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Alireza Hosseini

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Alireza Hosseini, M.Sc.

aus

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Abstract

The final rheological properties of the products of emulsion polymerization are highly correlated with the particle size distribution (PSD). This motivates the development of a control strategy to achieve a desired PSD in the presence of disturbances and model-plant mismatch. The first step towards controlling the PSD is providing a reliable model. The population balance equation (PBE) is the most commonly applied tool to investigate the state of the particles in particulate processes such as emulsion polymerization.

The focus of this dissertation is mainly on developing a reliable model to describe the evolution of the PSD and using that model to control the PSD in emulsion polymerization. In early stages of this research, it was observed that the standard deterministic PBE models of emulsion polymerizations do not predict the broadening of the PSD that is observed experimentally for the growth dominated semi-batch emulsion polymerization correctly. This insufficiency is hidden when a significant numerical diffusion occurs due to the use of unsuitable discretization methods, but is evident if a suitable discretization method such as the modified weighted essentially non-oscillatory method is used. A thorough investigation on the limitations of the classical PBE models and the potential sources of the observed discrepancy showed that there is a structural inadequacy in the growth model that cannot be surmounted even by parameter adaptation. To overcome this inadequacy of the classical PBE models of emulsion polymerization, a novel approach was proposed where a stochastic term is added to the growth kernel to account for the growth inhomogeneities which is not adequately treated in the original PBE models. The probability distribution of the resulting stochastic process (Langevin equation) evolves over time based on the Fokker-Planck equation (FPE).

Using the validated FPE model, a practical approach to control the PSD is developed. In this approach, the frequent measurements up to a specified time after the start of the batch (mid-course) are incorporated to estimate the lumped states (all states except PSD) of the system using a state estimator. The estimated states together with the measured PSD at the mid-course of the process are the observations. These observations are used as the initial condition for an optimization which is performed to obtain the trajectory of the monomer feed from the mid-course up to the end of the process. In this optimization, a hybrid model is used. This hybrid model comprises of the FPE model and a data-driven component which maps the observations at the mid-course to the residual of the states (difference between the plant and the model) at the end of the batch. This residual is used to correct the predictions of the FPE model during the optimization. The performance of the proposed control structure is evaluated under parametric and under structural plant-model mismatches.

Zusammenfassung

Die rheologischen Eigenschaften von Produkten aus Emulsionspolymerisationen werden stark von der Partikelgrößenverteilung (particle size distribution, PSD) beeinflusst. Dies motiviert die Entwicklung einer Regelstrategie, die eine gewünschte Partikelgrößenverteilung im Produkt trotz Unsicherheiten im Prozess und dem der Regelung unterlagerten Modell ermöglicht. Dieses Modell zu entwickeln ist dabei der erste Schritt.
Der Fokus dieser Dissertation liegt hauptsächlich auf der Entwicklung eines für modellbasierte Regelungen geeigneten Modells und dessen Verwendung zur Regelung der PSD. Es wurde festgestellt, dass das übliche deterministische Populationsbilanzmodell (population balance models, PBE) der Emulsionspolymerisation populationsverbreiternde Effekte der hier experimentell beobachteten wachstumsdominierten Semi-Batch Emulsionspolymerisation nicht zufriedenstellend abbildet. Diese Ungenauigkeit wird bei Wahl einer ungeeigneten Diskretisierungsmethode überlagert von numerischer Diffusion, ist aber signifikant, wenn ein diffusionsarmes Verfahren zur Lösung der partiellen Differentialgleichungen des Modells genutzt wird. Nach intensiven Studien mit den klassischen PBE-Modellen zur Untersuchung ihrer Gültigkeitsgrenzen und Identifizierung möglicher Quellen der unpräzisen Beschreibung verbreiternder Effekte wurde festgestellt, dass auch durch Parameteranpassung das Verhalten qualitativ nicht präzise genug dargestellt werden kann, sodass von einem strukturellen Modellfehler im Wachstumsmodell ausgegangen wird. Durch die hier vorgestellte Erweiterung des klassischen Modells um eine stochastische Beschreibung von Wachstumsinhomogenitäten kann diese strukturelle Ungenauigkeit kompensiert werden. Die Dynamik der Wahrscheinlichkeitsverteilung des resultierenden stochastischen Prozesses wird durch die Focker-Planck-Gleichung beschrieben (FPE).
Ausgehend von einem validierten FPE Modell wird eine Strategie zur Regelung der PSD entwickelt. Dabei werden basierend auf regelmäßigen Messungen bis zu einem bestimmten Zeitpunkt während der Batch-Polymerisation (Mid-Course) zunächst nur die durch einfache Differentialgleichungen beschriebenen Zustände mittels eines Zustandsschätzers geschätzt. Dieser geschätzte Zustand zusammen mit Messungen der PSD an diesem Zeitpunkt bildet die Anfangsbedingung für eine dynamische Optimierung zur optimalen Monomerzugabe bis zum Ende der Polymerisation. Der Optimierung liegt ein hybrides Modell zugrunde, in welchem das FPE Modell um ein datenbasiertes Untermodell zur Korrelation der Beobachtungen am Mid-Course (geschätzte und gemessene Zustände) mit der Abweichung zwischen Modell und System am Ende der Polymerisation erweitert wird. Dieses Fehlermodell wird zur Korrektur der Vorhersagen des FPE-Modells während der Optimierung verwendet. Das Regelkonzept wird unter parametrischen und strukturellen Modellfehlern evaluiert.

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