

Model Based Design of Structured Polymers Using the Reverse Design Approach

V. Soni,^S J. Abildskov^C G.E. Jonsson, and R. Gani

*CAPEC, Department of Chemical Engineering, Technical University of Denmark, Lyngby, Denmark
ja@kt.dtu.dk*

Karayiannis

Department of Chemical Engineering, University of Patras, Patras, Greece

Mavrantzas

Institute of Chemical Engineering and High Temperature Chemical Processes, ICE/HT-Forth, Patras, Greece

In polymer membrane separations, the design of structured polymers yielding desired separations is of interest. Two methods are common: either a trial-and-error procedure is followed, where different polymers are tested, and the design variables, which depend upon temperature, pressure, and composition, are the membrane permeability and mass flux; or a reverse approach is followed, where one designs a polymer with a microscopic structure optimally matching the specified permeability.

We assume that the permeability properties of a polymer system are intimately related to its microscopic structure (monomer composition) and/or polymer architecture. Thus, the design procedure involves fixing the degree of separation for the mixture, and selecting the optimal polymer based on a property model. Such models require property information (density, diffusivity, solubility, etc.) as a function of polymer architecture (e.g., the length and degree of branching). Obtaining this information from computer simulations seems appealing, since systematic/strategic data are rare, and true experiments are time consuming and expensive.

We give the results for the structural, volumetric, and dynamic properties of a simple polymer, such as poly-ethylene, as a function of the molecular architecture (branch length and branch frequency). The equilibrium radius of gyration of linear and branched poly-ethylene, the longest relaxation time, and the chain center-of-mass self-diffusion coefficient have been obtained, in this case, from Monte Carlo simulations, followed by molecular dynamics simulations with a multiple-time-step method. Analyzing these data using group contribution methods gives a closed-form analytical relationship between these properties and the polymer molecular structure and conformation. For poly-ethylene, these include the chain length (number of carbon atoms), branch lengths, and branch point frequencies. Results from this analysis and reverse calculations (and how they compare to simulation data that were masked in the group contribution step), to validate the proposed methodology, are given. In the future, we will extend the method to other polymers, such as polypropylene, cis-1,4-polybutadiene, poly-isobutylene, etc.