Modeling and Simulation in Polymer Reaction Engineering: A Personal Perspective

Siripon Anantawaraskul[1,2*]
[1]Department of Chemical Engineering, Faculty of Engineering, Kasetsart University, Bangkok 10900
[2]Center for Advanced Studies in Nanotechnology and Its Applications in Chemical, Food and Agricultural Industries, Kasetsart University, Bangkok 10900
Phone +66 2942 8555 ext. 1231, Fax +66 2561 4621, *E-Mail: fengsia@ku.ac.th

Abstract

Modeling and simulation can provide important insights on the polymerization process: how polymer chains were formed and how to control their microstructures. Such quantitative understanding can help determine appropriate operating conditions to tailor-make polymer chain microstructures (therefore, polymer properties) and aid the product development process. In this presentation, three modeling tools and example of their applications will be discussed: (1) method of moment, (2) Monte Carlo simulation, and (3) artificial neural network.

The polymerization reaction involves a large number of chemical species (i.e., monomer, active catalyst site, active chains with different lengths, and dead chains with different lengths). Therefore, it is a tedious and time-consuming task to keep monitoring all compositional changes in the system. Although this can be done by solving an extremely large system of ordinary differential equations, where each equation describes the transient material balance of each component, it is not practical in industry. This problem can be greatly simplified by using the method of moment, which greatly reduce the mathematical system in the manageable level of 10-20 equations in exchange with the reduce in information to only the average chain microstructures (i.e., average molecular weight, average comonomer content) instead of microstructural distribution. This approach is commonly considered in the polymerization process control and operations. Research example of the method of moment analysis in ethylene/1-olefin copolymerization produced in the tandem system (with no comonomer feed) will be illustrated.

If the polymerization system of interests is complicated and the details on the formation of chains with different microstructures are required, static and dynamic Monte Carlo simulations can address such requirements. Monte Carlo simulation use the stochastic approach by following the process of building each chain “unit by unit” according to the random selection of the reactions in polymerization mechanism. In this presentation, an example of dynamic Monte Carlo simulation of olefin block copolymers (OBCs) made with chain shuttling polymerization will be discussed to show how polymer population with different chain microstructures (e.g., number of block, comonomer content) were evolved.

Artificial neural network (ANN) offers new approach to describe the polymerization system. ANN is one of the black-box modeling concepts, which mimics how our nervous system operated and processed data in order to find the relationship between inputs and outputs. Although conventional phenomenological modeling approaches can be used to describe well the forward problem of how the operating conditions affect produced chain microstructures, these models cannot be used to directly solve invert problem of how to determine appropriate operating conditions to yield desired polymer microstructures. Example of ANN application in solving such problem in the ethylene/1-olefin copolymerization made with two site type system will be discussed.

Although the modeling and simulation of polymerization system cannot replace experiments, they can be of great complements. Beside the above examples, they can also be used to validate the proposed polymerization schemes (through systematic model discrimination), deconvolute the microstructures (to identify the number of site type and characteristics of site type), reduce number of experiments, and therefore provide the key to control the production process.

Keywords: Artificial Neural Network, Method of Moment, Monte Carlo Simulation, Polymer Reaction Engineering