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Reduced-order methodologies for feedback control of particle size distribution in semi-batch emulsion copolymerization

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Abstract

Within-batch feedback control strategies are developed for the regulation of the particle size distribution (PSD) in a semibatch vinyl acetate (VAc)/butyl acrylate (BuA) emulsion copolymerization system. These strategies are also applicable for regulation of distributions in other particulate systems governed by population balances. In the first strategy, PID controllers are employed for regulating nucleation and growth events through tracking the nominal trajectories of total number of particles and the solids content by manipulating the feed-rates of the more reactive monomer, BuA, and the surfactant. The second control strategy is based on tracking nominal trajectories of the moments of the distribution with a quadratic dynamic matrix controller (QDMC). To determine the appropriate number of moments to describe the PSD during various stages of a nominal batch, a maximum-entropy approach is utilized. In the final and most complex approach, a nonlinear model predictive controller is designed utilizing the detailed population balance model of the system. The ill-conditioning resulting from the high-dimensionality of the resulting dynamical system is removed by principal component analysis (PCA)-based model order reduction and a multi-rate estimator is designed to compensate for the measurement delay associated with the PSD measurements.

Keywords: Control of distributions; Population balances; Emulsion polymerization; Moments; Multi-rate estimation; Principal component analysis; Bimodal distribution

1. Introduction

In particulate processes, the quality of the products is a strong function of various properties of the particles distributed over internal coordinates. Particle size distribution (PSD), where the weight fraction of the particles is distributed over size, is closely related to product performance in industrial applications. For example, the PSD of the latex paints is closely related to film-forming behavior of the paint, and crystal size distribution is related to the porosity of the crystal products. Although consistent exercise of the optimal production procedure would always result with the desired PSD, various uncertainties and disturbances during the production might cause particulate end-products with different PSDs that have poor particulate product performance. The rejection of these disturbances for consistent product quality requires closed-loop feedback control of the PSD and this necessity is more pronounced when the shape of the target PSD is complex and/or multi-modal.

Emulsion polymerization is a method for carrying out free-radical polymerization in the dispersed particle phase inside a continuous aqueous phase. In emulsion polymerization processes, especially when latex is the final product, control of PSD is important due to the direct relation between the PSD and the packing of the particles (Shikata et al., 1998; Colombini et al., 2004). For example, desired packing of the latex particles may be achieved by a bimodal PSD providing a certain ratio of smaller particles forming a continuous phase around larger particles (Tzitzinou et al., 2000). Control of PSD in emulsion polymerization reactors suffers from the unavailability of frequent on-line measurements and heterogeneous nature of the process forming a challenging dynamic control problem. Another aspect is that emulsion polymerization is highly interactive due to the interplay between nucleation, growth, and coagulation of polymer particles shaping the PSD.

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A natural framework to model the evolution of PSD in particulate processes is provided by the population balance equations (PBE). The use of PBEs provides an accurate description of the evolution of internal properties (e.g. size, age) as well as the external properties (e.g. position in physical space) of a particle population (Ramkrishna, 2000; Ramkrishna and Mahoney, 2002). Coen et al. (1998) applied the finite difference approximation to model the size distribution of styrene on the zero–one styrene system. A moving finite element method is presented in Dafniotis (1996) to solve the population equations. Immanuel et al. (2002) used orthogonal collocation on finite elements to model the PSD in an emulsion copolymerization system and performed the parametric sensitivity analysis of the resulting model. Kumar and Ramkrishna (1996a,b) discretized the population balances by integrating the continuous population balance over discrete size intervals and assumed the particles are concentrated at representative points within each element. Kiparissides (2006) provides a recent summary on modeling, optimization, control of PBE processes and presents models for a vinyl chloride suspension polymerization and a methyl methacrylate free-radical batch polymerization system.

The control of systems governed by PBEs has been studied by many researchers. Emulsion polymerization systems control had been reviewed by Dimitratos et al. (1994) and more recently, the control of general polymerization systems was reviewed by Richards and Congalidis (2006). Controllability of the systems governed by PBEs was studied by Semino and Ray (1995a,b). They analyzed the controllability of PBE systems such as crystallization, human population, and emulsion polymerization systems without the use of distributed actuators. Simpler versions of the models developed by Rawlings and Ray (1988a,b) were used to analyze the controllability of the PSD in emulsion polymerization. They found that the use of feed concentrations of surfactant and initiator or inhibitor guaranteed the controllability in the unconstrained problem. Congalidis and Richards (1998) used a first principles model off-line, to determine the effects of various changes of operating conditions on the composition and viscosity control of an emulsion polymerization reactor. Liotta et al. (1997) demonstrated that growth was a utilizable tool for particle size control. Yabuki and MacGregor (1997) employed a mid-course correction policy to control the final product quality in a semi-batch emulsion polymerization of styrene–butadiene rubber. Saldívar and Ray (1997) formulated a multi-variable control problem and controlled the molecular weight and the copolymer composition in a semi-batch methyl methacrylate/vinyl acetate (VAc) system. Crowley et al. (2000) shaped the PSD in the semi-batch emulsion polymerization of styrene to a desired bimodal distribution. The optimal trajectory of surfactant feed flowrate or free surfactant concentration (surfactant concentration above critical micelle concentration) was found by using sequential quadratic programming (SQP). Immanuel and Doyle (2002) employed genetic algorithms to calculate the open-loop optimal feed profiles of surfactant and monomer (VAc) rates in a semi-batch VAc/BuA emulsion copolymerization reactor to obtain a target end-point PSD. Valappil and Georgakis used a static end-use property model to relate the weight and number averaged molecular weights and the average size to the selected end-use properties. The aim of their work was to move the controlled outputs to a target region rather than a specific setpoint. Park et al. (2004) used an MPC controller that utilizes a PLS model to predict and control the end-point bimodal PSD in an experimental semi-batch emulsion copolymerization reactor. Alhamad et al. (2005) applied a dynamic matrix controller to an experimental styrene/MMA emulsion copolymerization system, where the average radius, particle size polydispersity index, average molecular weight, and monomer conversion were regulated by the DMC to their optimal trajectories. Shi et al. (2006) designed model-based control algorithms for a continuous and a batch crystallizer, where they utilized reduced-order models based on moments of the PSD. For the continuous crystallizer, a hybrid predictive controller manipulated the feed solute concentration to regulate the first four moments of the PSD and the solute concentration. In the seeded batch crystallizer case, they designed an MPC controller that manipulated jacket temperature to minimize the third moment of the crystals formed by nucleation.

In this paper, three integrated strategies that exploit model reduction to control the PSD in a semi-batch emulsion copolymerization system are presented and compared. The first approach utilizes the total number of particles (i.e., third moment of the population density function) and the solids content information to regulate the PSD. As there are only two outputs, a PID controller is employed, forming a simple control strategy that can serve as a baseline for more advanced control algorithms. A more advanced algorithm is used for the regulation of the PSD through a finite number of its moments, where this number is decided by a solution of the classical moments problem. A quadratic dynamic matrix controller (QDMC) regulates the moments of the distribution by manipulating all the feedrates to the semi-batch system. In the final approach, principal component analysis (PCA) is used to reduce the PSD into its leading principal components (PC). The PCs of the distribution are controlled by a multi-rate nonlinear model predictive controller (MPC) that estimates the reduced states of the system, utilizing fast solids content and slow PSD measurements.

This paper is organized as follows. In the following section, the simulated system that was used as a benchmark PBE system in this study is introduced. In Section 3, the three control methodologies are presented. The disturbance rejection performances of each methodology against various disturbances are presented and discussed in Section 4. Finally, conclusions drawn from the performances of the algorithms are presented in Section 5.

2. Simulated system

In this study, a comprehensive dynamic model of a semi-batch VAc/butyl acrylate (BuA) emulsion copolymerization system is used as the plant. The PBE model of this system was developed by Immanuel et al. (2002). In modeling emulsion copolymerization, the dynamic behavior of the particle population is described by the particle density function, $f(r, t)$ that