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Development of soft-sensors for online quality prediction of sequential-reactor-multi-grade industrial processes

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HIGHLIGHTS

- Soft-sensors for a sequential-reactor-multi-grade (SRMG) process are developed.
- The virtual variables extract the info of input variables in an SRMG process.
- Just-in-time sequential nonlinear soft-sensors handle global & local regions.
- The proposed online quality soft-sensor outperforms the others in a real plant.

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ABSTRACT

Reliable online quality prediction of sequential-reactor-multi-grade (SRMG) chemical processes often encounters different challenges, including process nonlinearity, input variable selection/extraction, sequential relationship in reactors, and multiple grades in a production line. A novel just-in-time sequential nonlinear modeling method is proposed. It integrates input variable selection/extraction and quality prediction into a unified framework. First, the input variables in the previous reactors are substituted by "virtual" quality variables via least squares support vector regression (LSSVR) transform models. Then, the sequential relationship in a sequential-reactor process can be captured by a global sequential LSSVR model using an efficient training strategy. Furthermore, for a new test sample, an improved model is constructed by integrating just-in-time learning and the proposed sequential LSSVR model. Consequently, shifting into operating modes for multiple grades can perform better than a single global model. Finally, the proposed just-in-time sequential LSSVR (JS-LSSVR) model shows sequential, global–local, and quality-relevant characteristics for an SRMG process. The JS-LSSVR modeling method is applied to online prediction of melt index in an industrial polymerization production process in Taiwan. The prediction results show its superiority in terms of high prediction accuracy and reliability in comparison with other approaches.

1. Introduction

In recent years, there has been increasing demand for product diversification in the fine chemical and polymer industries because of the highly competitive market. This issue is particularly important in the polymer industry when multiple grades of products are produced (Kaneko et al., 2011; Kim et al., 2005; Liu, 2007). However, the development of a reliable and accurate model in polymerization processes using first principles is time-consuming (Kiparissides, 2006; Ohshima and Tanigaki, 2000; Richards and Congalidis, 2006; Sharmin et al., 2006). On the other hand, product qualities, such as melt index (MI), are often analyzed off-line and infrequently. Consequently, grade change-over is operated manually in many polymer plants, resulting in relatively large settling time, overshoots and off-spec products (Kim et al., 2005; Liu, 2007; Sharmin et al., 2006). Therefore, accurate online prediction of product qualities is critical for advanced control systems as it continuously characterizes the behavior of processes and provides useful information (Chitralekha and Shah, 2010; Kaneko et al., 2011; Kim et al., 2005; Kiparissides, 2006; Liu, 2007; McAuley and MacGregor, 1991; Ohshima and Tanigaki, 2000; Richards and Congalidis, 2006; Sharmin et al., 2006; Zhang et al., 2006).

As an alternative, data-driven soft sensors have been adopted to predict product qualities using process measurement data because they have become widely available in many chemical

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plants (Chen and Ren, 2009; Fortuna et al., 2007; Kadlec et al., 2009, 2011; Kaneko et al., 2011; Kano and Ogawa, 2010; Liu et al., 2009; Yu, 2012a, 2012b; Zhang et al., 2010; Zhao et al., 2010). Compared to comprehensive mechanistic models, one main advantage of soft sensor models is that they can be developed quickly without substantial understanding of the phenomenology involved. Therefore, increasing data-driven soft sensors have been applied to multi-grade chemical and polymer processes, including partial least-squares (PLS) (Ahmed et al., 2009; Sharmin et al., 2006), artificial neural networks (Gonzaga et al., 2009; Lou et al., 2012; Mat Noor et al., 2010; Shi and Liu, 2005; Zhang et al., 2006), support vector regression (SVR) and least squares SVR (LSSVR) (Chitralekha and Shah, 2010; Han et al., 2005; Kaneko and Funatsu, 2011; Lee et al., 2005; Shi and Liu, 2006), Gaussian process regression (GPR) (Chen and Ren, 2009; Ge et al., 2011; Yu, 2012b), clustering-based and other hybrid modeling methods (Kaneko et al., 2011; Kim et al., 2005; Liu, 2007).

For many polymerization production processes, there are several operating reactors in a sequence. Generally, product qualities in a reactor are mainly affected by related variables in themselves and by some variables in the previous reactors in this sequential process (Kiparissides, 2006; Lou et al., 2012; Ohshima and Tanigaki, 2000; Richards and Congalidis, 2006; Sharmin et al., 2006; Zhang et al., 2006). Actually, without enough process knowledge, it is difficult to choose suitable input variables for modeling of a sequential process, especially for the last reactor, whose quality properties are the most critical. Moreover, input variables should be preprocessing suitably because they often show co-linearity from the partial redundancy in the sensor arrangement and are corrupted with noise (Fortuna et al., 2007; Kadlec et al., 2009; Kano and Ogawa, 2010; Yu, 2012a). However, studies in the construction of a model seldom focused on suitable variable selection/extraction during a sequential process. Principal component analysis (PCA), a dominating latent variable (LV)-based method, can extract important LVs as a preprocessing step (Cao et al., 2003; Kadlec et al., 2009; Shi and Liu, 2005; Zamprogna et al., 2005). However, the extracted LVs may capture most of the process variation, but not necessarily explain quality properties (Gustafsson, 2005; Zhao et al., 2010).

Meanwhile, the production of products with multi-grade requires frequent change of operating conditions of a sequential-reactor process. Because of the change of operating conditions, process and quality measurements often exhibit different characteristics and show different nonlinearities (Kaneko et al., 2011; Kim et al., 2005; Liu, 2007; Yu, 2012b). Actually, it is important to accurately predict product qualities during transitional modes because it can provide useful information for operators to shorten the transitional period and reduce off-spec products. Nevertheless, a single model is insufficient to capture the actual process characteristics in different operating conditions (Kaneko et al., 2011; Kim et al., 2005; Liu, 2007; Yu, 2012b). However, few modeling methods in the past have been applied to quality prediction for a whole sequential-reactor polymerization production process with consisting of several steady-state grades.

In this work, a novel just-in-time sequential modeling method is proposed to address the aforementioned two issues in a sequential-reactor-multi-grade (SRMG) process. Among existing nonlinear modeling methods, because of the good modeling performance with limited training samples (Cawley and Talbot, 2004, 2007; Liu et al., 2009, 2012; Shi and Liu, 2006; Suykens et al., 2002), the LSSVR approach is adopted to construct the soft sensor model. First, a sequential LSSVR-based (SLSSVR) modeling method which can integrate the variable extraction and quality prediction into a unified framework is proposed. The input variables can be reduced and the sequential relationship in the process is captured. Furthermore, the just-in-time learning (JITL) method (Cheng and Chiu, 2004; Ge and Song, 2010; Hu et al., 2013; Liu et al., 2007, 2012) is integrated with the SLSSVR model for better description of an SRMG process with frequent change of operating conditions. In the JITL model structure, a local model is built using the most relevant samples from the historical data set around a query sample when the prediction of the sample is required. In this way, the current state of the process nonlinearity can be better tracked by the JITL model directly (Cheng and Chiu, 2004; Fujiwara et al., 2009; Kano and Ogawa, 2010; Liu et al., 2012).

The remainder of the paper is organized as follows. After the problem formulation of a sequential-reactor process, the traditional LSSVR-based soft sensor modeling methods are first described in Section 2. Section 3 presents the just-in-time sequential LSSVR modeling method for quality prediction of a whole SRMP process. In Section 4, the proposed method is evaluated through a case study of MI prediction in an industrial polymer plant in Taiwan. Comparison with other methods is also investigated in this section. Finally, concluding remarks are made in Section 5.

2. Traditional LSSVR-based soft sensors

2.1. Problem formulation of a sequential-reactor process

As for a sequential-reactor (SR) process, there are L operating reactors in a sequence, noted as $l=1,\cdots,L$. As shown in Fig. 1, the modeling data set of the first reactor can be denoted as

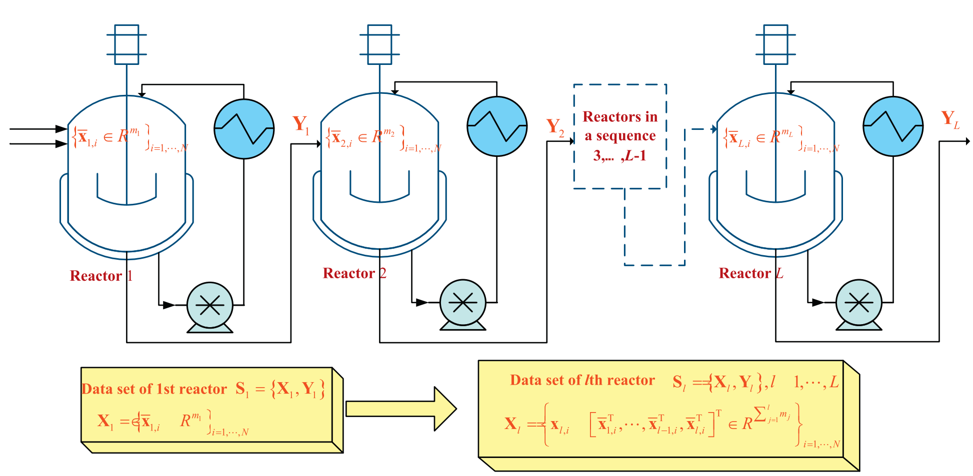

Fig. 1. A simplified flowchart of a sequential process with L operating reactors and the related modeling data set of the lth reactor ($\mathbf{S}_l=\{\mathbf{X}_l,\mathbf{Y}_l\}, l=1,\cdots,L$).