equivalent stochastic pore network models (PNM) of nanoporous structures are extracted from the high-resolution 2D SEM images.

To simulate single-phase flow, the pore topology method (PTM) is used. PTM is a fast micro-scale modeling approach that uses the medial surface of the 3D void space as the solution domain for flow simulation [Riasi et al. 2016]. After extracting the medial surface of the micropores, a local hydraulic conductivity and a solid matrix wall permeability coefficient is assigned to each voxel on the medial surface. The separation layer is then represented as a voxelized lattice structure assembled on top of the medial surface. The hydraulic conductivity of separation layer voxels and the wall permeability of solid matrix of support layer is acquired from the PNM analysis. Collectively, this provides the solution domain, which is then used for single-phase flow simulation. Absolute permeability of the membrane is computed and compared with the experimental measurements.

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