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Inner-phase and inter-phase analysis based operating performance assessment and nonoptimal cause identification for multiphase batch processes

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ABSTRACT

Batch processes play a significant role in modern industrial processes. Nevertheless, the process operating performance may degrade from optimal level, which cancels the economic profits of the plant, and effective techniques for operating performance assessment are essential. Although multimodel approaches are proposed to fit its multiphase characteristic, the effect of combined action of multiple phases on the operating performance of the overall batch, which is very important for operating performance assessment, is neglected. In this study, a novel inner-phase and inter-phase analysis based operating performance assessment and nonoptimal cause identification strategy is proposed to overcome it. The key characteristic of the proposed method is that the inter-phase assessment models are developed based on the inner-phase assessment models of each phase, which takes the correlations and interactions between phases into consideration and reveals the combined effect of multiple phases on the operating performance of the overall batch. Furthermore, online local and global assessments are performed to master the operating performance from different perspectives and improve the algorithm performance. Possible cause variables can be determined by variable contributions under nonoptimal level. The effectiveness of the proposed methodology is demonstrated through a fed-batch penicillin fermentation process and a injection molding process.

1. Introduction

In the aspect of producing low-volume and high-value added products, batch and semi-batch processes play an increasingly important role in modern industrial production. However, because of the disturbance, noise, and other uncertain causes, the process operating performance may deteriorate away from optimal level, which discounts the benefits of preliminary designs from process optimization and results in degraded operating behaviors. Hence, it is very necessary to put forward an effective operating performance assessment strategy for batch processes.

In the past several decades, many methods about process monitoring of batch processes have been developed (Louwerse and Smilde,

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2000; Nomikos and MacGregor, 1995; Meng et al., 2010; Jia et al., 2010), among which multiway principal component analysis (MPCA) is most widely used (Nomikos and MacGregor, 1994). Subsequently, several extensions to deal with various factors such as process dynamicity (Chen and Liu, 2002), nonlinearit (Lee et al., 2004), non-Gaussianity (Yoo et al., 2004) of batch processes are available. However, since conventional MPCA method takes the entire batch data as a single object, it is difficult to reveal the changes of process correlations between phases and often ill-suited for multiphase batch processes. So far, different phase division methods have been proposed (Zhang et al., 2018; Zhao and Sun, 2013; Yu and Qin, 2009) and different modeling methods have been developed that take the phase effects into consideration, including Undey and Cinar, Srinivasan et al., Lu et al., Zhao et al., Sang et al., etc. (Undey and Cinar, 2002; Lu et al., 2004a; Muthuswamy and Srinivasan, 2003; Doan and Srinivasan, 2008; Zhao et al., 2007a; Sang et al., 2008). These methods can be roughly summarized into two categories: multiblock methods and phase-divided methods (Yao and Gao, 2009). The multiblock methods characterize the multiphase batch process through a single model structure by grouping the batch process into several blocks, while the phase-divided methods build separated models for each phase. However, these studies ignore the inter-phase relationships and are incapable of modeling the correlations and interactions between phases, though they have significant impacts on process monitoring. More recently, Ng and Srinivasan (2009) recognized this issue and proposed the adjoined principal component analysis (AdPCA) by using the overlapping PCA model to characterize the transient operations between phases. Taking a different approach, Zhao et al. (2007a) developed the stage-based soft-transition multiple PCA method, and the transiting characteristics are monitored by weighting several sub-PCA models with the degree of membership as weight coefficients. The pioneer work has provided abundant theoretical bases for our following work.

In actual processes, the main task of process monitoring is to ensure the production safety under normal operating conditions, but it cannot satisfy the quest by enterprises for profits any longer. For most of plants, the production goal is to profit, and an effective way is to maintain the process on optimal operating level throughout the batch production. By this point, the operating performance assessment of industrial processes came into being (Ye et al., 2009). The purpose of process operating performance assessment is to get a measure on how far the current operating condition is from the optimum (or how optimal the current operating state is) on the premise of normal operating conditions. According to process characteristics and plant personnel's attitudes of the operating performance, the performance levels in the normal operating range can be further divided into several grades, such as optimal, suboptimal, general, and poor. Through operating performance assessment, operators and managers can make a deeper understanding and mastering with the process operating performance, and propose reference suggestions on the operating adjustment and performance improvement.

Some methods about operating performance assessment of industrial processes have been proposed in recent years. Depending on the natures of the information used, they are divided into two categories: quantitative information based methods and coexistence of quantitative and qualitative information based methods. The quantitative information refers to the numerical measurement data, while the qualitative information indicates the state descriptions or semantics, such as big, medium, small, and other fuzzy information. Therefore, the quantitative information based assessment methods are usually oriented to the processes with sufficient data collecting instruments and the process operating performance can be fully reflect by the measurements. Several assessment methods based on the quantitative information have been reported. The assessment methods based on performance-related information were developed (Liu et al., 2014, 2016a) for continuous processes, where the performance-related information of each performance grade was extracted by multivariate statistical technologies. With regard to multimode continuous processes, Gaussian mixture model (GMM) (Ye et al., 2009) and comprehensive economic index prediction based (Liu et al., 2015) methods were proposed sequentially on operating performance assessment. More recently, a multiple hypotheses testing (MHT) based assessment approach was developed for multiphase batch processes (Liu et al., 2016b), though it neglected the effect of the combined action of multiple phases on the operating performance of the overall batch run. The advantage of quantitative information based assessment methods is that more accurate, detailed and objective assessment results can be obtained when the quantitative information is used in evaluation. However, subjecting to the objective reasons, some actual production processes do not have sufficient instrumentations for data collection, while a wealth of qualitative information is available. In this case, the quantitative and qualitative information complement each other and should be used together to evaluate the operating performance of the processes. In view of this, Zou et al. (2017, 2018) proposed the assessment techniques based on dynamic causal diagram (DCD). The modified DCD was developed to deal with the qualitative information and Dempster–Shafer theory of evidence (DST) was used to handle the information fusion. Such approaches can be applied to many industrial processes, however, the assessment results usually appear rough and may be seriously affected by subjective factors and the adopted information fusion strategy. Thus, we focus on the research of quantitative information based assessment strategy in this study.

Although the batch process is usually considered as a kind of multimode processes due to its multiphase characteristic, it still has some special intrinsic characteristics that causes the existing assessment methods of multimode continuous processes to be unsuitable for multiphase batch processes. They are summarized as follows:

1) **Correlations between modes**. For continuous multimode processes, the multimode characteristic is usually due to changes in external environment, production conditions, and product specification, etc (Tan et al., 2011). Therefore, each mode exhibits an independent working state, and there is no necessary connections between different modes. By comparison, different phases of a batch serve the products with the same type, specification, and composition of a batch process. It is not independent among phases. They influence each other, restrict each other, and achieve the predetermined production goal through the organic synergy.
2) **Sequential nature between modes**. In continuous multimode processes, the active transformation from one mode to another usually depends on the change of the production scheme and has no particular order to be followed. On the contrary, in batch processes, switching from one phase to the next must adhere to a particular order strictly to achieve the predetermined production target. Thus, the sequential nature contains in batch processes.

In this study, a novel inner-phase and inter-phase analysis based operating performance assessment approach is proposed for multiphase batch processes with the consideration of the combined action of multiple phases on the operating performance of the overall batch. First, the Gaussian mixture model based phase successive division algorithm (GMM-PSD) (Liu et al., 2016b) is used for phase division on account of its advantages that can not only ensure each phase containing a series of consecutive sampling instants but also retain the uneven-length characteristics in each individual phase to achieve accurate process information. Then the influences of the process characteristics of each individual phase and the correlations and interactions between phases on the operating performance are analyzed by establishing two types of assessment models: inner-phase and inter-phase assessment models. The inner-phase assessment models are established for each phase based on its unique process characteristics extracted by total projection to latent structures (T-PLS) (Zhou et al., 2010). They reveal the impact of the behavior on the local operation performance and play a part in online phase identification and nonoptimal cause identification. By comparison, the inter-phase assessment models are built for a number of successive phases on the foundation of inner-phase assessment models. They characterize the combined behaviors of multiple phases under the consideration of the correlations and interactions among them and show their effect on the operating performance of the whole batch. In batch processes, since