Modeling, visualization and membrane development

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The advance of polymer synthesis, self-assembly, solution thermodynamics and characterization methods have been allowing an excellent control of membrane morphology[1] and adequate functionalization for applications, such as nano- and ultrafiltration in aqueous and organic medium. In collaboration with different groups we have been also taking advantage of theoretical tools of modeling and visualization to accelerate the path of developments in the field. The following examples have been explored. Membrane morphology can now be tailored with narrow pore size distribution by using block copolymers in selected solvent systems. Pore size could be varied from ultra- to nanofiltration range by simply blending with other copolymers. Dissipative particle dynamics (DPD)[2,3] proved to be an excellent tool to better understand and guide the self-assembly in solution, which is an essential step in the pore formation. DPD has been used in combination with electron microscopy and time-resolved small angle X-ray scattering for morphological characterization. Most membranes have an asymmetric, rather complex, morphology. Complete quantification of porosity and liquid flow speed in different layers is challenging. By combining electron microscopy and digital methods of visualization[4] we demonstrated how full porosity characterization can be done and performance can be predict[5].

References

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