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Iterative optimization for batch processes through online modeling

Jinjin Zhao*. Yi Yang*. Xi Chen*$^{\#}$.Furong Gao**

**Department of Control Science and Engineering, Zhejiang University, Hangzhou, China*
***Department of Chemical and Biomolecular Engineering, Hong Kong Univ. of Science and Technology, Hong Kong*
(*#Corresponding author. Email: xichen@iipc.zju.edu.cn*)

Abstract: Batch process optimization is of great significance in industrial applications. This paper proposes an iterative optimization method for batch processes through online modeling, in which, local models are iteratively developed to guide a trust-region optimization. The characteristics of the method are demonstrated through a numerical simulation. This method is also successfully implemented to the quality control of injection molding process with satisfactory performance and high efficiency.

1. INTRODUCTION

Batch process optimization is of great significance in reducing production costs, improving product quality, and meeting the requirements of different users. Model-based optimization (MBO) (Srinivasan *et al.,* 2003) is widely used to seek the optimal operating conditions for batch processes. This approach initially establishes a process model, which correlates operating conditions and product quality. An optimization algorithm is then used to determine the optimal solution. The model accuracy is of great importance for implementation. A number of studies have been reported in batch process modeling techniques, which can be categorized into two types, the first-principle models (Hangos & Cameron, 2001; Bonvin, 1998) and data-driven models (Chen, Nguang, & Chen *et al.,* 2004; Chen & Xi, 1998; Jaeckle & MacGregor, 1996, 2000; Sebzalli, 2001; Kulkarni, 2004). However, as a batch process requires a wide operation range, deriving an accurate model for a complex process is always difficult. Model-free optimization (MFO) (Box & Draper, 1987) is another technique for batch process optimization. Kong et al. proposed such a technique for rapid and low-cost batch processes (Kong *et al.,* 2011). Instead of building a process model, online measurements were directly used to guide the system toward the optimal solution. Efficient algorithms were also employed in the searching process. Owing to the existence of the measurement noise and process disturbance, MFO also faces a convergence challenge.

To overcome the limitations in MBO and MFO, a novel method called iterative modeling and trust-region-based optimization (IM&TO) is proposed for batch process optimization in this paper. Rather than building an accurate model for the whole range of a batch process, a local model (Bachtadze, *et al.,* 2007, 2010, 2011) based on limited run data is used. Trust-region optimization (Nocedal & Wright, 1999) is adapted to seek the optimal solution within a bounded range. After achieving new data running on the local solution, a new model can be obtained through an iterative modeling technique, based on which the optimization can be further conducted in the updated trust region. This process will be repeated until the model is no longer updated. Compared with MBO, the modeling cost, either the experimental cost for data-driven models or process knowledge for first-principle models, is reduced significantly because of the local accurate model. Good extrapolation and adaptability to changing conditions are achieved through iterative learning and modeling. Compared with MFO, the experimental cost in optimization is reduced, and the optimization direction is guaranteed with model guidance.

2. IM&TO METHOD

In this paper, the authors propose a new method called IM&TO for batch process optimization. To avoid the difficulties in building an accurate model for the whole range in traditional MBO methods, the method uses local models for optimization. The flowchart of the proposed method is shown in Fig. 1. With limited experimental data, a local model is first developed based on data-driven modeling techniques. The model is accurate only in a limited range. Thus, optimization is next conducted with a bounded trust region to ensure a reasonable step. After the experimental test on the derived solution, the model is updated with newly obtained data. The trust-region optimization can thus be conducted again within an updated region. The method stops when the local model is no longer updated. Iterative modeling and trust-region optimization are two keys to the proposed method and are elaborated as below.

2.1 Iterative modeling technique

A key to the proposed method is to use local models for optimization. An iterative modeling technique is used to ensure the local accuracy of the model and to move the local model toward the optimal point through iterative optimization.

Surrogate models based on experimental data are used during the optimization. The models are updated iteratively by least squares regression with new data. The surrogate model can employ several types of structure; a quadratic polynomial model is selected for its simplicity and efficiency.

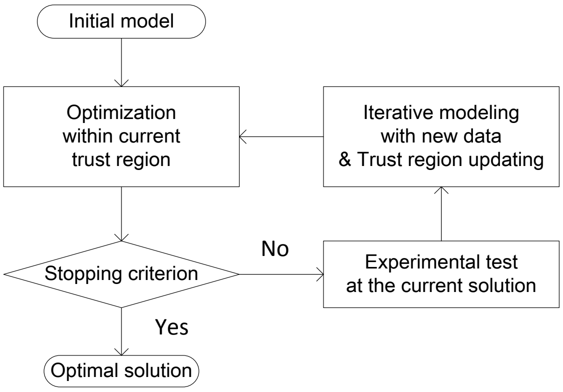
Initial model
Optimization within current trust region
Iterative modeling with new data & Trust region updating
No
Stopping criterion
Experimental test at the current solution
Yes
Optimal solution

Fig. 1. Flowchart of IM&TO method

A complete quadratic polynomial model with n variables is shown in Equation (1), where t_k^* is the model structure vector consisting of polynomial terms in the k-th iteration, and θ_k is the relevant parameter to be estimated.

$$\begin{aligned} & y_k = f_k = t_k^* \theta_k, \\ & t_k^* = \left(1, x_1, x_2, ..., x_n, x_1^2, ..., x_n^2, x_1 x_2, ..., x_1 x_n, x_2 x_3, ..., x_{n-1} x_n\right); \quad (1) \\ & \qquad \theta_k = (\theta_{k1}, \theta_{k2}, ..., \theta_{k(n(n-1)/2+2n+1)})^T \end{aligned}$$

The model is obtained based on limited data. Thus, iterative modeling is proposed to describe the process locally and to guide optimization. Consequently, the local model approaches the optimal zone through iterative optimization. During the iteration of optimization, both the model structure and modeling data are updated until optimization converges. In model structure updating, a strategy to set the priority of each polynomial term is necessary when the available data are limited to obtain a complete quadratic polynomial model, in which polynomial terms are chosen according to their importance based on the knowledge obtained from prior experiments. In data set updating, a strategy correlating the size and distance between the sample data and the current iterate is proposed. For example, in the k-th iteration, P_k is the sample set with S samples, and t_k is the model structure obtained based on the accumulated knowledge. A surrogate model f_k with n variables is obtained by least squares regression based on P_k and t_k. A new sample $p_{new}(x, y)$ is obtained after optimization on f_k and an experiment on solution x. In the (k+1)-th iteration, sample set and model structure will be updated to P_{k+1} and t_{k+1} based on the strategies (2) and (3), respectively.

In strategy (2), data set P_k is updated according to its size (S) and the data contained. If $S+1 \leq N$, $S=S+1$. N is the upper limit of the data size that satisfies $N > (n+1)(n+2)/2$. The sample data are added to the data set without losing any data. Otherwise, $S=N$, the size of the data set remains unchanged. The farthest point (except the trial point) from the current iterate is replaced by the newly added trial point, and the sample data are updated.

In strategy (3), model structure vector t_k is adjusted according to the size (S) of the current data set P_k, and knowledge from prior experiments, which is reflected from the parameters estimated by least squares regression. If $S \leq n+1$, linear terms are selected, and (S-1) variables are selected for the regression. If $n+1<S<(n+1)(n+2)/2$, nonlinear terms are selected based on the accumulated prior knowledge. Important terms should be added to the model structure as soon as possible during run-to-run optimization. Otherwise, $S \geq (n+1)(n+2)/2$, and a complete quadratic polynomial model is obtained.

$$P_{k+1} = \begin{cases} P_k \cup \{p_{new}\}, S = S+1; & \text{if } S+1 \leq N, \\ \{p_1, p_2, ..., p_{new}, ..., p_s\}, S = N. & \text{if } S+1 > N. \end{cases} \quad (2)$$

$$t_{k+1} = \begin{cases} \left(1, x_1, x_2, ..., x_{S-1}\right); \quad \text{if } S \leq n+1, \\ \left(1, x_1, x_2, ..., x_n, x_i^2, ..., x_j^2, x_t x_s, ..., x_p x_q\right); \\ \qquad \text{if } n+1 < S < \left(n+1\right)\left(n+2\right)/2, \\ \left(1, x_1, x_2, ..., x_n, x_1^2, ..., x_n^2, x_1 x_2, ..., x_1 x_n, x_2 x_3, ..., x_{n-1} x_n\right). \\ \qquad \text{if } S \geq \left(n+1\right)\left(n+2\right)/2. \end{cases} \quad (3)$$

2.2 Trust-region optimization based on iterative modeling

The surrogate model is built with limited data, making it unreliable in a large region. Thus, rather than search for the optimal solution on the whole range, optimization with a trust region is proposed to restrict the step length. In the traditional trust-region method, the objective function, f, is given. The approximate model m_k is commonly chosen as the second Taylor-series expansion of f. Optimization is conducted on the approximate model m_k with a trust region. The region size and region center are updated based on the agreement ρ_k between the approximate model m_k and the original model f within two iterates. The trust region not only restricts the step length, but also guarantees good reduction in f. As shown in Fig. 2, the irregular contours illustrate the curvature of the original model f. The elliptical contours illustrate the approximate model, m_k, which is built around the current iterate, x_k. If no trust region exists, the line search method based on the approximate model searches along the step direction to the minimizer of m_k as a new iterate x'_{k+1}, which results an increase in the objective model f. Bounded with a trust region, as shown by the dotted circle, the line search steps to the minimizer of m_k with a significant reduction in f as a better iterate x_{k+1}.

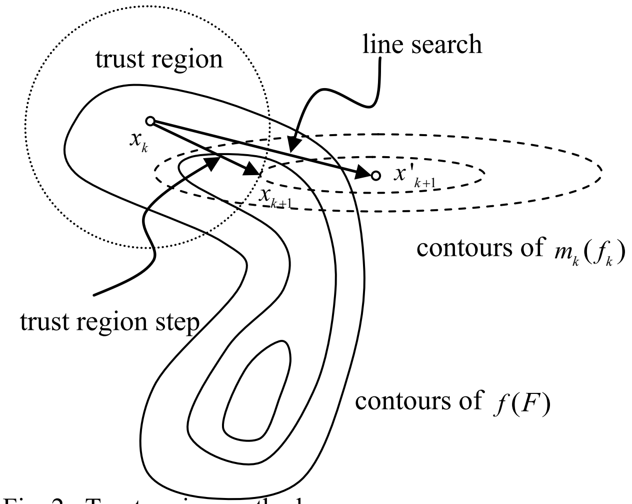

Fig. 2. Trust region methods

Unlike traditional trust-region optimization, the original model, f, in this case is unknown. However, we can still borrow this idea for iterative optimization. A local model is first built based on experimental data. By adding a trust region, iterative optimization can be conducted on the local model, which takes the role of the approximate model in traditional trust-region optimization. After obtaining the new iterate, the local model can be updated with newly obtained experimental data. This process continues until the model can no longer be updated.

In the IM&TO trust-region method, a reasonable region Δ_k, which is used to restrict the step length, is defined around the current iterate x_k and moves along iterates from batch to batch. In model updating, F is the unknown process model, the quadratic polynomial model f_k is trusted to be a good approximation of F in the region, which is updated iteratively. The two main steps of the method are described as follows: 1. Subproblem solving. The region size Δ_k remains a reasonable value, and the region center moves along with iterates. The current local model f_k is minimized within the trust region to obtain the next iterate x_{k+1}. 2. Model updating. Model f_k is updated with new data added. The subproblem is then solved again based on an updated model within a new trust region.

During the iterations, the local model accuracy is improved due to three aspects. First, an increasing amount of data is collected and used for modeling through run-to-run optimization, where the size of the data set is limited to an upper bound. Second, modeling data density increases through trust-region optimization and a data set updating strategy, where the step length is restricted in obtaining a new iterate, and the data far from the current iterate are discarded. The residual (R) defined in Eq. (4) describes the resemblance of the local model (SF) to the original model (OF) within the trust region, which is averaged on the verification points. Finally, the local model is modified in terms of structure and parameters with data accumulation.

$$R = \frac{1}{m}\sum_{i=1}^{m}\left|SF(x_i) - OF(x_i)\right| \tag{4}$$

where m is the sampling number of verification points x, which are evenly distributed within the trust region. We set the interval to be one-tenth of the trust region, m=11.

The differences between the traditional and IM&TO trust-region methods are listed in Table 1.

2.3 IM&TO Algorithm

The detailed algorithm of the proposed IM&TO method is described below.

Step0 (initialization): Choose an initial point x_o, an initial data set Y_o, and an initial model $f_0(x)$ derived from Y_o. Set a reasonable trust-region radius Δ. Set σ =10^{-6}. Set k = 0.

Step1 (step calculation and stopping criterion): Compute x_{k+1} to minimize the objective function $f_k(x)$ by solving the trust-region subproblem with bound constraint (5). If the stopping criterion (6) is satisfied under a stable model structure, the algorithm stops. Otherwise, go to the next step.

$$\begin{aligned} &\min \quad f_k(x) = t_k\theta_k \\ &\quad s.t.\ \left|x - x_k\right| \le B \ \ (B(x_k;\Delta_k) = \left\{x \in R^n : \left\|x - x_k\right\| \le \Delta_k\right\}) \end{aligned} \tag{5}$$

$$(t_k \subseteq \left\{1, x_1, x_2, \ldots, x_n, x_1^2, \ldots, x_n^2, x_1x_2, \ldots, x_{n-1}x_n\right\}; \theta_k, parameter)$$

$$\left|\theta_k - \theta_{k-1}\right| < \sigma \tag{6}$$

Step2 (experiment): conduct an experiment on x_{k+1} to obtain $F(x_{k+1})$. F is the real process. Obtain [$x_{k+1}, F(x_{k+1})$] as the new sample data and x_{k+1} as the trial point.

Step3 (model updating):

a. Data set is updated according to the size (S) of the current data set Y_k and the points contained:

If S+1 ≤ N, S=S+1. where N is the upper limit of the data size that satisfies N > (n+1)(n+2)/2 with n variables. The sample data are added to the data set without losing any data. Otherwise, S=N, the size of the data set remains unchanged. The farthest point (except the trial point) from the current iterate is replaced by the newly added trial point. The sample data are updated.

b. Model structure is adjusted according to the current data size and knowledge from prior experiments:

If S ≤n+1, linear terms are selected, and (S-1) variables are chosen to conduct the regression. The parameters estimated by least squares regression reflect the importance of each term, which is accumulated as knowledge to guide the upcoming term selection.

Else if n+1<S<(n+1)(n+2)/2, nonlinear terms are selected based on the accumulated prior knowledge. Important terms should be added to the model structure as soon as possible during run-to-run optimization.

Else, S ≥ (n+1)(n+2)/2, a complete quadratic polynomial model is obtained.

Step4 (trust region updating):

Table 1. Differences between traditional and IM&TO trust-region methods

method	Traditional trust-region method	IM&TO trust-region method
Sub-problem solving	f , known as the objective model; m_k , the second Taylor-series expansion of f ; min $\quad m_k(x_k) = f_k + \nabla f_k^T s + \frac{1}{2} s^T \nabla^2 f_k s$ $s.t.\ \ s \le B\ \ (B(x_k;\Delta_k) = \{x \in R^n : \|x - x_k\| \le \Delta_k\})$ $(f_k, the\ f\ value\ on\ x_k; s = \lvert x - x_k \rvert)$	F , unknown as a process model; f_k , quadratic polynomial model, obtained by least squares regression to represent F ; min $\quad f_k(x) = t_k \theta_k$ $s.t.\ \ \lvert x - x_k \rvert \le B\ \ (B(x_k;\Delta_k) = \{x \in R^n : \|x - x_k\| \le \Delta_k\})$ $(t_k \subseteq \{1, x_1, x_2, ..., x_n, x_1^2, ..., x_n^2, x_1 x_2, ..., x_{n-1} x_n\}; \theta_k, parameter)$
region changing strategies	region size Δ_k and region center x_k , updated based on the agreement criterion: $\rho_k = \frac{f(x_k) - f(x_{k+1})}{m_k(x_k) - m_k(x_{k+1})}$ $\Delta_{k+1} = \begin{cases} \gamma_2 \Delta_k;\ if\ \rho_k > \mu_2 \\ \Delta_k \quad ;\ if\ \rho_k > \mu_1 \\ \gamma_1 \Delta_k;\ if\ \rho_k < \mu_1 \end{cases}; x_{k+1} = \begin{cases} x_k + s\ ; if\ \rho_k > \mu_1 \\ x_k \quad ;otherwise \end{cases}$ $(0 < \mu_1 < \mu_2 < 1; 0 < \gamma_1 < 1; \gamma_2 > 1)$	region size Δ_k , remains a reasonable value to restrict the step length; region center x_k , updated to x_{k+1}

Region size remains unchanged. The trial point is accepted and the iterate moves to x_{k+1} as the region center in the next optimization. Increase *k* by one, and go to step 1.

3. SIMULATION

A numerical simulation is conducted first to illustrate the proposed IM&TO method. A quadratic polynomial model *SF* is used to approximate a cubic model *OF* locally to determine the minimum of the *OF* in an iterative manner. Models are set below.

Objective function, $OF = x^3 + 10x^2\ (-5 < x < 5)$ with minimizer (0,0), which is assumed to be the unknown process model; Surrogate Function, $SF = p(1)x^2 + p(2)x + p(3)$. The algorithm stops when the difference between the current *SF* and the prior one is less than the tolerance, $\sigma = 10^{-6}$.

Initializations and the steps are detailed as follows: Set the trust region Δ =2. Set initial iterate x1=-3. Three data sets (s1, s2, and s3), as shown in Run #1 of Table 2, are obtained randomly before optimization. Based on these data, a quadratic polynomial model is first obtained. By conducting trust region optimization on this local model, a new iterate, x_1*=-2, can be obtained. With the newly obtained data, the local model is updated. Further trust region optimization iterates to a new point, x_2*=-1. After the third iteration, the accumulated data number exceeds the maximum data number used for modeling, and the farthest point from current iterate will be replaced by the new data. As shown in Run # 3 and Run # 4 of Table 2, point s1=-5, which is the farthest point from the current iterate, x4=-0.3653, is replaced by s1'=-0.3653 in the fourth iteration. This iterative trust-region optimization repeats until it converges at Run #14, when a preset tolerance is reached, resulting in a stable local model and the optimal solution s13=[-4.8882e-6, 2.3895e-10]. The detailed procedure is listed in Table 2, where column 1 denotes the run number, column 2 is the current iterate, columns 3 to 7 denote the data set used for modeling, column 8 is the optimal result obtained at each iteration, and column 9 is the step calculated within two iterates.

Several characteristics of the IM&TO method are illustrated by this simulation. First, a good optimization direction is obtained through IM&TO, as the iterate x moves toward the optimal solution with a stable trend. Second, the method performs well from different initials. In another test, a similar process is conducted with a different initial iterate x1'=3, and the optimal solution s12=[9.4670e-005, 8.9626e-008] is ultimately obtained within 12 iterations. Third, the local model accuracy is improved significantly to describe the true process within the trust region better. As shown in Fig. 3, during the model verification, the residual decreases to a stable value from the third iteration with small oscillations as the sample data become denser with iterative modeling strategy, which indicates better resemblance.

4. APPLICATION TO INJECTION MOLDING PROCESS

Injection molding is a typical batch process to produce plastic parts at a high production rate with tight tolerances. As a major plastic processing technique for converting thermoplastic into all types of products, injection molding consists of four stages: filling, packing, holding, and cooling. For each cycle, the plastic resin is melted and then injected into a mold with the desired shape. High pressure is maintained to compensate for the shrinkage during the packing and holding stages. When the molded part is cooled and sufficiently rigid, the mold is opened, and the product is ejected. The cycle is then repeated to manufacture more products. Similar to other batch processes, quality optimization is a critical issue for successful molding. Given the machine, mold, and material, product quality is determined by the operating conditions. Optimal settings of

Table 2. Samples and iterates

runs	iterate(x)	s1	s2	s3	s4	s5	s[x*,	y]	step
1	-3	-5(s1)	2	-3	-	-	-2	32	1
2	-2	-5	2	-3	-2	-	-1	9	1
3	-1	-5	2	-3	-2	-1	-0.3653	1.2859	0.6347
4	-0.3653	-0.3653(s1')	2	-3	-2	-1	-0.2885	0.8084	0.0768
5	-0.2885	-0.3653	2	-0.2885	-2	-1	-0.2015	0.3979	0.087
6	-0.2015	-0.3653	-0.2015	-0.2885	-2	-1	0.1979	0.3994	0.3994
7	0.1979	-0.3653	-0.2015	-0.2885	0.1979	-1	0.0027	7.1838e-05	-0.1952
8	0.0027	-0.3653	-0.2015	-0.2885	0.1979	0.0027	-0.0023	5.4649e-05	-0.005
9	-0.0023	-0.0023(s1'')	-0.2015	-0.2885	0.1979	0.0027	-0.0023	5.4649e-05	0
10	-0.0023	-0.0023	-0.2015	-0.0023	0.1979	0.0027	-0.0019	3.6420e-05	0.0004
11	-0.0019	-0.0023	-0.2015	-0.0023	-0.0019	0.0027	-4.888e-06	2.3895e-10	0.0019
12	-4.888e-06	-0.0023	-4.888e-06	-0.0023	-0.0019	0.0027	-4.888e-06	2.3895e-10	0
13	-4.888e-06	-0.0023	-4.888e-06	-0.0023	-0.0019	-4.888e-06	-4.888e-06	2.3895e-10	0
14	-4.888e-06	-0.0023	-4.888e-06	-0.0023	-0.0019	-4.888e-06			

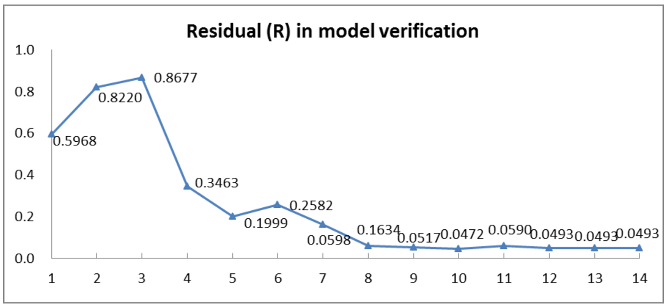

Fig. 3. Residual in model verification within trust region

the key process variables are essential to obtain quality products. The rapidly varying market requires a flexible manufacturing system with which molds and materials have to be changed frequently, resulting in difficulties in first-principle model development and application. Meanwhile, as each cycle of the injection molding process is normally short with relatively low costs, this example is suitable to demonstrate the online optimization method proposed in this project. In addition, the experiment results of MFO method under the same experimental environment is stated for comparison.

4.1 Problem Formulation

In the following experimental test, the target is to obtain the optimal settings to achieve a satisfactory quality requirement. Injection and holding are two major phases for the product quality. Thus, five process variables (operation range), including first injection pressure (90bar-120bar), second injection pressure (90bar-120bar), switch point (30%-60%), holding pressure (60bar-75bar), and holding time (5s-9s), are selected as the variables to be optimized. The weight of the product is set as the quality target variable, which is a good indication of process stability and has close relationship with other quality properties. Q_w is the desired weight, which is the quality requirement. $f(x)$ is the map between the optimized variables and the target variable. The min-max normalization is used to ensure the equal weighting of each variable during data pre-processing. As described above, the optimal setting problem, aiming at moving the weight as close as possible to the target value, can be formulated as (7).

$$\begin{aligned} &\min J = \left| f(x) - Q_w \right|^2 \\ &s.t. \quad 0 \le x_i \le 1 \quad (i = 1, 2, ..., 5) \end{aligned} \tag{7}$$

An ordinary round plastic part is chosen as the molding product, which well reflects the process characteristics. The machine used is the Hai-Tai reciprocating screw injection molding machine HTL68/JD with a shot weight of 82 g, which is a typical low-end machine with an open-loop controller. The material used is polymethyl methacrylate. During the experimental test, six random initial experiments are designed before optimization.

4.2 Results and Analysis

The experimental results are shown in Figs. 4 and 5, where Fig. 4 shows the trajectory of the optimized variables, whereas Fig. 5 plots two different optimization paths with two significantly different initial points. Fig. 4 shows that the first to the sixth iterates were considered to form the initial model with five optimized variables. After the initial model is obtained, the trust region optimization is guided consistently toward the optimal. After only six rounds of IM&TO, i.e., in the 12th iteration, the stopping criterion is met, and the optimization is terminated. The resultant product weight trajectory is shown by the solid curve in Fig. 5.

During the iteration of optimization shown in Fig. 4, iterates from the 6th to 11th iterations approach the desired target stably and rapidly, which indicates a clear optimization direction and high efficiency through the IM&TO method. The dotted curve in Fig. 5 shows the optimization procedure with a significantly different initial setting. The result again shows a consistent and efficient convergence to the target value, proving that the IM&TO works well for different initial points.

Fig.6 shows the different optimization procedures by applying MFO and IM&TO under the same experimental environment. After obtaining the same initial model with the first 6 iterates, the trajectories differ until the optimal requirement of quality weight is met, respectively. It is obvious that IM&TO method reduces the experiment cost to get the desired product, and the optimization direction is much clearer and more stable.

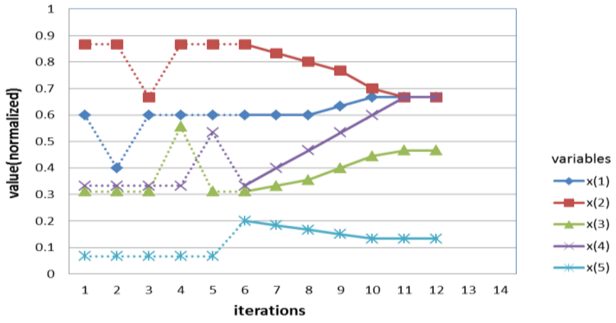

Fig. 4. Trajectories of optimized variables

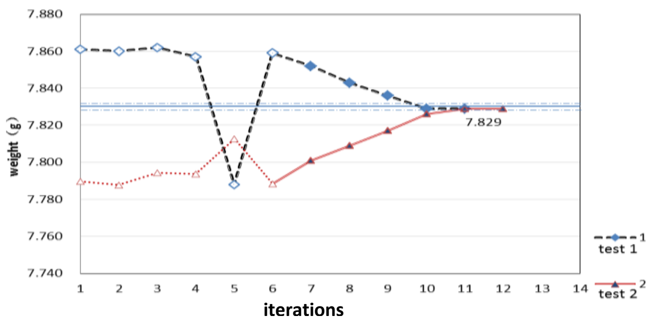

Fig. 5. Weight trajectories from different initials

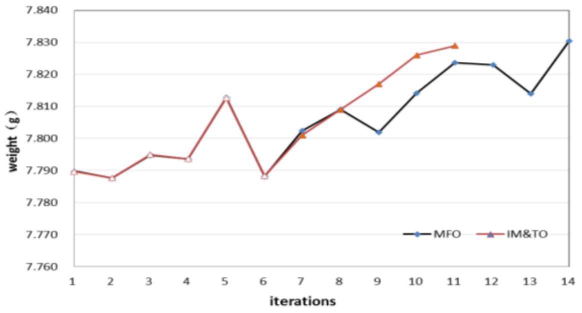

Fig. 6. Weight trajectories of IM&TO and MFO

5. CONCLUSIONS

An iterative modeling and trust-region-based optimization method for batch processes is proposed in this paper. The proposed method uses a local accurate model to guide trust-region optimization with an iterative modeling technique. The cost of solving optimization problems using the IM&TO method is reduced significantly. Moreover, the optimal direction is reliable during the iterations, and good extrapolation and performance with different initials are achieved through iterative modeling and optimization. The method has been demonstrated through a numerical simulation and an industrial example, both of which confirm the good performance of the proposed approach.

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