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A dual modifier adaptation optimization strategy based on process transfer model for new batch process

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Abstract: In this paper, a novel dual optimization method based on process transfer model is proposed for the quality optimization control for new batch process, which combines within batch optimization method and batch-to-batch modifier-adapt strategy. Firstly, a process transfer model, JY-PLS, is applied to solve the problem that the number of new batch process data is not sufficient to built reliable latent variable process model, which transfer the data information from a based and similar batch process to the aimed new process. However, there are always difference between similar batch processes, which lead to serious plant-model mismatch. In order to cope with this problem, MCC control method is utilized to determine the optimization points and optimal setting compensation method is used to eliminate the gap between suboptimal and optimal, especially for solving the within-batch mismatch. In addition, batch-to-batch modifier adaptation is used to further overcome the batch-to-batch disturbance and solve the plant-model mismatch. Finally, the proposed approach is illustrated on the cobalt oxalate synthesis process.

***Keywords**:* Optimization control, Batch process, Similar, Process Transfer Model, Compensation.

1. INTRODUCTION

Batch and semi-batch processes are commonly used to manufacture high-value products with low quantities[1]. A large number of specialty chemicals, polymers, and pharmaceuticals are produced in batch process. In order to obtain the maximum benefit from batch processes, it is necessary to optimize operation[2]. Although sophisticated online measurements of product qualities are available, application in practical industrial processes is rather limited. Moreover, the uncertainties in the process behaviour, the absence of steady state, nonlinear and time-varying dynamics over a wide range of operation conditions complicate the optimization of these kinds of processes[3].

Multivariate statistical process control techniques have been applied successfully in several industrial applications for online process modeling, control and optimization et al.[4-7]. In order to build a reliable process optimization model, these techniques require that the data representing the common cause variability (CCV) to which the process is subject to be available. However, process data are usually insufficient to build a process model for new process based on multivariate statistical techniques. Experimental campaigns designed to produce CCV data are carried out very rarely, especially if the cost of raw materials is high or the product manufacturing is subject to a rigid regulatory environment (as in the case of the food and pharmaceutical industries, for example). Some researchers have studied the problems and proposed few methods, Chunhui Zhao tackled adaptive monitoring method for batch processes based on phase dissimilarity updating with limited modeling data, where statistical analysis models are developed implicitly based on the Gaussian-distribution assumption from batch to batch[8], in order to solve independent factors that underlie sets of non-Gaussian process measurements, independent component analysis （ICA） is used to build monitoring model with limited modeling data[9]. However, these methods do not solve the problem of insufficient data.

There are a large number of similar processes in modern industry, which storages a wealth of process data. Traditional multivariate statistical techniques just consider the single process, the process is treated as a completely independent process, and there is no correlation between similar processes. This leads to a contradiction: the old process data is rich, but the new process is seriously inadequate.

Is it possible to transfer process data from old and similar process to a new process to aid the optimization of the new process? In general, two plants dedicated to the same manufacturing process may share several characteristics. For example, they may be geometrically similar or have some common measured variables. Most importantly, the fundamental laws describing the physics of the system are expected to be the same in both plants, because the underlying physical phenomena driving the process are the same. Theidea of transfer has been used in the actual industrial process, Jaeckle and MacGregor [10]tackled the product transfer problem, and proposed a methodology based on latent variable models (LVMs) to transfer products between different manufacturing plants. García-Muñoz et al [11] further investigated and proposed a new modeling technique, called joint-Y partial least squares (JY-PLS) regression, to model the correlation between the operating conditions in different plants through the latent space generated by the quality of the manufactured products. The effectiveness of this method has been tested industrially in different applications, for product scale-up and data standardization purposes [12, 13]. However, the product transfer problem considered in all the above studies is fundamentally different from the process transfer problem considered in the present work. Tomba and Facco [14]explore the issue of the transfer of process monitoring models between different plants that exploit the same manufacturing process to manufacture the same product and combining fundamental knowledge and latent variable techniques to transfer process monitoring models between plants. Methodologies for transferring a model to a new process have been recently proposed by Lu and coworkers[15, 16]. Although these procedures are effective, they just refer to the transfer of predictive models and monitoring models, there is no work published on the process transfer for the quality optimization of batch processes.

In this paper, a dual modifier adaptation optimization strategy based on process transfer model for the quality optimization of new batch process is proposed. First of all, the similar processes data are transfer to the new process data by process transfer model (PTM), which is chosen as JY-PLS in this paper. Further, the model-plant mismatch of the process transfer based quality optimization control is firstly proposed and solved by using just-in-time model to compensate the gap between suboptimal and optimal. In simulation studies, a population balance model for a cobalt oxalate synthesis process is modeled by the method of moments and used for the simulation study. The proposed optimization strategy results in improved optimization performances compared to that of the method without transfer data from batch to batch.

This paper is organized as follows. In Section 2, the PTM based similar batch process transfer is introduced. Then PTM based dual modifier adaptation optimization strategy is described in Section 3. Section 4 analyzes the optimization performances, and the conclusions are given in Section 5.

2. PROCESS TRANSFER STRATEGY

2.1 Process similarity

In industrial production, there are a large number of similar production process which product the same production, use the same raw materials and the similar equipment. The most important is the physical principle or chemical principle, driving the entire production process, is the same .From data level, data of similar processes is highly correlated. The methods that commonly used to measure similarity is mainly based on the definition of distance, such as euclidean distance, Minkowski distance, Chebyshev distance. Although the production process is similar and final quality is the same, there are many difference between different plants include the number of monitoring variables, the types of monitoring variables, and differences of environment. It is not appropriate to directly use distance to judge the similarity.

Latent variable techniques have received a great deal of attention from researchers in the past decades. The multivariate projection to latent variable space can effectively reduce the dimension and obtain several completely independent latent variables. It is suitable to measure process similarity by calculating distance of latent variable. For two similar batch process, a represents the new process and b is based process. Their times is same , but the number and type of variable and number of batches are different. Flores-Cerrillo discuss the unfolded way of batch process data, as shown in the paper [17].

2.2 Process Transfer Model JY-PLS

After batch data is unfolded, four data matrices available are X_a , X_b, Y_a, Y_b (subscript “a” represent new process, “b” represent based process). Due to the similarity of plant a and b, the same latent variable is owned and T_b is transferred to solve the problem of data lack. It is assumed that matrices Y_a and Y_b lie in a common latent variable (LV) plane, then the loadings Q_a and Q_b for the two PLS models built should be just a rotation of each other and can therefore be defined by a single joint loading matrix Q_J, Q_J can be obtained by the joint quality Y_J . The only restriction in the JYPLS is that Y_a and Y_b must have the same quality variables defining their columns[11]. However, the JYPLS model does not impose restrictions on the number of columns in X_a and X_b, nor on the nature of the variables in X_a and X_b, nor on the number of observations per site.

The weights and loadings for the X_a and X_b matrices (P_a,W_a , P_b, W_b,) have the same interpretation as in the usual PLS regression models, but with respect to the combined plane mapped by the Joint Y matrix and defined by the common loadings matrix Q_J [11] .The JYPLS model is defined by Eq.（1）-（6）

$$\mathbf{X_a} = \mathbf{T_a}\mathbf{P_a^T} + \mathbf{E_a} \tag{1}$$

$$\mathbf{Y_J} = \begin{bmatrix} \mathbf{T_a} \\ \mathbf{T_b} \end{bmatrix} \mathbf{Q_J^T} + \mathbf{E_{JY}} \tag{2}$$

$$\mathbf{T_a} = \mathbf{X_a}\mathbf{W_a}^* \tag{3}$$

$$\mathbf{T_b} = \mathbf{X_b}\mathbf{W_b}^* \tag{4}$$

E_{YJ} represent the prediction errors. when x_{new} is obtained, prediction is

$$\mathbf{B} = \mathbf{Wa}^* \times \mathbf{Q_J^T} \tag{5}$$

$$\mathbf{y}_{new} = \mathbf{x}_{new} \cdot \mathbf{B^T} \tag{6}$$

2.3 Model Update

By acquired new data [X_a ,Y_a]and based data [X_b ,Y_b], the initial regression function can be obtained. With the operation of the new process, available data is used to fill data set of new process and update the model. If the k new batch data from the optimization steps is obtained, the model updating step can be achieved by eq.7

$$\mathbf{X}_{(k)} = \begin{bmatrix} \mathbf{X}_{(k-1)} \\ \mathbf{x}_{(k)} \end{bmatrix}, \quad \mathbf{Y}_{(k)} = \begin{bmatrix} \mathbf{Y}_{(k-1)} \\ \mathbf{y}_{(k)} \end{bmatrix} \quad (7)$$

and refitting the JY-PLS model

$$\begin{bmatrix} \mathbf{X}_{(k)} & \mathbf{Y}_{(k)} \end{bmatrix} \xrightarrow{JY-\mathrm{PLS}} \mathbf{Q}_{\mathbf{J}(k)} \quad (8)$$

With production going on, new data are constantly add and furtherly meet quantity requirements. Nevertheless, process transfer model, which includes based process, can't perfectly match new process and will affect optimization performance. In order to further improve the online optimization performance of the new batch plant. The based data are replaced one by one.

3. OPTIMIZATION STRATEGY

In Section 2, the process transfer model（JY-PLS）is applied to transfer data from old process to solve the problem that new process data is insufficient. However, it is unavoidable that there are differences between the old process and the new process, which further leads to the model-plant mismatch . whatever within-batch or/and batch-to-batch. In order to overcome this problem, a dual modifier-adaptation strategy for batch optimization is proposed in this section. Firstly, optimization problem is formulized. Then, within-batch optimization with data-based compensation method is used to modifier batch mismatch in real time. Finally, batch-to-batch optimization is used to further improve final product quality.

3.1 Formulation of the Optimization Problem

The optimization of batch process have caused many researches, which can be summarized as three types as followed 1) within-batch optimization 2) batch-to-batch optimization 3) within-batch and batch-to-batch optimization[18]. These optimization methods just take single plant into consideration. However, PTM based on optimization include two similar processes. In process transfer, similar processes exist difference include equipment differences, circumstance differences, technology differences. These differencees lead to the model-plant mismatch. In practice, a static map can be used to describe the relationship between the process inputs $u \in \mathbb{R}^N$ and the final quality measurements $y_p \in \mathbb{R}^N$ [19].Here, the subscript "p" represents a quantity related to the plant. Hence, the static batch optimization problem based on PTM can be formulated as follows

$$\begin{aligned} &\min_{\mathbf{u}} \quad \Phi_p(\mathbf{u}) := \phi\left(\mathbf{u}, \mathbf{y_p}\right) \\ &s.t. \quad \mathbf{G}_p(\mathbf{u}) := \mathbf{g}\left(\mathbf{u}, \mathbf{y_p}\right) \le 0 \end{aligned} \quad (9)$$

where $\phi(\cdot)$ is the plant performance index, and $g(\cdot)$ is the constraints imposed on the inputs and quality variables.

According to the mapping relating the process inputs and the qualities, an approximation of JY-PLS model is available in the form

$$\mathbf{y}\left(\mathbf{u},\ \mathbf{B}\right) = \boldsymbol{\sigma}_{\mathbf{y}} \circ \left(\mathbf{B}^{\mathbf{T}} \mathbf{u}\right) + \boldsymbol{\mu}_{\mathbf{y}} \quad (10)$$

where μ_y and σ_y are the mean and the standard deviation of the quality variables, $\hat{y}$ is the predicted product qualities, $\circ$ means Hadamard product.

It can get suboptimality to minimize the mean-square-error of prediction. These can't solve the plant-model mismatch, which results from process transfer. Another problems that need to pay attention to is such mismatch is existing in batch-to-batch and /or within batch process.

3.2 Within-batch Optimization

In practical industries, disturbance often affects the operation of the batch process, which make the final product

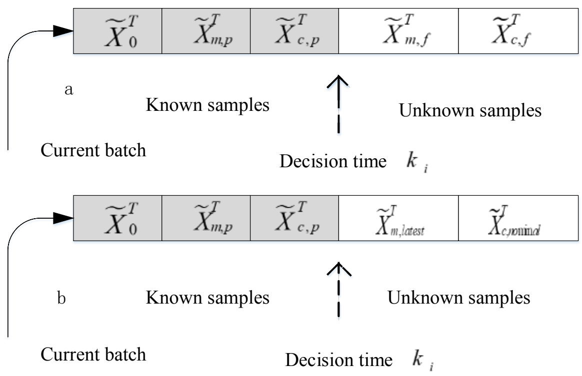

Fig.1 Data used for model prediction

quality outside of a defined in-control region. In addition, because process transfer model include two similar process data which make model-plant mismatch always exists. MCC is usually used for within-batch optimization and acquire great optimization results [20]. In MCC, a complete batch variable is divided by several decision points. Once reaching decision points, a optimization action is utilized to adjust manipulated variable. When a new batch is under processed, at decision point k_i, there exist a regressor vector X^T (Fig. 1) described as

$$x^T = \begin{bmatrix} x_0^T \ x_m^T \ x_c^T \end{bmatrix} = \begin{bmatrix} x_0^T \ x_{m,p}^T \ x_{m,f}^T \ x_{c,p}^T \ x_{c,f}^T \end{bmatrix} \quad (11)$$

where $x_{m,p}^T$ is a vector of all measured variables available up to time k_i, $x_{m,f}^T$ is a vector of unmeasured variables not available at k_i but that will available in the future, $x_{c,p}^T$ is a vector of the known manipulated variables and $x_{c,f}^T$ is a vector of the future manipulated variables which will determined by the control approach. Unavailable data $x_{m,f}^T$ and $x_{c,f}^T$ can get by way of PCA prediction [20]. If directly optimize new process, it only get suboptimal u^* because of plant-model mismatch. However, the similarity between the transfer processes makes suboptimal near to the optimal solution u_p^* .The following relation can be obtained by using Taylor formula expansion

$$J\left(\mathbf{u}_p^*\right) = J\left(\mathbf{u}^*\right) + \frac{\partial J}{\partial \mathbf{u}}\left(\mathbf{u}_p^* - \mathbf{u}^*\right) + \delta \quad (12)$$

where $J(\bullet)$ is comprehensive performance index, δ is infinitesimal of higher order,

$$\Delta J = H\left(\Delta \mathbf{u}\right) \tag{13}$$

where $\Delta J = J\left(u_p^*\right) - J\left(u^*\right)$, $\Delta u = u_p^* - u^*$,JITL(Just-In-Time Learning) PLS proposed by LI Kang [21]can obtain the relationship between u and J, and can compensate for the plant-model mismatch. The optimization problem is transformed into the following formula

$$\begin{aligned} \max_{\Delta u} \quad & \Delta J = H\left(\Delta \mathbf{u}\right) \\ s.t. \quad & g\left(\Delta \mathbf{u}\right) \le 0 \\ & \Delta \mathbf{u}_{\min} \le \Delta \mathbf{u} \le \Delta \mathbf{u}_{\max} \end{aligned} \tag{14}$$

3.3 batch-to-batch optimization

To limit the deterioration of control performance due to model plant mismatches and unknown disturbance, a batch-to-batch control strategy is used at the end of the current batch. It utilizes the information of the current and previous batch run to enhance the operation of the next batch.

In order to solve the model-plant mismatch, modifier-adaptation methodology was proposed and have developed a variety of methods[17-20]. Generally, two methods are summarized as followed ,1) modifying the cost 2) modifying the constraints of the optimization problem. In such a way that the necessary condition of optimization of the model and the plant can match.

In this work, a linear modification is used based on the JY-PLS model. Letting $u_{(k)}$ denote the kth scaled operation point, the model output is modified as

$$\mathbf{y_m}\left(\mathbf{u}, \mathbf{B_{(k)}}\right) = \mathbf{y}\left(\mathbf{u}, \mathbf{B_{(k)}}\right) + \boldsymbol{\varepsilon}_{(k)} + \boldsymbol{\lambda}_{(k)} \cdot \left(\boldsymbol{\sigma}_{\mathrm{u}} \circ \left(\mathbf{u} - \mathbf{u_{(k)}}\right)\right) \tag{15}$$

where σ_u is the standard deviation of the input matrix, and $\varepsilon_{(k)} \in \mathbb{R}^M$ and $\lambda_{(k)} \in \mathbb{R}^{M\times N}$ are the kth model modifiers, which can be calculated as follows

$$\boldsymbol{\varepsilon}_{\mathbf{(k)}} = \mathbf{y_p}\left(\mathbf{u_{(k)}}\right) - \mathbf{y}\left(\mathbf{u}, \mathbf{B_{(k)}}\right) \tag{16}$$

$$\boldsymbol{\lambda}_{\mathbf{(k)}} = \frac{\partial \mathbf{y_p}}{\partial \mathbf{u}}\left(\mathbf{u_{(k)}}\right) - \frac{\partial \mathbf{y}}{\partial \mathbf{u}}\left(\mathbf{u_{(k)}}, \mathbf{B_{(k)}}\right) \tag{17}$$

According to problem (9),optimization problem with modifier is translated into

$$\begin{aligned} \min_{\mathbf{u}} \quad & \Phi_{\mathrm{m}}(\mathbf{u}) := \phi\left(\mathbf{u}, \mathbf{y}_{\mathrm{m}}\left(\mathbf{u}_{(k)}, \mathbf{B}_{(k)}\right)\right) \\ s.t. \quad & G_m(\mathbf{u}) := \mathbf{g}\left(\mathbf{u}, \mathbf{y}_{\mathrm{m}}\left(\mathbf{u}_{(k)}, \mathbf{B}_{(k)}\right)\right) \le 0 \end{aligned} \tag{18}$$

The simplest adaptation strategy is to implement the rescaled optimal solution $u^*_{(k+1)}$ obtained from Eq. (18). However, this simple way may lead to excessive correction when the operation is far away from the optimum, and also it may make the adaptation strategy very sensitive to measurement noise. A better choice consists of filtering the next operating point with a first-order exponential filter

$$\mathbf{u}_{(k+1)} = (\mathbf{I} - \mathbf{K})\mathbf{u}_{(k)} + \mathbf{K}\mathbf{u}^*_{(k+1)} + g \cdot \boldsymbol{\rho}_{(k+1)} \tag{19}$$

where $\mathbf{K} \in \mathbb{R}^{N\times N}$ is a diagonal gain matrix. $\boldsymbol{\rho}_{(k+1)}$ is a vector of N original excitation signals composed of 1's and −1's, and g is the amplitude associated with the inputs.

4. CASE STUDY

4.1 Process Description

A cobalt oxalate synthesis process in cobalt hydrometallurgy industrial is a liquid phase reaction of cobalt chloride and ammonium oxalate, and cobalt oxalate is produced by the following reaction

$$\underset{\mathrm{A}}{CoCl_2} + \underset{\mathrm{B}}{(NH_4)_2C_2O_4} \rightarrow \underset{\mathrm{C}}{CoC_2O_4} \downarrow + \underset{\mathrm{D}}{2NH_4Cl} \tag{20}$$

The process flow sheet is shown in Fig.2 .The process consists of two important parts which are ammonium oxalate dissolver and crystallizer. The process of cobalt oxalate is carried out in the crystallizer operated with continuously stirring. In order to maintain the constant temperature in the crystallizer, a heating jacket and PI controller are used. Specific procedures can be seen in the article [22].

The moment model of the crystallization process is shown by the following set of ordinary differential equations:

$$\frac{dV}{dt} = F_B \tag{21}$$

$$\frac{d\mu_0}{dt} = B - \frac{F_B\mu_0}{V} \tag{22}$$

$$\frac{d\mu_j}{dt} = jG\mu_{j-1} - \frac{F_B\mu_j}{V} \qquad j = 1,2 \tag{23}$$

$$\frac{dC}{dt} = \frac{F_B C_{BI} V_{AI}}{(V_{AI} + F_B t)^2} - 3\rho_c k_v G\mu_2 - \frac{F_B C}{V} \tag{24}$$

where V is the suspension volume, u_j is the jth moment of the PSD, and C is the solution concentration. $B$and G are the crystal nucleation rate and growth rate, respectively, V_0 is the initial volume of cobalt chloride, ρ_c is the crystal density, and k_v is the volumetric shape factor. The model parameters of the synthesis process are given as followed.

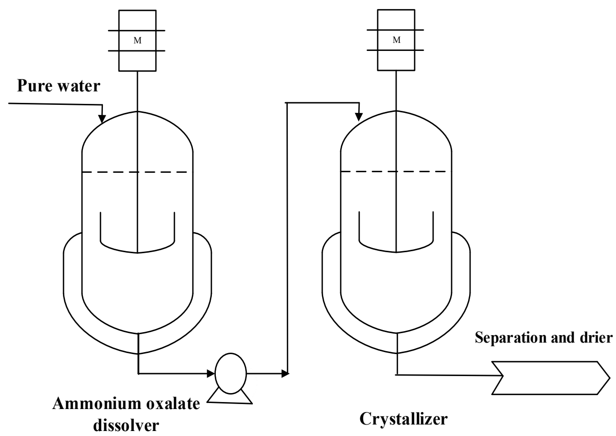

Fig.2The schematic diagram of the cobalt oxalate synthesis process

Table1 variable setting between new and based process

	Variable	Based process	New process
Circumstances Difference	Concentration of $CoCl_2$ (mol/m3)	1089.6---1111.6	1092.6—1114.6
	Concentration of $(NH_4)_2C_2O_4$ (mol/m3)	1676.6---1710.4	1666.7---1700.3
	Initial volume of $CoCl_2$ (m3)	1.39----1.42	1.40----1.44
Technology Difference	K_b(k)	1.3621×10^4	1.352×10^4
	K_g(k)	1.5840×10^4	1.5730×10^4
	k_g $(s^{-1} \cdot \mu m)$	2.70×10^{14}	2.83×10^{14}

$$C_s = 0.0001(T-273)^2 + 0.001(T-273) + 0.1 \quad (25)$$

$$B = 6.31\times10^{31}\exp(-1.3621\times10^4/T)\Delta C^{2.775} \quad (26)$$

$$G = 2.80\times10^{14}\exp(-1.584\times10^4/T)\Delta C \quad (27)$$

In this paper, the objective function is to maximize the mean crystal size defined in Equation (28), leading to the optimization problem (29)

$$Ln = \frac{\mu_1(t_f)}{\mu_0(t_f)} \quad (28)$$

$$\begin{aligned} &\max_{F(t)} \quad Ln \\ &s.t.. \quad \int_0^{t_f} F(t)C_2 dt \geq C_{2,\min} \\ &\qquad F_L \leq F(t) \leq F_U \end{aligned} \quad (29)$$

where F_L and F_U are the lower and upper bounds on the feed rate of ammonium oxalate, and $C_{2,min}$ is the minimum quantity of ammonium oxalate added in the crystallizer

4.2 *Within-batch optimization*

In order to optimize the batch process in time and obtain optimal solution , the MCC control strategy with optimal setting compensation is used. 0.1% disturbance is added to the input variables. Fig.3 shows that the PSD of cobalt oxalate increases with the batch going and gradually converge to 2.3. In order to compare the batch optimization effects, the method without within-batch optimization is used for comparison. As shown in Fig.4, within-batch optimization can greatly improve the PSD of cobalt oxalate. The 10th, 50th, and 80th batches are randomly selected. Witnin-batch optimization can optimize the batch process and improve the final quality.

4.3 *Batch-to-batch optimization*

Within-batch optimization can optimize the batch process in real time and control the final quality in the effective area. However, batch process is constantly repeated and there is a strong link between current batch and previous batch, previous batch condition will affect current batch performance. In addition, plant-model mismatch and disturbance between batches may cause the next batch away optimal quality. Therefore, batch-to-batch optimization is a necessary part. Fig.4 shows crystal size of cobalt oxalate with batch evolution, while Fig.5 show comparison of the feeding law trajectories for different iterations. With batch process running, crystal size of cobalt oxalate gradually improve , at

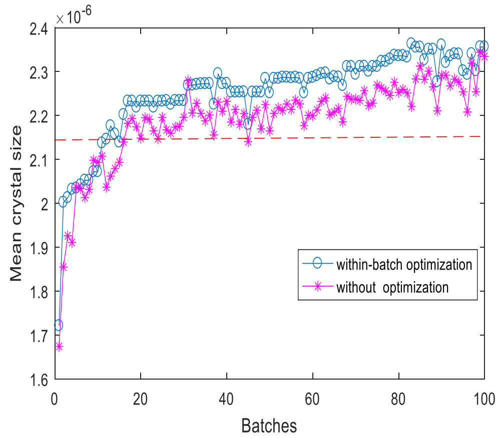

Fig.3 Comparison between within-batch optimization and without optimization

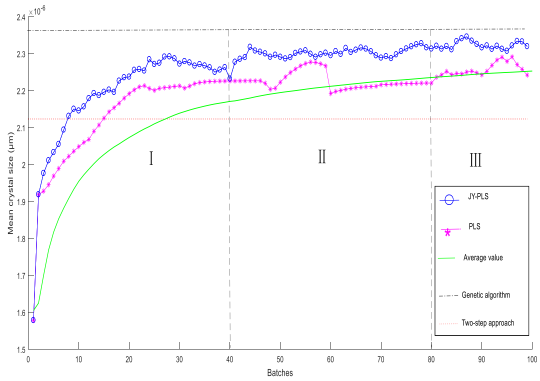

Fig.4 batch-to-batch optimization

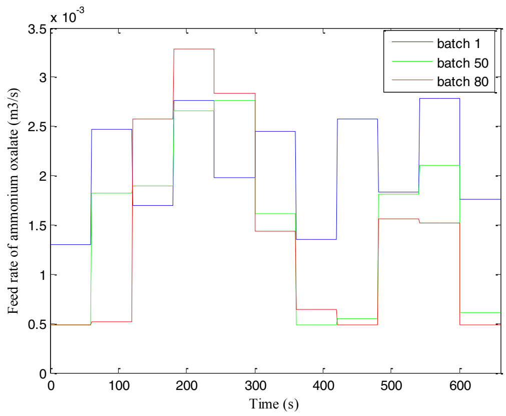

Fig.5 Comparison of the feeding law trajectories for different iterations

the same time, Evolution of the total quantity of ammonium oxalate added in crystallizer is gradually decrease and converge to 1500.

5. CONCLUSIONS

In this paper, a novel dual optimization method between similar batch processes based on PTM is proposed. It combines the optimal setting compensation method and batch-to-batch modifier-adapt strategy. During the evolution of a batch, MCC control method is utilized to determine the optimization points and compensate the error between suboptimal and optimal. Batch-to-batch optimization is used to overcome plant-model mismatch. A PTM is applied to solve the problem that new process data is lack, which transfer similar based process data to the new process. The proposed method can solve the plant-model mismatch due to process transfer, especially for solving the within-batch mismatch. The proposed approach is illustrated on cobalt oxalate synthesis process. Simulation results demonstrate that the proposed method can effectively improve final quality prediction and further optimize final quality.

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