Society of Plastics Engineers
PLASTICS RESEARCH ONLINE

10.1002/spepro.003037

# Selecting latex characteristics

**Mohammad Shahrokhi, Ehsan Vafa, and Hossein Abedini**

*Emulsion polymer properties can be regulated by a simultaneous inferential control strategy, even in the presence of some modeling errors.*

Emulsion polymerization is one of the most important processes in polymer industries for producing a wide range of special products such as latex paints, coating, adhesive, and synthetic rubber. Control of end-use properties in emulsion polymerization is a crucial issue because of a lack of on-line measurements. Since these properties are in close relation to molecular and morphological characteristics of the latex product, such as molecular weight distribution (MWD) and particle size distribution (PSD), they can be used as controlled variables to provide products with desired end-use properties.

A considerable number of studies[1–4] address the optimal open-loop control of polymerization reactors. The open-loop control of PSD or MWD is based on the process model without measuring the process output, and so this strategy is very sensitive to model mismatch and external disturbances. To tackle this problem, some researchers have proposed efficient closed-loop control strategies that, unlike open-loop control, use information on the output to control the desired polymer properties.[5,6] In almost all schemes proposed for control of PSD and MWD in emulsion polymerization reactors, the major restriction in closed-loop control is the time delay inherent in measuring devices. We addressed this with an inferential control strategy. We control PSD and MWD by regulating the solution conductivity and concentration of unreacted chain transfer agent (CTA) via surfactant and CTA inlet flow rates as manipulated variables.

Using a comprehensive dynamic model of styrene emulsion polymerization under non-isothermal conditions, we predicted the evolution of both PSD and MWD in a semi-batch reactor. To reduce the computational load for simulation and optimization, we applied the method of moments to solve population balance equations. We assessed the accuracy of our model for predicting polymer PSD and MWD by comparison with experimental data.

We performed a sensitivity analysis to identify suitable manipulated variables for closed-loop control of the reactor. We found that surfactant and CTA inlet flow rates are the most suitable candidates for controlling PSD and MWD, respectively.

We used a pattern search algorithm optimization technique to generate optimal feed rates of surfactant and CTA for the target PSD and MWD. Subsequently, we obtained the desired profiles of unreacted CTA and free surfactant concentrations in the reactor corresponding to the optimal PSD and MWD, and we used these as set-points

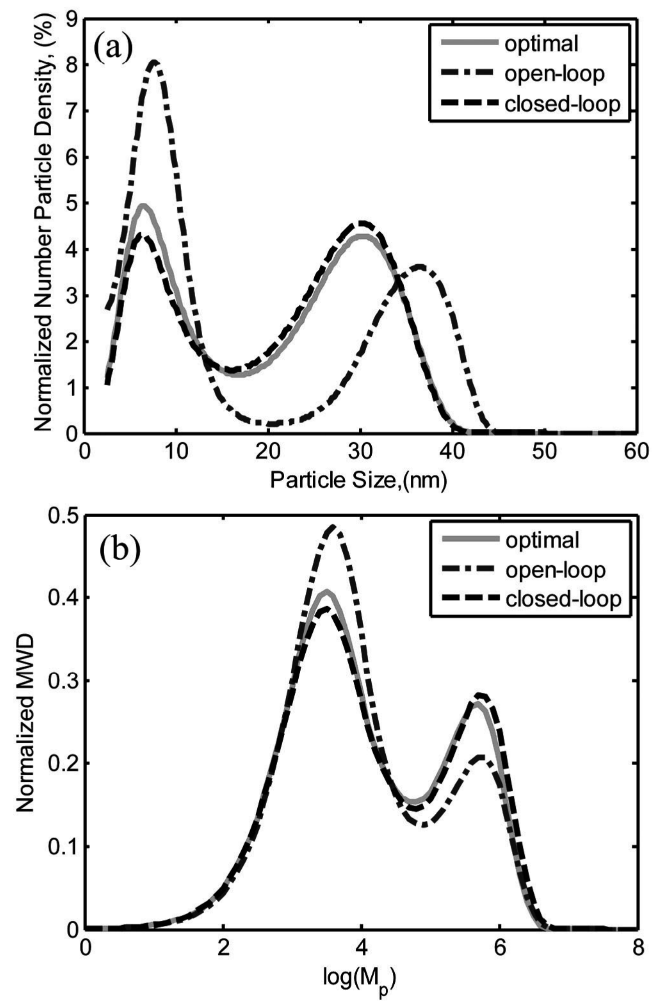


***Figure 1.*** *Comparison of final particle size distribution (PSD) and molecular weight distribution (MWD) obtained by the proposed closed-loop control scheme with those achieved by the open-loop strategy for 10% impurities in surfactant and CTA in reactor feed and −40% errors in their initial values: (a) Final PSD (b) Final MWD.*

*Continued on next page*

Society of Plastics Engineers
PLASTICS RESEARCH ONLINE



to implement the inferential control strategy. We estimated the unreacted CTA concentrations by designing a multi-rate observer that uses frequent on-line temperature measurements and infrequent measurements of CTA concentration. It is difficult to measure ionic free surfactant concentration, so we measured solution conductivity instead, which is a good indication of free-surfactant concentration. Once we had identified the optimal trajectories of conductivity and unreacted CTA concentration, we used an inferential closed-loop strategy to control PSD and MWD simultaneously. We used two single-loop PI controllers to control conductivity and unreacted CTA concentration by adjusting surfactant and CTA inlet flow rates, respectively.

Our results show that the performance of the proposed closed-loop control schemes for regulating PSD and MWD are much better than the open-loop ones (see Figure 1).

In summary, control of molecular and morphological characteristics of emulsion polymers (such as PSD and MWD of the latex product) is very important, but difficult because of a lack of real-time measurements. We have shown that satisfactory control of PSD and MWD can be achieved by regulating the solution conductivity and the concentration of unreacted CTA. Since modeling error is unavoidable, it is desirable to develop a control strategy that efficiently takes into account all kinds of parameter uncertainties. This topic will be considered in future work.

## Author Information

**Mohammad Shahrokhi and Ehsan Vafa**
Sharif University of Technology
Tehran, Iran

**Hossein Abedini**
Iranian Polymer and Petrochemical Institute
Tehran, Iran

**References**

1. T. J. Crowly, E. S. Meadows, E. Kostouas, and F. J. Doyle III, *Control of particle size distribution described by a population balance model of semibatch emulsion polymerization*, **J. Process control 10**, p. 419, 2000. doi:10.1016/S0959-1524(00)00017-2.
2. C. Sayer, G. Arzamendi, J. M. Asua, E. L. Lima, and J. C. Pinto, *Dynamic optimization of semi-continuous emulsion copolymerization reactions: composition and molecular weight distribution*, **Comput. Chem. Eng. 25**, p. 839, 2001. doi:10.1016/S0098-1354(01)00658-5.
3. C. D. Immanuel and F. J. Doyle III, *Open-loop control of particle size distribution in semi-batch emulsion copolymerization using a genetic algorithm*, **Chem. Eng. Sci. 57**, p. 4415, 2002. doi:10.1016/S0009-2509(02)00355-X.
4. C. D. Immanuel and F. J. Doyle III, *Hierarchical multi-objective strategy for particle size distribution control*, **AIChE J. 49**, p. 2383, 2003.
5. B. Alhamad, J. A. Romagnoli, and V. G. Gomes, *Online multi-variable predictive control of molar mass and particle size distributions in free-radical emulsion copolymerization*, **Chem. Eng. Sci. 60**, p. 6596, 2005. doi:10.1016/j.ces.2005.05.053.
6. J. Zeaiter, J. A. Romagnoli, and V. G. Gomes, *Online control of molar mass and particle size distribution in emulsion polymerization*, **AIChE J. 52**, p. 1770, 2006.