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Fast and reliable computational strategy for developing a rigorous model-driven soft sensor of dynamic molecular weight distribution

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ABSTRACT

Key polymer properties are substantially directly related to the polymer molecular weight distribution (MWD). On-line monitoring and prediction of dynamic MWD profiles are highly important for on-line quality control of polymerization processes. In this study, a fast and reliable computational strategy for an equation-oriented model-based soft sensor for the high-density polyethylene grade transition process is developed. The simultaneous collocation approach is adopted to discretize the dynamic model. A novel moving finite element method is proposed to improve the on-line performance of the derived large-scale nonlinear equation systems. The sensitivity information of the nonlinear equation systems contributes to a convergence enhancement strategy for the sensor. The prediction accuracy and computational efficiency are demonstrated using industrial data. A potential application to extend the polymerization process with changeable flowsheet is also tested through simulation.

1. Introduction

Continuous slurry polymerization with heterogeneous Ziegler–Natta catalysts is a common process in high-density polyethylene (HDPE) production, in which polymers grow at the active sites of the catalyst. How the monomer molecules are connected in the polymer chain determines the molecular architecture of the resulting polyolefins as well as their various properties and applications. The molecular weight distribution (MWD) is a key microstructure index because it significantly affects the mechanical and rheological properties of the polymer [1]. Once the MWD is determined, several other quality indices, such as the polydispersity index (PDI) and weight average molecular weight (Mw), can also be determined. Thus, considering MWD in polymer quality prediction and control is necessary. To achieve different end-use polymer specifications, a plant generally produces products with various grades through the same equipment. To save material and energy, grade transition requires continuous changes from one steady state to another as fast as possible [2]. Given that grade transition is highly nonlinear and time-variant, it requires continuous monitoring by experienced operators. The operating conditions, such as temperature, pressure, and feed flowrates, are measured on-line. Meanwhile, product quality should be promptly determined to reduce unnecessary waste. However, performing on-line measurement of the polymer quality, particularly for MWD determination, is difficult. The conventional high-temperature gel permeation chromatography (GPC) method requires highly accurate sensors and long experiment durations. GPC measurement is often performed in the steady state after grade transition is completed and is seldom performed during the transition. During this delay, polymers are regarded as off-grade materials and are unnecessarily wasted. Thus, an early and accurate assessment of polymer quality is highly important [3].

Soft sensors are widely used to estimate process variables that are difficult to measure on-line in chemical processes. Research efforts have been made to develop data-driven soft sensors for polymerization processes. Numerous data-driven modeling methods [4], such as principal component regression (PCR) [5], artificial neural network (ANN) [6,7], partial least squares (PLS) [3,8,9], support vector machine (SVM) [3,10], and the Bayesian method [10,11], have been adopted for soft sensors. However, constructing data-driven models with high prediction performance for grade transition processes is difficult. To address the time-variant and highly nonlinear relationship between

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Nomenclature

x^*	Exact solution of soft sensing problems
$\hat{x}$	First-order estimate of x^*
J^*	Jacobian of soft sensing problem $\mathcal{P}$ at x^*

Greek letters

α	Vector of initial state of differential variables
β^*	Regression constant vector
γ^*	Correlation parameter vector
ζ	Flory distribution parameter
η	Tolerance of disturbance mode
θ	Vector of operating conditions
ξ	Vector of training samples
ω	Parameter of Gaussian correlation function

Latin scripts

$\mathcal{P}(k, k-1)$	Soft sensing problem with parameter θ_k *and* α_{k-1}
$\mathcal{S}$	Solution set of problem $\mathcal{P}$
$\hat{x}$	ASP for problem $\mathcal{P}$

the polymer quality and process variables, effort has been made in developing dynamic models. Gonzaga et al. [6] utilized an ANN-based soft sensor to provide estimates of the polymer viscosity. Tsen et al. [7] employed hybrid ANN models to predict the PDI of polyvinyl acetate in batch reactors. Facco et al. [9] developed a multi-phase PLS model to predict the polymer viscosity in batch reactors and indicated that the estimate accuracy can be substantially improved if some forms of dynamic information are included in the models. Shang et al. [10] developed a dynamic model based on SVM within a Bayesian framework to predict the MI of polypropylene. Kaneko and Funatsu [12] constructed time difference models to estimate the melt index (MI) of the polymer. Kim et al. [13] developed a clustering-based hybrid model to monitor the MI of polypropylene during grade transition operations. Ohshima and Tanigaki [14] applied the extended Kalman filter technique in the on-line sensing of the polymer MI. Among the reviewed data-driven methods for polymer grade transition processes, none of them used MWD as a polymer quality index. Unlike other quality indices, such as MI [3,10,13,14], viscosity [6,9], and PDI [7], MWD has a large-scale feature. The typical maximum chain length to represent the MWD profile can be as large as 10^5, or sometimes even larger. Meanwhile, GPC data during grade transition are very scarce because of measurement limits in the industrial field. Thus, developing data-driven models is very difficult for the high-dimensional output and data scarcity in this case. As an alternative, the first-principle model can play an important role with good accuracy over a broad range of operating conditions. The challenge in first-principle models is that their development requires considerable expertise and process knowledge. Besides, the model solution is difficult and costly due to the complexity of polymerization and MWD. Several comprehensive models have been developed to describe the mechanics of ethylene polymerization processes [15,16]. MWD modeling has also been considered in recent years [17]. The prediction accuracy can be improved by correcting the model parameters through off-line measurement. However, to the best of our knowledge, MWD monitoring using first-principles models has not been reported. Furthermore, solving large-scale models in real-time is problematic.

The computational time required for first-principles models can span from minutes to hours depending on the model complexity. However, model-based soft sensors require fast and reliable implementation, which can be improved through efficient modeling and solving strategies. The equation-oriented (EO) approach is one of the most competitive strategies in process simulation. The process model is often stiff and large, and solving EO models is difficult. Hashemian and Armaou [18] employed the Carleman linearization technique to obtain fast dynamic systems. Touretzky and Baldea [19] derived non-stiff reduced-order models from multiple time-scale processes for real-time computation. Zavala et al. [20] developed real-time iterative strategies for a simultaneous solving approach based on nonlinear programming sensitivity. These strategies have potential in modeling and solving for the on-line computation of dynamic models.

This study addresses fast and reliable computational strategies for the on-line monitoring of dynamic MWD based on first-principles models. A complete EO model is developed for an industrial HDPE slurry process. Fast surrogate models for thermodynamics and efficient modeling for dynamic MWD calculation reduce the scale of the process model. A novel moving finite element method is proposed to improve the on-line performance. The sensitivity information of nonlinear equation systems contributes to a convergence enhancement strategy for the sensor. This integrated framework is implemented on plant data to demonstrate the prediction accuracy and computational efficiency. A potential application to extend the polymerization process with a changeable flowsheet is also tested through simulation.

2. Dynamic model development

Fig. 1 illustrates the flowsheet of an industrial HDPE slurry process with two continuous stirred tank reactors (CSTRs) in series. The five-site Ziegler–Natta catalyst system and the other feed streams, including ethylene, hydrogen, and n-hexane, are fed continuously into the CSTRs. The product of the first reactor is fed into the second reactor. The vapor streams leaving the reactors are recycled to the feed streams through coolers, flash drums and compressors to achieve high monomer conversion. The final product that leaves the second reactor is dried and pelletized.

Intuitively, the dynamics of the process and MWD depend on the operating conditions of the process units (such as temperature, pressure, liquid level and feed flowrates). A predictive model relating the operating conditions that can be measured on-line to the process dynamics and MWD is developed. The process units (i.e., reactors, flash drums, coolers, and compressors) are modeled with equations that describe the thermodynamics, polymerization kinetics, and mass and energy balances. Unlike data-driven models, this first-principle