

Reactor Modeling for Polymerization Processes

Carlos M Villa

The engineering principles that apply to polymerization reactions are extensions of well established principles for the study of reactions involving small molecules. Macromolecules are so attractive because through changes in their molecular architecture one can influence end-user properties that small molecules do not have, like melt strength, crystallinity, and clarity, to name a few. This additional degree of freedom comes at a cost, however, since it introduces a level of complexity that one needs to be careful about during reactor design, analysis, and/or operation. There are many practical problems in Polymer Reaction Engineering that can be handled using traditional tools. Very little additional expertise is required from the Reaction Engineer. There are other problems that demand this expertise and, as they do, it becomes harder to stay away from empirical components and to tell when an observation should be predicted by the model or handled as a measurement artifact. This talk tries to define the borders that separate these two types of problems, and discusses the challenges and opportunities we often face. There are still practical problems to solve in the area of commodity polymers and there are many opportunities to apply the same engineering principles to specialty polymers.