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Periodic Learning of B-spline Models for Output PDF Control: Application to MWD Control

H. Wang*, J. F. Zhang and H. Yue

***Abstract*—Periodic learning of B-spline basis functions model for the output probability density function (PDF) control of non-Gaussian systems is studied in this paper using the recursive least square algorithm. Within each control interval, the basis functions are fixed and the control input design is performed that controls the shape of the output PDFs. However, between each control interval, periodic learning techniques are used to tune the shape of the basis functions. This has been shown to be able to improve the accuracy of the B-spline approximation model. As such, the overall B-spline model of the output PDFs becomes a dual-model related to both time and space variables. The algorithm has been applied to a simulation study of the molecular weight distribution (MWD) control of a styrene polymerization process, leading to some interesting results.**

I. INTRODUCTION

In recent years, the control of the whole shape of the output probability density function (PDF) has been studied in response to the increased demand from many practical systems. The typical processes include the web solid distribution control in papermaking [1], the particle size distribution (PSD) control in milling processes [2,3,4,5], and the molecular weight distribution (MWD) control [6,7,8] and particle size distribution control [9,10,11] in polymerization processes.

For this type of systems, the actual controlled output is the shape of the output probability density functions and the inputs are only related to time (such as flow rate and valve opening, etc). In this regard, the following partial differential equation (PDE) can be generally used to represent the dynamical evolution of the output PDFs

$$0 = \xi\left(\frac{\partial^n \gamma}{\partial y^n}, \frac{\partial^{n-1}\gamma}{\partial y^{n-1}}, \cdots, \frac{\partial \gamma}{\partial y}, \gamma, \frac{\partial^m \gamma}{\partial t^m}, \frac{\partial^{m-1}\gamma}{\partial t^{m-1}}, \cdots \frac{\partial \gamma}{\partial t}\right) \quad (1)$$

where $\xi(\cdots)$ is a general nonlinear function and $\gamma(\cdot)$ denotes the output PDF. This PDE model is a general expression of many population balance equations such as the following widely used particulate system model [12]

$$\frac{\partial W(\zeta,t)}{\partial t} + \frac{\partial[k(\zeta,t)W(\zeta,t)]}{\partial \zeta} = h(\zeta,t) \quad (2)$$

where t is time; ζ is the internal coordinate; $W(\zeta,t)$ is the number density of particles; $k(\zeta,t)$ is the particle growth rate; and $h(\zeta,t)$ is the net creation of particles.

Direct use of the PDE model is difficult in practice in that either such a model is difficult to establish through the first principle approaches due to the complicated nature of the process, or the obtained control algorithms are too complicated to be applied in the real-time situations. To solve this problem, the B-spline approximation to $\gamma(\cdot)$ has been proposed since 1998 as one of the main groups of methods to control the output PDFs for non-Gaussian stochastic systems [13,14,15]. The idea is to use a set of fixed basis functions together with a group of time-varying weights to approximate the output PDFs at each time instant. The control input can therefore be designed to simply control the weights in the time-domain. This is equivalent to solving a PDE model by using the separation of variables technique with a fixed set of basis functions. That is, there are no space related differential equations in terms of the evolution of the shape of the basis functions. Several B-spline models have been developed ever since and have been shown capable of controlling the output PDFs to a good accuracy [16,17,18,19], albeit the number of B-spline basis functions can be quite high for complicated output PDF shapes and the accuracy to the PDF tracking may not be guaranteed. Since the PDF of a process can vary widely over operation, it may be difficult to capture the behaviour over an extended operating period with fixed basis functions. As a result, it would be ideal if the basis functions can be regularly updated according to the output PDF changes during the control process.

In this paper, the periodic learning and repetitive control are combined to perform the tuning of the basis functions for the output PDF control. In this context, the control horizon is divided into a number of intervals $\left[(j-1)(T+\Delta T), j(T+\Delta T)\right]$ $(j=1,2,\cdots)$ with T being the control interval length and ΔT being the time period to tune

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*H. Wang, the corresponding author, is with the Control Systems Centre, The University of Manchester, Manchester, M60 1QD, United Kingdom hong.wang@umist.ac.uk

J. Zhang is with the Institute of Automation, Chinese Academy of Sciences, Beijing 100080, China jinfang.zhang@mail.ia.a.cn

H. Yue is with the Institute of Automation and the University of MAnchester, Manchester M60 1QD, United Kingdom h.yue@umist.ac.uk

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the B-spline basis functions. Within each interval $\left[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T\right]$, the linear B-spline functions with FIXED basis functions are used to generate the required control inputs that control the output PDF shape. In the interval $\left[jT+(j\text{-}1)\Delta T, j(T+\Delta T)\right]$, the basis functions are updated to obtain a better approximation accuracy to the output PDFs. Such a set of updated basis functions will be used as the fixed basis functions for the next control interval. This means that the basis functions are tuned periodically and the following figure shows such a tuning phase.

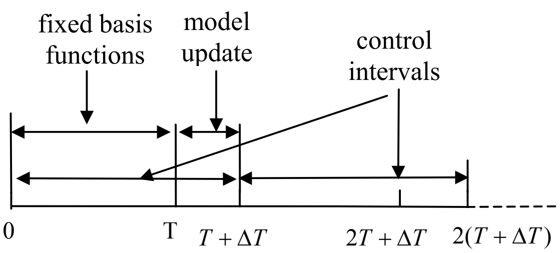

Fig. 1. Illustrative tuning principle

To start with, in the period of [0,T] the control inputs are designed with a set of FIXED B-spline functions, whereby the control is realized via the control of the weights in the B-spline approximation. When the sample time reaches T, the tuning of the basis functions is activated. This will last for a period of ΔT, during which the control law stays the same as that of [0, T]. This enables the tuning to be focused on the basis functions and the parameters of the weights dynamics. Once the tuning is completed, the second control interval will start from the sample instant T+ΔT by using the updated basis functions and the model parameters. This process will repeat until the end of control horizon is reached.

II. Model presentation

Assume that the output PDF of the considered stochastic systems, $\gamma_k(y,j)$, is defined in a known interval denoted by [a, b] (i.e. $y\in[a,b]$). In this paper, the following linear B-spline function model [15] will be used to represent the dynamic relationship between the inputs and the output PDFs for each control instant k $\in\left[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T\right]$

$$\begin{cases} V_k^j = G^j V_{k-1}^j + H^j u_{k-1}^j \\ \gamma_k(y,j) = C(y,j)V_k^j + L(y,j) \end{cases}$$
$$j=1,2,\cdots;\quad k=1,2,\cdots \tag{3}$$

where $V_k^j\in R^{n-1}$ is the weights vector that groups all the independent weights in the B-spline model; n is the number of basis functions chosen for approximation; u_{k-1}^j is a scalar input to the system; G^j and H^j are the parameter matrices which represent the system dynamics for k $\in\left[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T\right]$. As presented in [15], let $B_i(y,j)$ (i = 1, 2, …, n) stand for the fixed basis functions for the *j*th control interval satisfying

$$b_i^j = \int_a^b B_i(y,j)dy \qquad i=1,2,...n;\ j=1,2,... \tag{4}$$

then in equation (3)

$$L(y,j) = \frac{B_n(y,j)}{b_n^j} \tag{5}$$

$$C(y,j) = \left[B_1(y,j) - \frac{b_1^j}{b_n^j}B_n(y,j),\quad B_2(y,j) - \frac{b_2^j}{b_n^j}B_n(y,j),\right.$$
$$\left. \cdots,\quad B_{n-1}(y,j) - \frac{b_{n-1}^j}{b_n^j}B_n(y,j) \right] \tag{6}$$

To simplify the following expression, denote

$$f_k(y,j) = \gamma_k(y,j) - L(y,j) \tag{7}$$

then the model in (3) can be further expressed in a one-step-ahead input and output form to read

$$f_{k+1}(y,j) = a_1^j f_k(y,j) + \cdots + a_{n-1}^j f_{k-n+2}(y,j) + C(y,j)D_0^j u_k^j$$
$$+C(y,j)D_1^j u_{k-1}^j + \cdots + C(y,j)D_{n-2}^j u_{k-n+2}^j \tag{8}$$

a_i^j ($i=1,\cdots,n-1$) and D_l^j ($l=0,\cdots,n-2$) are the parameters and parameter vectors formulated from the state space model of equation (3) using information of G^j and H^j for k $\in\left[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T\right]$. Similar to G^j and H^j, a_i^j and D_i^j are fixed within each control interval. However, their values are updated simultaneously with the tuning of the basis functions. The following performance function is used to measure the functional distance between the output PDF and the target PDF $g(y)$ (also defined on [a, b])

$$J^j = \int_a^b (\gamma_{k+1}(y,j) - g(y))^2 dy \tag{9}$$

where $\gamma_{k+1}(y,j)$ is the output PDF of the stochastic system at time instant $k+1$ for the *j*th control interval. To minimize J^j, u_k^j can be obtained by solving

$$\frac{\partial J^j}{\partial u_k^j} = 0 \tag{10}$$

to give the following feedback format

$$u_k^j = \frac{\int_a^b C(y,j)D_0^j \breve{g}(y,j)dy}{\int_a^b \left(C(y,j)D_0^j\right)^2 dy} \tag{11}$$

where

$$\tilde{g}(y,j) = -\sum_{i=2}^{n-1}\left(a_i^j f_{k-i+1}(y,j) + C(y,j) D_{i-1}^j u_{k-i+1}^j\right) - L(y,j) + g(y) - a_1^j f_k(y,j) \quad (12)$$

This control law can be used together with the measured output PDFs so as to formulate a set of necessary information for the update of the basis functions as well as a_i^j and D_l^j within the jth tuning period $\left[jT+(j\text{-}1)\Delta T, j(T+T\Delta)\right]$.

III. UPDATE BASIS FUNCTIONS AND { a_i^j , D_l^j }

Assume that the control function (11) is applied to the system for k∈ $[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T]$, then according to figure 1 the update of the basis functions and { a_i^j , D_l^j } should take place in $\left[jT+(j\text{-}1)\Delta T, j(T+\Delta T)\right]$. For such an update, the information available should be

$$\Omega = \{f_{k+1}(y,j), a_i^j f_{k-i+1}(y,j), D_0^j u_k^j, D_1^j u_{k-1}^j, \cdots, D_{n-2}^j u_{k-n+2}^j\} \quad (13)$$

It is also important to note that in $\left[jT+(j\text{-}1)\Delta T, j(T+\Delta T)\right]$, the control inputs are still calculated using (11) with the same set of basis functions and parameters { a_i^j , D_l^j } for the jth control interval $[(j\text{-}1)(T+\Delta T), jT+(j-1)\Delta T]$, where Ω should satisfy equation (8).

Denote

$$T_k(y,j) = f_{k+1}(y,j) - \sum_{i=1}^{n-1} a_i^j f_{k-i+1}(y,j) \in R^{1\times 1} \quad (14)$$

$$\Pi_k^j = \left[\Pi_k^j(1) \quad \Pi_k^j(2) \quad \cdots \quad \Pi_k^j(n)\right]^T \in R^{n\times 1} \quad (15)$$

$$\pi(y,j) = [C(y,j) \quad L(y,j)] \in R^{1\times n} \quad (16)$$

$$\Pi_k^j(i) = D_0^j(i)u_k^j + D_1^j(i)u_{k-1}^j + \cdots + D_{n-2}^j(i)u_{k-n+2}^j, \quad i = 1,2,\cdots,n-1 \quad (17)$$

$$\Pi_k^j(n) = 1 \quad (18)$$

where $D_l^j(i)\,(l = 0,1,\cdots,n-2)$ is the ith component of vector D_l^j. Using the above notations and by fixing { a_i^j , D_l^j }, equation (8) becomes

$$T_k(y,j) = \pi(y,j)\Pi_k^j \in R^{1\times 1} \quad (19)$$

This is a linear model where the update of $\pi(y,j)$ should take place by using the data collected during [(j-1) (T+ ΔT), jT+ (j-1) ΔT]. Similar to the scanning parameter estimation technique used in [15], a set of y_p are selected from the [a, b] interval for p = 1, 2, …., M, so that the following equation hold for each y_p

$$T_k(y_p,j) = \pi(y_p,j)\Pi_k^j, \quad p = 1,2,....,M \quad (20)$$

where M is a pre-specified positive integer. As $T_k(y_p,j)$ and Π_k^j are available at jth interval, $\pi(y_p,j+1)$ for the (j+1)th control interval can be directly updated by using a standard least square identification, leading to the following recursive least square algorithm:

$$\pi(y_p,j+1)^T|_{k+1} = \pi(y_p,j+1)^T|_k + \frac{P(k)\Pi_k^j e(k,y_p)}{1+\Pi_k^{jT}P(k)\Pi_k^j} \quad (21)$$

$$e(k,y_p) = T_k(y_p,j) - \pi(y_p,j+1)|_k \cdot \Pi_k^j \quad (22)$$

$$P(k) = P(k-1) - \frac{P(k-1)\Pi_k^j\Pi_k^{jT}}{\Pi_k^{jT}P(k-1)\Pi_k^j}P(k-1) \quad (23)$$

$$k = 1,\cdots,N; \quad p = 1,2,\cdots M$$

where N is the number of sampling points along the time axis [$(j-1)(T+\Delta T)$, $jT+(j\text{-}1)\Delta T$]; $\pi(y_p,j+1)^T|_k$ is the updated value of $\pi(y_p,j+1)^T$ at sample instant k. The initial value of $\pi(y_p,j+1)$ is evaluated from the most recent fixed basis functions and $P(0) = 10^{3-6}I_n$.

The procedures for the update of the B-spline functions (namely in the form of $\pi(y_p,j+1)$) is therefore given by:-

1. At sample time k, collect $T_k(y,j)$ and Π_k^j at the j th control interval;
2. Use equations (21)-(23) to calculate $\pi(y_p,j+1)$ with $p = 1,2,...M$;
3. Increase k by 1 and go back to step 1 until $k = N$. Here N is the number of data pairs sampled at each control interval.

Once the basis functions are updated, the next scan for the jth interval should be implemented to update the model parameters { a_i^j , D_l^j }. This can also be realized by the recursive least square algorithm. For this purpose, denote

$$\theta^j = \left[a_1^j,\cdots,a_{n-1}^j, D_0^j(1),\cdots,D_0^j(n-1),\cdots,D_{n-2}^j(1),\cdots, D_{n-2}^j(n-1)\right]^T \in R^{1\times(n^2-n)} \quad (24)$$

$$\phi(y,j,k) = \left[f_k(y,j),\cdots,f_{k-n+2}(y,j), u_k^j C_1(y,j),\cdots,u_k^j C_{n-1}(y,j), \cdots, u_{k-n+2}^j C_1(y,j),\cdots,u_{k-n+2}^j C_{n-1}^j(y,j)\right]^T \in R^{(n^2-n)\times 1} \quad (25)$$

where $\phi(y,j,k)$ is composed of the updated basis functions. As a result, the modification of θ^j is carried out using the following algorithm:

$$\theta^{j+1}(k+1) = \theta^{j+1}(k) + \frac{P_P(k)\phi(y_p,j,k)e_p(k,y_p)}{1+\phi(y_p,j,k)^T P_P(k)\phi(y_p,j,k)} \quad (26)$$

$$e_p(k,y_p) = f_{k+1}(y_p,j) - \theta^{j+1}(k)^T \phi(y_p,j,k) \qquad (27)$$

$$P_p(k) = \left(I - \frac{P_P(k-1)\phi(y_p,j,k)\phi(y,j,k)^T}{1+\phi(y_p,j,k)^T P_P(k-1)\phi(y_p,j,k)}\right)P_P(k-1) \qquad (28)$$

where $P_p(0) = 10^{3-6} I_{n\times(n-1)}$, the initial value of θ^{j+1} is the value of θ used in the j th control interval.

The procedures used to update the parameter vector θ^{j+1} can be summarized as follows:

1. At sample instant k (=1, 2, $\cdots$, N), formulate $f_{k+1}(y_p,j)$ and $\phi(y_p,j,k)$;
2. Calculate $\theta^{j+1}(k)$ for $p=1,2,...,M$ with equations (26)-(28);
3. Increase k by 1 and go back to step 1 until $k=N$.

The control and tuning of basis function and parameters can be illustrated in figure 2.

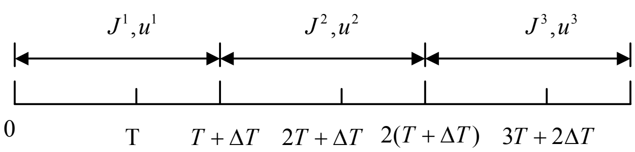

Fig. 2. The control and parameters modification time series

The complete updating algorithm can be summarized as follows:

Step1: During [0, T], the closed-loop system uses a set of fixed basis functions and parameter vector θ to realize the control action as described in (11), where the data (namely u_k and $f_{k+1}(y)$) are stored for the updating operation of the basis functions;

Step2: From the time instant T to T+ ΔT, the saved data are used to calculate the B-spline basis functions with equations (21)-(23).

Step3. Using the updated B-spline basis functions in step 2, the saved data of [0, T] are used again to tune the model parameters via equations (26)-(28).

During step 2 and step 3, the system is controlled with the same model parameters and B-spline functions as those in [0, T];

The procedure will carry on until the pre-specified control horizon ends. This constitutes a periodic learning process, which regularly updates the basis functions and the model parameters for the weight dynamics.

IV. A SIMUATION STUDY OF MWD CONTROL

The proposed algorithm is applied to a simulation example of an MWD control system. The process of interest is a styrene bulk polymerization reaction in a pilot-plant continuous stirred tank reactor (CSTR) as shown in figure 3, in which styrene is the monomer for polymerization and azobisisobutyronitrile is used as the initiator. These two flows are injected into the CSTR with the ratio adjusted by a pump. The energy for the reaction is provided by the heated oil in the CSTR's jacket and the oil temperature is controlled to be constant. The total flow rate to the system, F, is composed of the flow of monomer, F_m, and the flow of initiator, F_i, i.e., $F = F_m + F_i$. The monomer input ratio is defined as $C = \frac{F_m}{F}$. In this work, adjustment of C is considered to be the means to control the MWD of the polymer. The model of this system can be seen in [20].

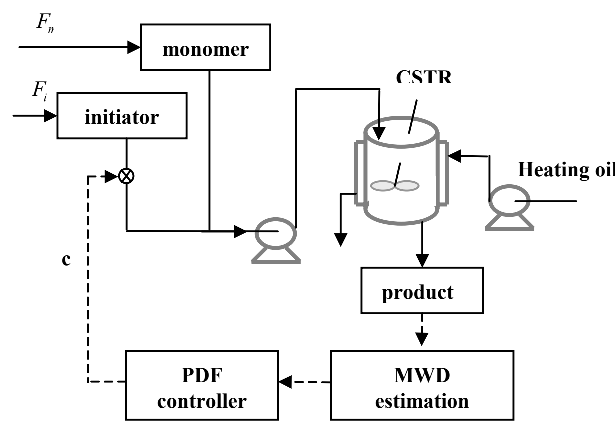

Fig. 3. Styrene polymerization system in a pilot CSTR

For the above polymerization process, seven third-order polynomial B-spline functions are chosen for the MWD approximation. The B-spline model is established based on the data provided by a previously developed first-principle MWD model. The control input is designed so that the output MWD will follow a desired MWD. The periodic learning of the B-spline functions is carried out as illustrated in the previous section. Simulation results are shown in figure 4 to figure 7.

Fig. 4 shows the target MWD, the initial MWD and the output MWD of the system at the end of the control horizon, where it is clear that the output MWD can follow the shape of the target MWD. Fig. 5 displays the responses of the MWD in terms of a 3D mesh format, showing the periodic learning and batch-to-batch process. In this figure there are ten control intervals, each consists of fifteen MWD responses. In fig. 6, the responses of the control input calculated from equation (11) are given, from which the periodic learning operation can be seen. For this system, the real control input to the process is limited in a range from 0.2 to 0.8. In fig. 7, the closed-loop performance, namely Js_j

$$Js_j = \int_{(j-1)(T+\Delta T)}^{j(T+\Delta T)} \int_a^b (\gamma_{k+1}(y,j) - g_t(y))^2 dydt, \quad j = 1, \cdots, 10$$

is displayed, indicating the consecutive improvement of the control results.

As such, it can be seen from these figures that when applying the periodic learning algorithm to the MWD control of the polymerization system, the process has an improvement in terms of batch-to-batch operation.

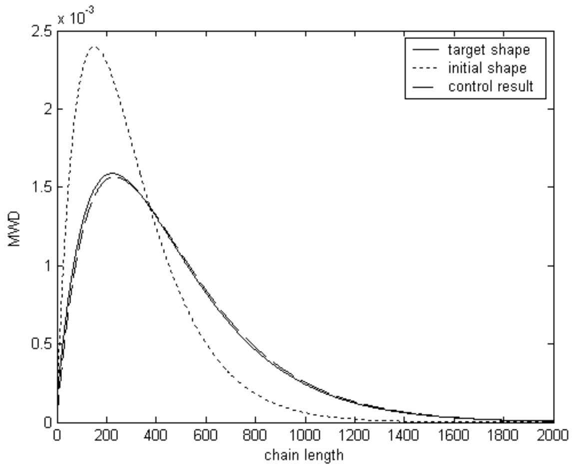

Fig. 4. The desired MWD and the output MWD at the end of control

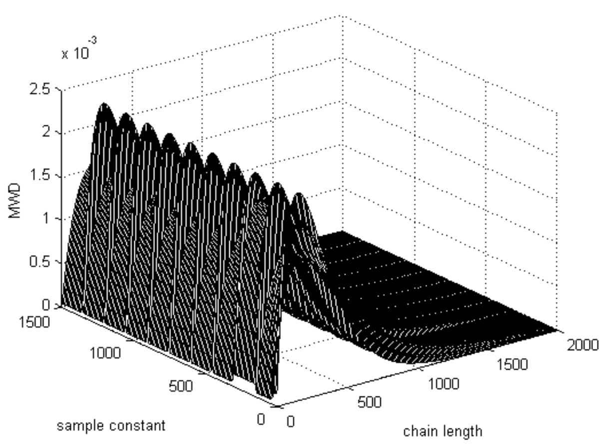

Fig. 5. The output MWD during the whole control process

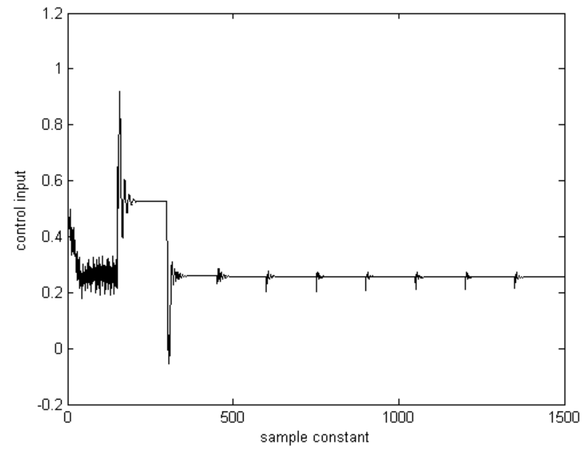

Fig. 6. The control input during the control process

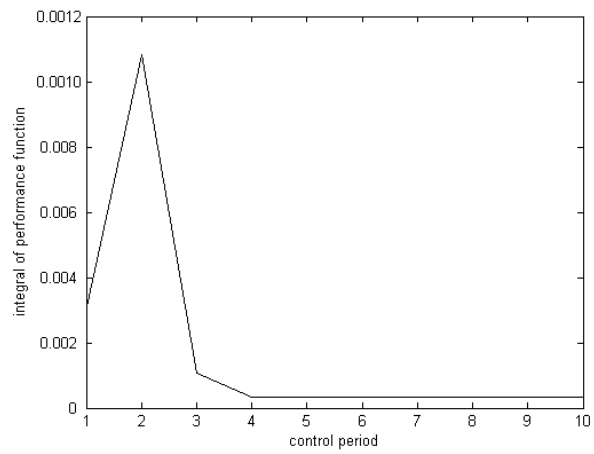

Fig. 7. The integral of performance function during each control period

V. Conclusions

A periodic learning algorithm is proposed for the output PDF control based on the B-spline approximation model. With this control strategy, the output PDF model not only relates to time but also relates to space. With the update of the B-spline functions, the variation of PDF during operation can be considered and therefore the model accuracy of the PDF approximation can be improved. This algorithm is applied to the simulation study of a batch-to-batch MWD control system. Simulation results show the convergence and effectiveness of the algorithm.

The current method is only a periodic learning algorithm, in which the basis functions are updated by a least square identification rule. For a more effective update of the basis functions, certain iterative learning rules should be considered to modify the width and height of the bais functions. In the future work, the modification of the basis functions and the model parameters will be studied further to form a general expression for the output PDF control.

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