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Quality Analysis and Prediction for Start-up Process of Injection Molding Processes

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Abstract: As a typical batch process, injection molding process plays an important role in industry. This work focuses on the start-up process of injection molding process. Based on a deep study of the start-up process of injection molding process, a phase-shift sliding window modelling scheme is proposed in this paper for quality prediction. Firstly, to deal with the time-varying problem during the start-up process, sliding windows are built in the batch direction, and multiple continuous models are established to capture the relationship between the process variables and the quality respectively. Secondly, according to the operational characteristics of the plastication phase of injection molding process, a hypothesis that the plastication phase of the current batch has a greater impact on the quality of the next batch than the quality of the current batch is proposed, and the existence of this assumption is verified by the simulation with experimental data. Under the premise of the above assumptions, a new quality prediction scheme is proposed and is verified to be more accurate than the traditional methods.

Keywords: Multiphase batch processes, start-up process, quality prediction, injection molding process.

1. INTRODUCTION

Batch processes are widely used today for producing higher value-added products to meet rapidly changing market. Semiconductor processing, injection molding, fermentation, and most bio-processes are all batch processes in nature. Competition and demand for consistent and high-quality product have spurred the development of quality-related researches for batch processes.

As a typical batch process, injection molding process has played an important role in industry for many years. A typical injection molding process consists of four major operation phases, injection, packing-holding, plastication and cooling. First, molten plastic is injected into the mold, second, the material is packed and held in the mold under pressure, and at last the plastic is cooled down in the mold until the part becomes sufficiently rigid for ejection, during the early part of which plastication phase takes place in the barrel, where polymer is melted and conveyed to the barrel front by screw rotation, preparing for next cycle.

Significant efforts have been made for the development of methods for quality prediction, among which, multivariate statistical modelling is widely used as it is derived directly from historical data with little prior process knowledge, and it has superior ability in handling high-dimensional and correlated process data. Multi-way partial least square (MPLS) (Nomikos et al. (1995)) models were first proposed using the whole process variables to build the model for quality prediction. After, critical-to-quality time periods were focused to enhance the prediction accuracy (Duchesne et al. (2000)). Considering the multiplicity of phases, phase-based statistical modelling methods were developed to improve the performances of process analysis and quality control, and after that many works have been done (Lu et al. (2005), Zhao et al. (2008), Ge et al. (2014), Zhao et al. (2014a)). Recently, based on the understanding that previous phases may have influence on the following phases as well as the final process qualities, all the critical-to-quality phases were connected by the regression residuals of the phase-based recursions in the quality-regression modelling (Zhao et al. (2017)), which is called a phase-based recursive statistical quality regression method.

Besides the process variation along the time direction within a batch, the process variation along the batch direction within a whole process has also drawn researchers' attention. In batch processes, the process variation in the batch direction throughout the whole operation leads to different process states with different process characteristics. Some techniques have been proposed to handle process variations by model adaptation (Lee et al. (2003), Lee et al. (2005)). The batch process can be divided into different periods of which the process characteristics are constant and time-varying, respectively. In the slow time-varying batch process, the relationship between the batch process variables and the quality variables is not basically the same all the time, but varies as the batch operation progresses or process mechanism characteristic changes (Zhao et al. (2014b)). Distant batches have different process variable trajectories, operating patterns, and correlation characteristics. In the start-up process of injection molding processes, the variation is serious and difficult to analyze. However, few works have been done focused on the start-up process. To deal with this, a natural idea is to divide the whole batch operation into various windows. Each window obtains a series of continuous batches. Then those different models respectively analyze the potential essential characteristics. Therefore, sliding windows are built in the batch direction, and multiple

continuous models are established to capture the relationship between the process variables and the quality respectively.

Moreover, in traditional phase-based modelling methods for batch processes, phases within a batch are analyzed together with the corresponding quality of the batch to find out how the process variables of the phases influence the final quality. Although many modelling strategies have been proposed to solve different problems, the accordance between the process variables of the phases and the final quality has never been broken in the analysis of batch processes. However, with a deep understanding of batch process characteristics, it should be noticed that batches are successive and not necessary to be physically divided during a whole process, and although the concept of phase or batch division is helpful for operation and understanding, it is superficial. As a part of the whole process, previous batches definitely can influence and provide useful information for the subsequent batches. Thus, it is reasonable to believe that the previous batches or phases may influence the quality of the subsequent batches and should be involved in the modelling. Further, in some batch processes, due to process characteristics such as process mechanism or time delay, the process variables of some certain phases may have greater impact on the quality of the next batch than the current batch. Particularly, for the injection molding process, the plasitication phase should have significant influence on the final quality of the next batch because of the physical meaning of this phase that it takes place in the barrel and the polymer is melted and conveyed to the barrel front by screw rotation, preparing for next batch cycle. Therefore, in this paper, based on the characteristic of the injection molding process, a phase-shift model development strategy is proposed, where the relationship between the process variables of previous batches and the quality of the current batch, and both the process variables of the previous and the current batch are involved in the quality prediction for the current batch.

So in this paper, aiming at the start-up process of injection molding processes, a phase-shift sliding window modelling scheme is proposed. The sliding window method is used to divide the batches of the whole process into successive groups of windows in batches, and then performs quality analysis and prediction for each window. Furthermore, according to the operational characteristics of the plastication phase, a hypothesis of that the plastication phase of the current batch has a greater impact on the quality of the next batch than the quality of the current batch is proposed, and the existence of this assumption is verified according to the simulation with experimental data. The simulation also illustrates the feasibility and performance of the proposed algorithm.

The rest work of this paper includes the following aspects: First, the proposed method is presented in Section 2, including critical-to-quality phase identification, sliding window model development, and phase-shift model development. In Section 3, the application of the proposed method to a real injection molding start-up process is presented and discussions are conducted based on the illustration results. At last, the conclusion is drawn.

2. METHODOLOGY

2.1 Critical-to-quality phase identification

Due to the multi-phase characteristic, each batch cycle is divided into multiple phases by indicator variables. Knowledge of the concrete process and basic process analysis may be necessary to decide the indicator variables. Also, it is assumed the batches considered have even durations for each phase within different batch cycles. If not, some data alignment technology would be necessary to make the corresponding phases from different batches have the same number of sample points.

If one phase has significantly contributed to the final qualities, a strong relationship exists between the process variables in this phase and the corresponding quality index. Therefore, a quality regression model which well reflects such relationship can provide good predication results. Thus, the fitness of time-slice models has been utilized to judge if the process variables of each time interval have significant impact on the final quality in previous works (Lu et al. (2005)). The multiple coefficient of determination is utilized to evaluate the prediction precision of each time-slice model.

In this part, first, the time-slice-based regression model is established and then the index is calculated to evaluate the prediction precision of each time-slice model. The mean of the index of all the time-slice models in a phase is taken as the magnitude of the effect of that phase. The details are presented below.

First, a time-slice quality regression model is built between the process variables of that time slice and the final qualities. Batch process data are usually collected as a three-dimensional matrix $\underline{\mathbf{X}}(I \times J_x \times K)$, where I refers to the number of batches, J_x refers to the number of process variables and K refers to the sample times within each batch. The measurements of J_y final quality variables in I batches are summarized into a matrix $\underline{\mathbf{Y}}(I \times J_y)$. The variables are first centered and scaled across the batches. After that, the process data and the final qualities are denoted as $\mathbf{X}(I \times J_x \times K)$ and $\mathbf{Y}(I \times J_y)$. $\mathbf{X}$ is decomposed along the time axis to obtain k time-slice matrices $\tilde{\mathbf{X}}_k(I \times J_x)$ $(k = 1, 2, ..., K)$. The correlation between the process variables and the quality variables can be extracted from matrices $\tilde{\mathbf{X}}_k$ and $\mathbf{Y}$. By applying PLS, the time-slice PLS model is achieved as below:

$$\tilde{\mathbf{X}}_k = \tilde{\mathbf{T}}_k (\tilde{\mathbf{P}}_k)^{\mathrm{T}} + \mathbf{E} \tag{1}$$

$$\mathbf{Y} = \tilde{\mathbf{U}}_k (\tilde{\mathbf{Q}}_k)^{\mathrm{T}} + \mathbf{F} \tag{2}$$

The above model can be abbreviated to the regression form as

$$\hat{\mathbf{Y}}_k = \tilde{\mathbf{X}}_k \tilde{\Theta}_k \tag{3}$$

where $\tilde{\mathbf{T}}_k$ and $\tilde{\mathbf{U}}_k$ are the score matrices, $\tilde{\mathbf{P}}_k$ and $\tilde{\mathbf{Q}}_k$ are the loading matrices, $\mathbf{E}$ and $\mathbf{F}$ are the residual matrices, $\tilde{\Theta}_k$ is the regression parameter matrix, and $k = 1, 2, \ldots, K$, K is the total number of time-slices. When a single quality variable $\mathbf{y}(I \times 1)$ is considered, the regression model is

$$\hat{\mathbf{y}}_k = \tilde{\mathbf{X}}_k \boldsymbol{\beta}_k \tag{4}$$

where $\boldsymbol{\beta}_k$ is the regression parameter.

Then, the multiple coefficient of determination, R_k^2, is utilized to evaluate the prediction precision of the kth time-slice model and reflect the regression fitness of the model:

$$R_k^2 = \frac{\sum_{i=1}^{I} (\hat{y}_{i,k} - \bar{y})^2}{\sum_{i=1}^{I} (y_i - \bar{y})^2} \tag{5}$$

where y_i is the measurement of the final quality of the ith batch, $\bar{y}$ is the average of measurements of the final quality of I batches, $\hat{y}_{i,k}$ is the quality prediction for the kth time-slice in the ith phase. R_k^2 ranges from 0 to 1. A larger R_k^2 indicates a better model prediction.

Within the cth phase, the average phase R^2 index of phase c is calculated based on R_k^2 within the phase,

$$\bar{R}_c^2 = \frac{1}{K_c} \sum_{k=1}^{K_c} R_k^2 \tag{6}$$

where K_c is the number of the time intervals within phase c.

2.2 Sliding window model development

In this part, the slow time-varying batch process is divided into different windows along the batch direction to capture their different characteristics by different models reasonably. To achieve this, sliding window model building method is utilized.

As shown in Fig. 1, the left is the process variable matrix $\mathbf{X}(I \times J_x \times K)$ and the right is the quality variable matrix $\mathbf{Y}(I \times J_y)$. The batch direction i is from the top to the bottom, i=1, 2,…, I. The time direction k is from the left to the right, k=1, 2,…, K. The direction perpendicular to the paper represents the direction of variables, which is omitted in this figure for brevity. In view of the characteristics of the slow time-varying processes, it can be approximated that the relationship between process variables and quality variables is the same in the adjacent batches, while the characteristics of the distant batches are different. First, the length of the window I_w is set properly to cover enough but close batches within a window to obtain accurate models. Then, the moving distance of the sliding window, L, is determined, which represents how many batches the sliding window moves downward relative to the previous sliding window. L determines the total number of windows to build and should be decided carefully not to make the computation load too heavy. To ensure that all batches are included at least by one sliding window, the value of L should be less than I_w. Concretely, Window 1 consisting of I_w batches starts from the first batch and ends at the I_w batch. Then, the sliding window moves down L batches, and Window 2 is obtained. Each time L batches are slid through until the last batch is covered in the window, resulting in N windows.

Within the nth window, a PLS model can be built between the process variables and the final quality variables. Consequently, the average phase R^2 index can be calculated. It should be noticed that in Fig. 1, only one individual phase is considered to focus on the time-varying characteristic rather than the multi-phase characteristic, that is, the relationship between the process variables within the cth phase and the final quality variable is captured individually but the phase predictions need to be connected together when obtaining the final prediction.

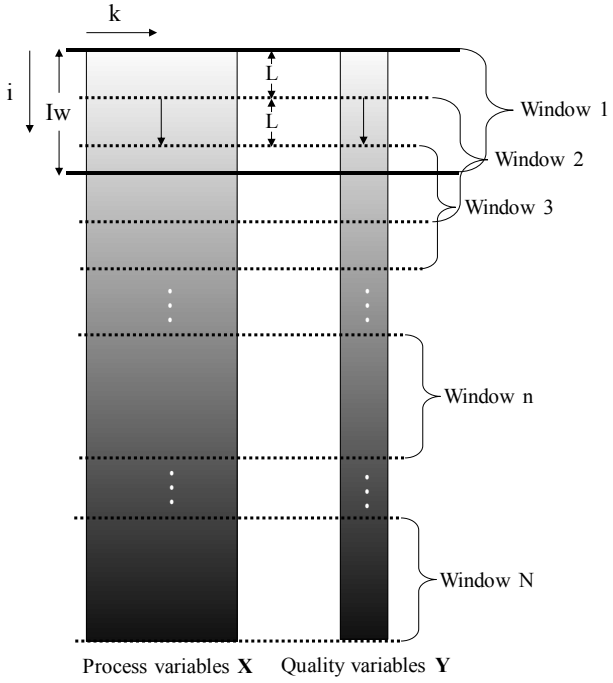

Fig. 1. Schematic diagram of sliding window model development.

2.3 Phase-shift model development

In this part, a novel modelling strategy is developed for the injection molding process, where one phase is shifted along the batch direction. The main idea is to capture the relationship between the process variables of a phase belonging to the previous batch and the final quality of the current batch, since that phase may have more important influence on the final quality than the phase belonging to the current phase.

The sliding model development has been illustrated in Fig.1 by one phase. For multiple phases, several models are built in a repeated way in traditional methods. In this part, in order to

predict the quality accurately, the corresponding relation between the process variables and the quality variables in the sliding window model can be adjusted accordingly. That is, the process variables of one phase belonging to the previous batch are shifted to the current batch and matched with the quality of the current batch. In Fig. 2, the phase-shift modelling strategy is shown. It is assumed that a batch process has such characteristics at phase A which needs to shift. Set the start time slice for this phase A to be k = a, and the width of the phase is d time slices. First, move the process variables at this phase down by one batch along the batch direction, so that the relationship between the process data of the last batch at the phase A and the quality of the current batch will be captured and analyzed. Then, the data which cannot constitute a complete batch are eliminated, and a new process variable matrix $\mathbf{X}_{new}$ and quality variable matrix $\mathbf{Y}_{new}$ are formed. So the sliding window method in the last section can be used on these new matrices to build quality prediction model for analysing and predicting the quality. Finally, after building model for each phase concerned, overall quality prediction can be obtained based on the phase predictions.

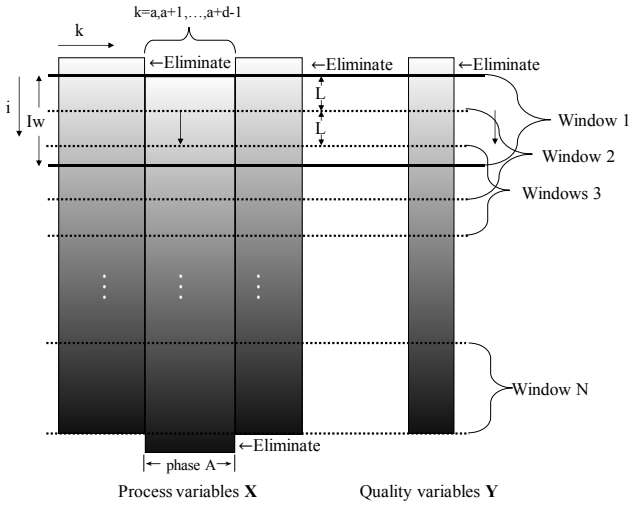

Fig. 2. Schematic diagram of phase-shift model development.

3. ILLUSTRATION AND DISCUSSION

3.1 Process description

The proposed algorithm is illustrated by the stat-up process of a real injection molding processes. All key process conditions can be online measured by their corresponding transducers. One dimension index, weight (g) is chosen to evaluate the product quality since the product weight is a direct index of quality defect such as flash or hollow. The material used in this work is high-density polyethylene (HDPE). Six process variables and one quality variable as shown in Table 1 are selected for modelling. Servo valve 1 (SV1) and servo valve 2 (SV2) are connected to the barrel and injection cylinder. Critical variables are used for quality prediction.

Table 1. Process variables for injection molding process

Process No.	Description	Unit
1	Nozzle temperature	℃
2	Screw velocity	mm/s
3	Injection cylinder pressure	Bar
4	Plastication pressure	Bar
5	SV1 opening	%
6	SV2 opening	%
Quality No.	**Description**	**Unit**
1	Weight	g

3.2 Phase division and sliding window parameter selection

As introduced before, phase division is implemented to divide a batch cycle into phases. Using indicator variables, each batch cycle can be divided into four phases. The process variables, screw velocity and SV1 opening are chosen to be indicator variables based on process knowledge. When the value of screw velocity is greater than zero, it means the screw moves forward, revealing the starting of one batch cycle. Meanwhile, SV1 opening can be used to indicate the end of the main part of a batch cycle. Screw velocity can indicate the switch points of phases. In Fig. 3, the phase division results are shown where the four phases (I–IV), injection, packing-holding, plastication and cooling, are separated from each other.

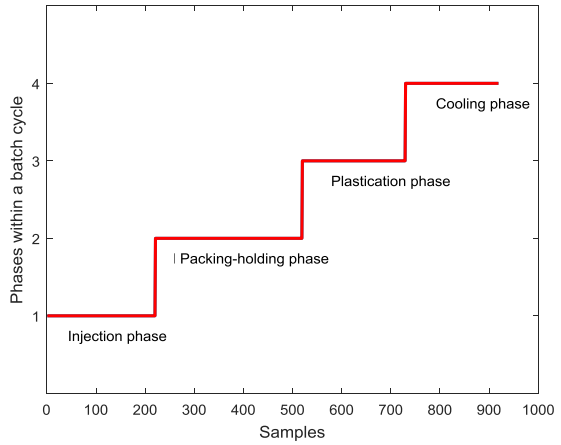

Fig. 3. Final results of phase division within a batch cycle.

In this paper, we set the width of the sliding window I_w = 20, the number of batches that slide down each time is L = 1. According to the number of batches obtained by the experiment I = 100, the total number of windows is N = 81.

3.3 Critical-to-quality phase identification

After window division, in each window, the time-slice-based model is established and then R^2 index is calculated to identify the contribution of each time-slice to the quality. Calculate the mean of the indexes in each phase. Three of these windows are selected and shown in Fig. 4.

As can be seen from the figures, in each window the mean values of R^2 within the four phases are different, so the contribution rate shows a phase characteristic change.

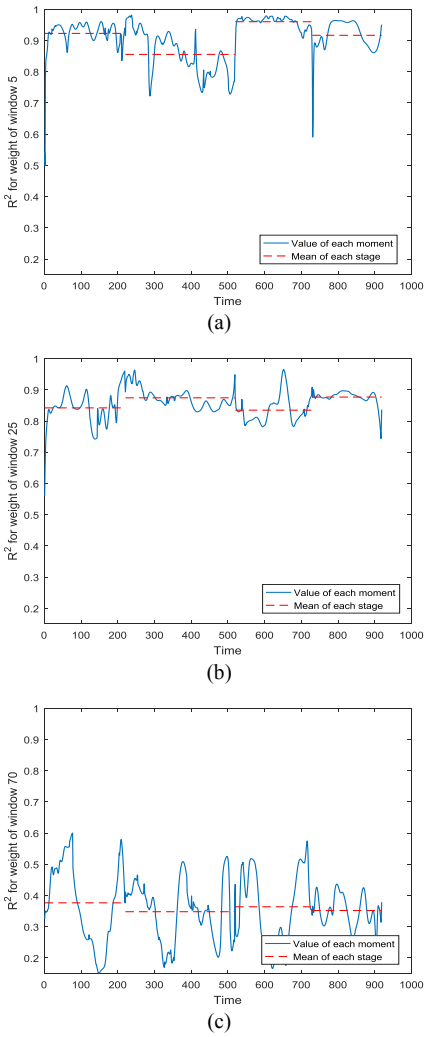

Fig. 4. R^2 index of different windows.

3.4 Online quality prediction

In the third phase of the injection molding process, namely plastication phase, melt fluid in the screw was not fully into the casting mold during the current batch. There is a large part of the material gathered in the screw waiting for the next batch of mold injection. Naturally, it can be assumed that the impact of this phase on the quality of the next batch will be greater than the current batch.

Two sliding window models are utilized to calculate the multiple coefficient of determination R_c^2 to show the influence of the plastication phase on the quality of the current batch (case 1) and the next batch (case 2). Two groups of windows, window 35 and 75 are selected to show the comparison, as shown in Fig. 5. In Table 2, the mean R_c^2 of the two cases are compared, represented by the two sets of windows and all windows. It can be seen that the mean R_c^2 of case 2 are higher than corresponding ones of case 1, which means that the influence of the plastication phase on the next batch is greater than that on the current batch.

Fig. 6 is the results of quality prediction of three types of methods, the traditional method without sliding windows, the sliding window method without phase-shift, and the proposed phase-shift sliding window method. Among them, the solid line is the measurement of quality, and the dotted line is the predictive value of quality. In addition, the root mean square error (RMSE) between the predicted and actual values of the quality is calculated as shown in Table 3. Obviously, the RMSE of the two methods using the sliding window method is much smaller than that of the traditional method without batch division. And for the characteristics of the plastication phase, the improved new sliding window method has the least RMSE. Therefore, it can be concluded that the proposed method is better than the traditional PLS methods.

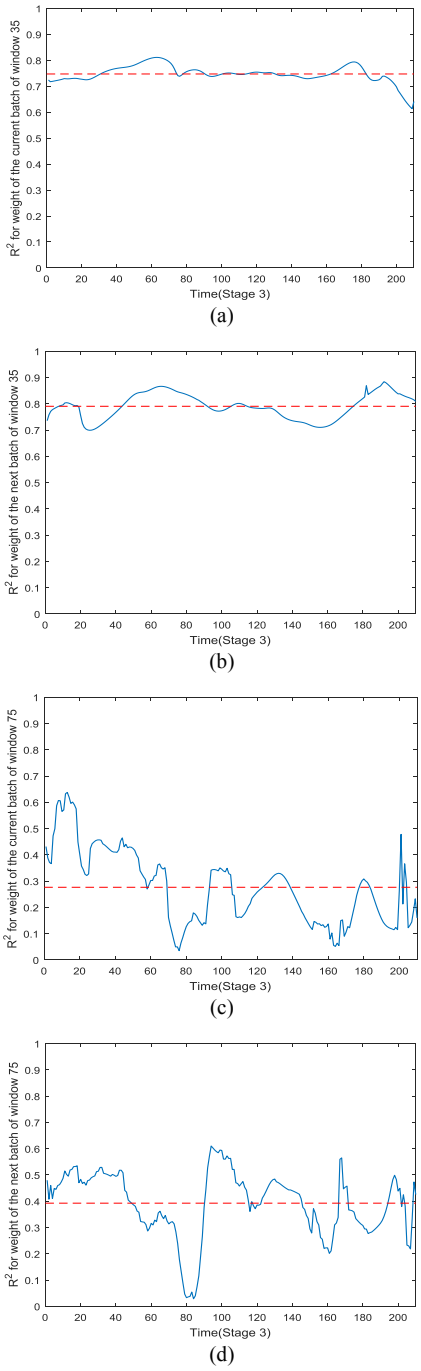

Fig. 5. Contrast diagram of the influence of the plastication phase.

Table 2. Comparison of mean R_c^2 of plastication phase

Window	Current Batch	Next Batch
35	0.7473	0.7903
75	0.2765	0.3926
all	0.6611	0.6823

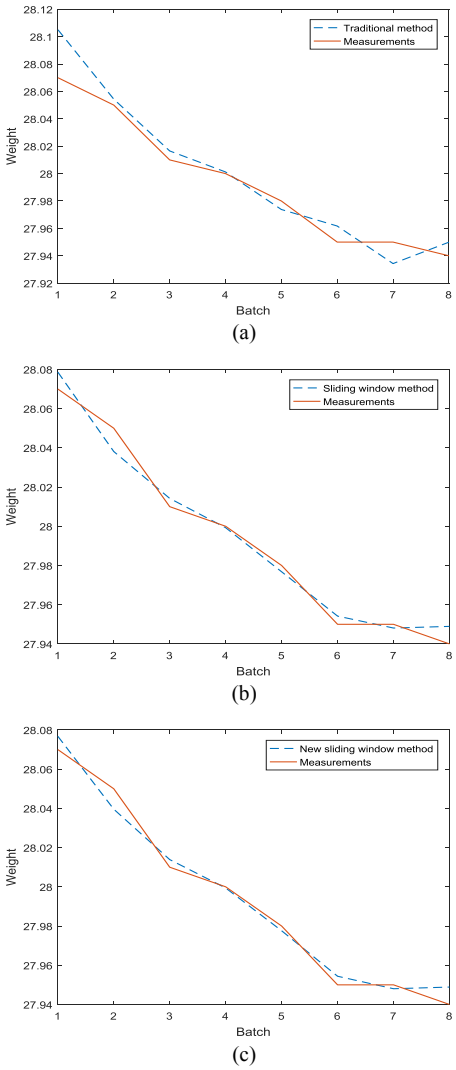

Fig. 6. Final quality prediction results for test batches.

Table 3. Comparison of RMSE of the three methods

Method	RMSE
Traditional	0.0150
Sliding window	0.0066
New sliding window	0.0059

4. CONCLUSION

In this paper, a phase-shift sliding window model is established based on the characteristics of the start-up process of injection molding processes. The sliding window model is used to capture the time-varying characteristics along the batch direction. In addition, according to the characteristic of the plastication phase that the variable impact on the quality of the next batch is greater than the quality of the current batch, a phase-shift modelling method is proposed. In the application to a real injection molding process, it is verified that the proposed method is more accurate than traditional methods. The obtained prediction result will be used for self-regulation of the process, which is the work in the future.

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