Modeling and Control of Emulsion Polymerization Processes with Evaporative Cooling

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Sachin Arora

Abstract

Emulsion polymerization is an important industrial process, which is used for producing a wide range of polymeric materials. From an industrial perspective, one of the major objectives is that of fast and safe operation with consistent polymer product quality. The polymerization usually proceeds as a double bond addition reaction initiated via a free-radical mechanism. The polymerization reaction kinetics is normally quite fast and is extremely exothermic. The latter restricts the speed of the process to the maximum cooling capacity available. The aim of this dissertation is to explore the possibility of extending the bottleneck of limited cooling capacity of jacketed reactors by the use of evaporative cooling.

The mentioned goal is pursued in a stepwise manner, starting from the development of a mathematical model that extends the physical and chemical phenomena involved in a conventional emulsion polymerization process by the vaporization phenomenon. The multicomponent gas-liquid mass transfer is described by the Maxwell-Stefan diffusion equations. First principle models are used that help to understand the underlying mechanisms and also for providing a solid basis for the development of model based optimization and control techniques.

The developed model is then validated by several experimental data sets from the literature as well as from own experiments. To gain further insight into the role of the parameters involved in the gas-liquid mass transfer, a local sensitivity analysis is performed.

Based on the extended model, a novel process operation strategy is developed. Controlled vaporization is done by which additional heat is removed from the reaction system running in a time optimal manner. This enables to extend the restrictions imposed by the heat removal capacity of the cooling jacket considerably.

In order to maximize the productivity with the minimum usage of nitrogen, an online optimizing control problem is then formulated in the model predictive control framework. Due to the online optimization of performance criteria, the scheme has a distinct advantage of adapting according to the changing conditions without depending on fixed setpoints.

Applicability and robustness of the control schemes are demonstrated by simulation studies on homopolymerization of vinyl acetate in an industrial sized reactor. The results show that a significant amount of heat can be removed by evaporative cooling thus leading to a higher productivity. Although, this dissertation is focussed on emulsion polymerization processes, it also serves as a guide to general polymerization modeling principles and devising control strategies for complex processes, which require stringent control and optimized production processes.

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