

# A New PDF Modelling Algorithm and Predictive Controller Design <sup>\*</sup>

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**Abstract:** Output distribution control is required in many industrial processes mainly for the purpose of improving product qualities. Different from the traditional mean and variance control of stochastic processes, the probability density function (PDF) control provides a comprehensive solution to deal with outputs with general distributions. Various models based on B-splines have been developed to approximate the output PDF required for closed-loop control, among them the rational square-root (RSR) B-spline model can guarantee the nonnegativeness and the integration constraint of a PDF. In this paper, the relationship between the so-called *actual weights* and *pseudo weights* of the RSR B-spline PDF model is investigated so as to explore a simplified modelling algorithm for the very complex nonlinear PDF modelling problem. Based on the proposed modelling algorithm, a predictive PDF control strategy has been established and applied to an exemplar system of closed-loop molecular weight distribution (MWD) control in a polymerisation process. The merit of predictive control over conventional PDF control is clearly demonstrated through the simulation study.

**Keywords:** Output probability density function (PDF), B-spline approximation, parameter estimation, model predictive control, molecular weight distribution (MWD)

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## 1. INTRODUCTION

Probability density function (PDF) control has various applications in industrial processes, such as molecular weight distribution (MWD) control and particle size distribution (PSD) control in polymerization processes, pulp fibre length distribution control in paper industries, PSD control in powder industries, crystallisation processes, etc. Taking the MWD control as an example, MWD of a polymer is one of the most important variables to be controlled in industrial polymerization processes since it directly affects many of the polymer's end-use properties such as thermal properties, stress – strain properties, impact resistance, strength, and hardness (Crowley and Choi, 1998; Takamatsu et al., 1988). One challenge in MWD control is the lack of on-line measurement of the distribution. Mathematical models of MWD developed on reaction mechanisms are normally nonlinear and of high dimensions. A number of methods have been developed to control MWD (Crowley and Choi, 1997; Echevarria et al., 1998; Clarke-Pingle and MacGregor, 1998; Wang et al., 2011; Wu et al., 2012), but most of them are in an open-loop control manner.

B-spline models are often used to approximate the output PDF of a dynamic system. The major advantage of a B-spline PDF model is the decoupling of time and space in formulation (Wang, 2000). There are different types of B-spline based PDF models developed. The simplest one is the linear B-spline PDF model

$$\gamma(y, u) = \sum_{i=1}^n \omega_i(u) B_i(y) \quad (1)$$

where  $\gamma(y, u)$  is the output PDF defined in a bounded region  $[a, b]$ ,  $y$  is an independent variable,  $u$  is the control input.  $B_i(y)$  ( $i = 1 \dots n$ ) are the B-spline basis functions defined in a specific range,  $\omega_i(u)$  is the weight associated with  $B_i(y)$ .  $n$  is the number of basis functions, increasing which will improve approximation accuracy but cost the computational efforts. Considering the example of MWD modelling,  $y$  stands for the chain length,  $u$  is the manipulated control input such as the ratio of monomer and catalyst flows,  $\gamma(y, u)$  is the MWD to be controlled. When the input, output data and PDF information are available, the linear B-spline PDF model can be easily established with a least-square (LS) estimation algorithm. Linear B-spline models have been used in our earlier studies of MWD modelling and closed-loop control system design (Yue et al., 2004, 2006, 2008; Zhang and Yue, 2007).

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One numerical issue of a linear B-spline model in (1) is that the approximated function could be less than zero at certain points in its definition domain, which is not acceptable for a PDF. An alternative square-root model is developed to address this issue (Wang et al., 2001).

$$\sqrt{\gamma(y, u)} = \sum_{i=1}^n \omega_i(u) B_i(y) \quad (2)$$

There is an integration constraint of  $\int_a^b \gamma(y, u) dy = 1$ , with  $a$  and  $b$  being the upper and lower bounds of  $y$ . On handling the integration constraint, the rational B-spline model is proposed (Wang and Yue, 2003).

$$\sqrt{\gamma(y, u)} = \frac{\sum_{i=1}^n \omega_i(u) B_i(y)}{\sum_{i=1}^n \int_a^b B_i(y) dy} \quad (3)$$

Combining (2) and (3) together, the rational square-root (RSR) B-spline model is developed (Zhou et al., 2005), which guarantees both the non-negativeness and integration constraint of a PDF.

$$\sqrt{\gamma(y, u)} = \frac{\sum_{i=1}^n \omega_i(u) B_i(y)}{\sqrt{\sum_{i,j=1}^n \omega_i \omega_j \int_a^b B_i(y) B_j(y) dy}} \quad (4)$$

In this paper, the RSR B-spline PDF modelling is further investigated with the aim to simplify the estimation of model parameters (B-spline weights and parameters associated with the weights dynamics). In Section 2, a new RSR B-spline model is proposed and the modelling procedure is presented. Section 3 briefs the standard output PDF control solution. In Section 4, a predictive PDF controller is designed based on the RSR B-spline model. Simulation study of an exemplar MWD control system is carried out in Section 5 to discuss the modelling efficiency and evaluate the predictive PDF control strategy.

## 2. RSR B-SPLINE PDF APPROXIMATION

### 2.1 Pseudo Weights and Actual Weights

Considering linear dynamics in weights vector, the discrete-time RSR B-spline PDF model (4) can be expressed as follows:

$$V(k+1) = AV(k) + Bu(k) \quad (5)$$

$$\sqrt{\gamma(y, k)} = \frac{C(y)V(k)}{\sqrt{V(k)^T EV(k)}} \quad (6)$$

where

$$C(y) = [B_1(y), B_2(y), \dots, B_n(y)] \quad (7)$$

$$E = \int_a^b C^T(y)C(y)dy \quad (8)$$

$A$  and  $B$  are matrices of proper dimensions.  $k$  is the time instance. The  $n$  B-spline basis functions in  $C(y)$ , cannot all be zeros simultaneously, therefore matrix  $E$  is invertible. Here  $V(k) = [\omega_1(k), \omega_2(k), \dots, \omega_n(k)]^T$  is called the *pseudo weights* vector in the RSR B-spline model (5)-(6) since it is only a middle term in PDF approximation and its value is not unique. The *actual weights* vector is defined as (Zhou et al., 2005)

$$V_r(k) = \frac{V(k)}{\sqrt{V(k)^T EV(k)}}. \quad (9)$$

It is apparent that  $V_r^T EV_r = 1$ . Using the *actual weights*, the PDF approximation in (6) can be rewritten as

$$\sqrt{\gamma(y, k)} = C(y)V_r(k) \quad (10)$$

To establish a complete dynamic model in (5)-(6) using input-output data and output PDF, one needs to calculate  $V(k)$  to obtain the PDF approximation weights, and estimate parameters in  $A$  and  $B$  to establish the weights dynamics. It can be seen from (6) that the *pseudo weights* vector is difficult to be determined since the model regarding  $V(k)$  is nonlinear and also  $V(k)$  is not unique, however, the *actual weights*,  $V_r(k)$ , can be uniquely calculated from the PDF function  $\gamma(y, k)$  as follows.

Left multiplying  $C^T(y)$  to both sides of (10) leads to

$$C^T(y)\sqrt{\gamma(y, k)} = C^T(y)C(y)V_r(k) \quad (11)$$

Take integration for  $y$  on both sides of (11) to get

$$\int_a^b C^T(y)\sqrt{\gamma(y, k)}dy = \int_a^b C^T(y)C(y)dyV_r(k) = EV_r(k) \quad (12)$$

As discussed earlier  $E$  is invertible, therefore the *actual weights* vector can be calculated by

$$V_r(k) = E^{-1} \int_a^b C^T(y)\sqrt{\gamma(y, k)}dy \quad (13)$$

### 2.2 Observer Estimation of Pseudo Weights

Since the *pseudo weights*,  $V$ , cannot be practically recovered from the output PDF, it will be difficult to establish the parameterised RSR B-spline model in the form of (5)-(6). However, if the model is known, i.e.,  $A$  and  $B$  are given, it is then possible to estimate  $V$  through model-based observer design, and use the estimated *pseudo weights* for controller development.

Assume matrix  $A$  is stable, construct the following nonlinear observer to estimate  $V$ :

$$\hat{V}(k+1) = A\hat{V}(k) + Bu(k) + L\varepsilon(k) \quad (14)$$

where  $\hat{V}(k) = [\hat{\omega}_1(k), \hat{\omega}_2(k), \dots, \hat{\omega}_n(k)]^T$  stands for the estimated state vector,  $L$  is the observer gain matrix,  $\varepsilon(k)$  is the output residual defined as

$$\varepsilon(k) = \int_a^b \left( \sqrt{\gamma(y, k)} - \sqrt{\hat{\gamma}(y, k)} \right)^2 dy \quad (15)$$

From (6), the square root of the estimated output PDF can be written as

$$\sqrt{\hat{\gamma}(y, k)} = \frac{C(y)\hat{V}(k)}{\sqrt{\hat{V}(k)^T E\hat{V}(k)}} \quad (16)$$

Therefore the residual function in (15) can be further expressed as

$$\begin{aligned} \varepsilon(k) &= \int_a^b \left( \sqrt{\gamma(y, k)} - \sqrt{\hat{\gamma}(y, k)} \right)^2 dy \\ &= 2 - 2 \int_a^b \sqrt{\gamma(y, k)} \sqrt{\hat{\gamma}(y, k)} dy \\ &= 2 - 2 \frac{V(k)^T E\hat{V}(k)}{\sqrt{V(k)^T EV(k)} \sqrt{\hat{V}(k)^T E\hat{V}(k)}} \end{aligned} \quad (17)$$

Consider a function for  $x$  and  $y$

$$f(x, y) = \frac{x^T E y}{\sqrt{x^T E x y^T E y}}$$

it is obviously that

$$\begin{aligned} \|f(x, y)\| &= \left\| \frac{x^T E y}{\sqrt{x^T E x y^T E y}} \right\| \\ &\leq \frac{\lambda_{\max}(E) \|x\| \|y\|}{\lambda_{\min}(E) \|x\| \|y\|} = \frac{\lambda_{\max}(E)}{\lambda_{\min}(E)} \end{aligned}$$

This means  $f(x, y)$  has the maximum and minimum value. Fixing  $y$ , from the first-order derivative of  $f(x, y)$  to  $x$

$$\frac{\partial f}{\partial x} = \frac{E y x^T E x - E x x^T E y}{x^T E x \sqrt{x^T E x y^T E y}} = 0$$

the extremum points are obtained at  $x = \pm y$ . It can be proved that when  $x = y$ ,  $f(x, y)$  reaches the maximum and when  $x = -y$ ,  $f(x, y)$  reaches the minimum. Applying this conclusion to (17), we have

$$0 \leq \varepsilon \leq 4.$$

Denoting  $\tilde{V}(k) = V(k) - \hat{V}(k)$ , the error dynamics can be described as

$$\tilde{V}(k+1) = A\tilde{V}(k) - L\varepsilon(k) \quad (18)$$

**Theorem 1** Assume the system matrix  $A$  is stable, and  $\|L\| \leq \delta$ , where  $\delta$  is a pre-specified small positive number, then the 2-norm of the stable solution to (18) will not exceed a pre-specified positive number.

Proof: Since  $A$  is stable,  $0 \leq \varepsilon \leq 4$ , and  $\|L\| \leq \delta$ , from the theory of ordinary differential equation, the solution of (18) is bounded. Assume  $\|\tilde{V}\| \leq M (M > 0)$ , there exists a unique positive definite symmetrical matrix  $P$  such that

$$A^T P A - P = -I \quad (19)$$

Choose the following Lyapunov function

$$\pi(\tilde{V}(k)) = \tilde{V}(k)^T P \tilde{V}(k) \quad (20)$$

then

$$\begin{aligned} \Delta\pi &= \pi(\tilde{V}(k+1)) - \pi(\tilde{V}(k)) \\ &= -\|\tilde{V}\|^2 - 2\tilde{V}^T A^T P L \varepsilon + (L\varepsilon)^T P L \varepsilon \end{aligned} \quad (21)$$

$$\begin{aligned} \Delta\pi &\leq -\|\tilde{V}\|^2 + 2\|\tilde{V}\| \|A\| \|P\| \|L\| \|\varepsilon\| + \|L\|^2 \|\varepsilon\|^2 \|P\| \\ &\leq -\|\tilde{V}\|^2 + 2\|\tilde{V}\| \|P\| \|L\| \|\varepsilon\| + \|L\|^2 \|\varepsilon\|^2 \|P\| \end{aligned}$$

Let  $L = \frac{-M\|P\| + \sqrt{M^2\|P\|^2 + \phi^2\|P\|}}{4\|P\|}$ , in which  $\|\phi\| \leq \|P\| (16\delta^2 + 8M\delta)$ . It is clear that the stable value of  $\|\tilde{V}\|$  will not grow larger than  $\sqrt{\|\phi\|}$ . This is because if  $\|\tilde{V}\| > \sqrt{\|\phi\|}$ ,  $\Delta\pi < 0$  holds and  $\pi(\tilde{V})$  will decrease.

From Theorem 1 it is known that when  $A$  is stable, the boundedness of  $\tilde{V}$  is guaranteed by the boundedness of  $L$ . This indicates the feasibility of using an estimated  $\hat{V}$  to replace the *pseudo weights* for controller design.

Although observer estimation of the *pseudo weights* is feasible if the model is given, it is not our intention

to develop controller based on the estimated  $V$ . This is mainly because it is not assumed a model is known, on the contrary, the model needs to be established using measurement data. Instead of using the *pseudo weights*, we'll make use of the convenient calculation of the *actual weights*,  $V_r$ , to establish an alternative RSR B-spline model.

### 2.3 New RSR B-spline Model and Modelling Algorithm

The following RSR B-spline model is proposed

$$V_r(k+1) = \bar{A}V_r(k) + \bar{B}u(k) \quad (22)$$

$$\sqrt{\gamma(y, k)} = \frac{C(y)V_r(k)}{\sqrt{V_r(k)^T E V_r(k)}} \quad (23)$$

$\bar{A}$  and  $\bar{B}$  are of the same dimensions as  $A$  and  $B$  in (5). It is argued that for the same input, this model is regarded as 'practically equivalent' to model (5)-(6), i.e., in the transient process, the output error between these two models are within an acceptable small range, and in the steady state, their outputs are the same. The use of 'practically equivalent' or 'characteristic' model in real engineering control systems was discussed in (Wu et al., 2007). In the rest of the paper, the new RSR B-spline model in (22)-(23) will be used for parameter estimation and controller design.

Denote

$$f(y, k) = \sqrt{V_r(k)^T E V_r(k) \gamma(y, k)}, \quad (24)$$

Taking into account of (22)-(23), we have

$$\begin{aligned} f(y, k) &= C(y)V_r(k) \\ &= C(y)(I - z^{-1}\bar{A})^{-1}\bar{B}u(k-1) \end{aligned} \quad (25)$$

Expanding (25) brings the parameterised model

$$\begin{aligned} f(y, k) &= a_1 f(y, k-1) + \dots + a_n f(y, k-n) \\ &\quad + C(y)D_0 u(k-1) + C(y)D_1 u(k-2) + \dots \\ &\quad + C(y)D_{n-1} u(k-n) \end{aligned} \quad (26)$$

where  $a_1, a_2, \dots, a_n, D_0, D_1, \dots, D_{n-1}$  are parameters to be estimated. Note each  $D_i (i = 1, \dots, n)$  is an  $n$ -dimensional vector. Denoting the  $j$ -th component of  $D_i$  as  $d_{ij}$ , the parameter vector for (26) can be written as

$$\theta_1 = [a_1, \dots, a_n, d_{01}, \dots, d_{0n}, d_{11}, \dots, d_{1n}, \dots, d_{(n-1)1}, \dots, d_{(n-1)n}]^T$$

Let

$$\begin{aligned} \Phi_1(y, k) &= [f(y, k-1), \dots, f(y, k-n), \\ &\quad u(k-1)B_1(y), \dots, u(k-1)B_n(y), \dots, \\ &\quad u(k-n)B_1(y), \dots, u(k-n)B_n(y)]^T \end{aligned}$$

then (26) can be rewritten into a compact form

$$f(y, k) = \theta_1^T \Phi_1(y, k) \quad (27)$$

A recursive least-square (RLS) algorithm can be used to estimate  $\theta_1$  in (27):

$$\hat{\theta}_1(i+1) = \hat{\theta}_1(i) + \frac{P(i-1)\Phi_1(y_i, k)\varepsilon(i)}{1 + \Phi_1^T(y_i, k)P(i-1)\Phi_1(y_i, k)} \quad (28)$$

$$\varepsilon(i) = f_k(y_i) - \theta_1^T(i)\Phi_1(y_i, k) \quad (29)$$

$$P(i) = \left( I - \frac{P(i-1)\Phi_1(y_i, k)\Phi_1^T(y_i, k)}{1 + \Phi_1^T(y_i, k)P(i-1)\Phi_1(y_i, k)} \right) P(i-1) \quad (30)$$

The procedures for establishing the RSR B-spline PDF model can be summarized as follows.

Step 1: Collect the input and output data pair  $(u(k), y_{i,k})$  and output PDF  $\gamma(y_i, k)$  at sampling time  $k$ .

Step 2: Calculate the *actual weights*  $V_r(k)$  by (13).

Step 3: Calculate  $f(y_i, k)$  according to its definition in (24).

Step 4: Choose data set  $Y = \{y_{i,k}\}, i = 1, 2, \dots, M$  in the definition interval  $[a, b]$  of  $y$ .

Step 5: Identify the parameter vector  $\theta$  with RLS algorithm in (28)-(30).

Step 6: Increase  $k$  to  $k + 1$  and repeat steps 1-5 until the end of the recursive calculation.

### 3. STANDARD PDF CONTROLLER DESIGN

A general PDF control target is to drive the output PDF to the desired distribution. Using the following performance function

$$J(u(k)) = \int_a^b \left( \sqrt{\gamma(y, k)} - \sqrt{g(y)} \right)^2 dy + Ru(k)^2 \quad (31)$$

where  $g(y)$  is the target distribution,  $R$  is a weighting factor for control input, the optimal control input  $u$  is obtained by taking  $\frac{dJ}{du} = 0$  to give

$$u(k) = \frac{\int_a^b C(y)D_0\bar{g}(y)dy}{\int_a^b (C(y)D_0)^2 dy + R} \quad (32)$$

where

$$\begin{aligned} \bar{g}(y) = & - \sum_{i=2}^n a_i f(y, k-i+1) - C(y)D_{i-1}u(k-i+1) \\ & + \sqrt{g(y)} - a_1 f(y, k) \end{aligned} \quad (33)$$

### 4. PREDICTIVE PDF CONTROL STRATEGY

#### 4.1 The Input-output Model of the Output PDF

Equation (26) can be written as

$$f(y, k) = \sum_{i=1}^n a_i f(y, k-i) + \sum_{j=0}^{n-1} C(y)D_j u(k-j-1) \quad (34)$$

The second term in (34) can be further expanded as

$$C(y)D_j u(k-j-1) = \sum_{i=1}^n d_{ji} u(k-j-1)C_i(y) \quad (35)$$

Introducing the back-shift operator  $z^{-1}$ , denote

$$\alpha(z^{-1}) = 1 - \sum_{i=1}^n a_i z^{-i}, \beta(z^{-1}, y) = \sum_{j=0}^{n-1} C(y)D_j z^{-j} \quad (36)$$

equation (34) can be represented as

$$\alpha(z^{-1})f(y, k) = \beta(z^{-1}, y)u(k-1) \quad (37)$$

Equation (37) is the input-output model of the output PDF. All the coefficients can be estimated by LS identification when the *pseudo weights* and the input-output data pairs are available.

#### 4.2 The Predictive Model of the Output PDF

The following Diophantine equation is introduced to construct the predictive PDF model

$$1 = G_q(z^{-1})\alpha(z^{-1}) + H_q(z^{-1})z^{-q} \quad (38)$$

where  $q$  is the step for model prediction.

$$G_q(z^{-1}) = 1 + \sum_{i=1}^{q-1} g_{q,i} z^{-i}, H_q(z^{-1}) = 1 + \sum_{j=0}^{n-1} h_{q,j} z^{-j} \quad (39)$$

Multiplying  $G_q(z^{-1})$  to both sides of equation (37) and taking equation (38) into account, we have

$$\begin{aligned} f(y, k+q) = & H_q(z^{-1})f(y, k) \\ & + G_q(z^{-1})\beta(z^{-1}, y)u(k+q-1) \end{aligned} \quad (40)$$

Write

$$G_q(z^{-1})\beta(z^{-1}, y) = \sum_{i=0}^{n-1+q-1} s_{q,i}(y)z^{-i} \quad (41)$$

and take  $q = 1, 2, \dots, p$  ( $p$  is the predictive control step), the multi-step predictive PDF model can be established from (40) in the following matrix form

$$\Pi(y, k, p) = \hat{H}f(y, k) + \Omega(y)U(k) + \Phi(y)\eta(k) \quad (42)$$

where

$$\Pi(y, k, p) = \begin{bmatrix} f(y, k+1) \\ f(y, k+2) \\ \vdots \\ f(y, k+p) \end{bmatrix}, \hat{H} = \begin{bmatrix} H_1(z^{-1}) \\ H_2(z^{-1}) \\ \vdots \\ H_p(z^{-1}) \end{bmatrix}$$

$$\Omega(y) = \begin{bmatrix} s_{1,0}(y) & 0 & 0 & \cdots & 0 \\ s_{2,1}(y) & s_{2,0}(y) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ s_{p,p-1}(y) & s_{p,p-2}(y) & \cdots & s_{p,1}(y) & s_{p,0}(y) \end{bmatrix}$$

$$\Phi(y) = \begin{bmatrix} s_{1,1}(y) & s_{1,2}(y) & \cdots & s_{1,n-1}(y) \\ s_{2,2}(y) & s_{2,3}(y) & \cdots & s_{2,n-1+1}(y) \\ \vdots & \vdots & \ddots & \vdots \\ s_{p,p}(y) & s_{p,p+1}(y) & \cdots & s_{p,n-1+p-1}(y) \end{bmatrix}$$

$$U(k) = \begin{bmatrix} u(k) \\ u(k+1) \\ \vdots \\ u(k+p-1) \end{bmatrix}, \eta(k) = \begin{bmatrix} u(k-1) \\ u(k-2) \\ \vdots \\ u(k-n+1) \end{bmatrix}$$

Equation (42) gives the predictive model of the output PDF. The coefficients in the Diophantine equation can be obtained by recursive development.

#### 4.3 The Predictive Controller for Output PDF

The following performance index is formulated for the purpose of predictive PDF control

$$\begin{aligned} J_1 = & \int_a^b [\Pi(y, k, p) - \Gamma(y)]^T [\Pi(y, k, p) - \Gamma(y)] dy \\ & + U(k)^T Q U(k) \end{aligned} \quad (43)$$

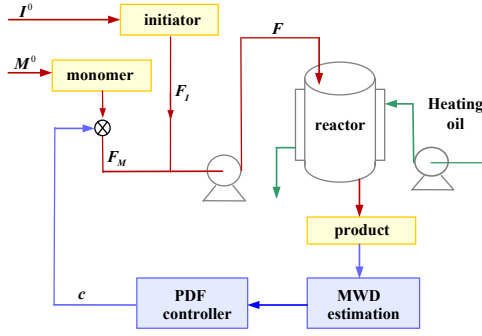


Fig. 1. The sketch of the example polymerization process

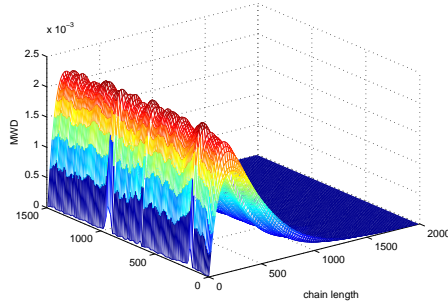


Fig. 2. The created data for PDF modelling

where  $\Gamma = [\sqrt{g(y)}, \dots, \sqrt{g(y)}]^T$ ,  $Q$  is the weighting matrix for control input. Taking (42) into (43) and denoting

$$\xi(y) = \hat{H}f(y, k) + \Phi(y)\eta(k) \quad (44)$$

as the known term at sampling time  $k$ , the optimisation solution to (43) is

$$U(k) = - \left( \int_a^b \Omega^T(y) \Omega(y) dy + Q \right)^{-1} \cdot \left( \int_a^b \Omega^T(y) (\xi(y) - \Gamma(y)) dy \right) \quad (45)$$

Equation (45) gives the  $p$ -step predictive controller.

## 5. SIMULATION STUDY

The above output PDF modelling and controller design algorithm are integrated and applied to the simulation study of the exemplar styrene polymerization process.

Fig. 1 illustrates a sketch of a lab-scaled polymerization process. The reaction takes place in a continuous stirring tank reactor (CSTR). The input flow  $F$  to the tank is the sum flow rate of the monomer ( $F_M$ ) and the initiator ( $F_I$ ). The monomer and the initiator is fed into the reactor with a ratio of  $C = \frac{F_M}{F_I + F_M}$ , which is used as the control input. The output is the MWD of the produced polymer. In the simulation, the sum flow rate  $F$  is kept constant, only the ratio  $C$  between the monomer and the initiator is adjusted. The development details of the first-principle model and the MWD formulation can be found in (Yue et al., 2004), from which the input-output data pairs and the MWD data used for PDF modelling in this simulation are produced.

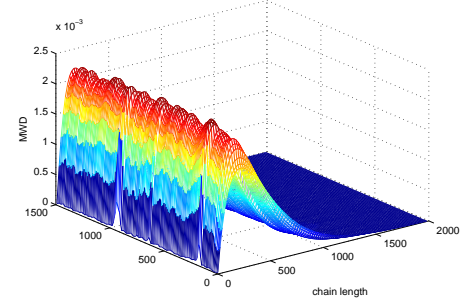


Fig. 3. MWD evolution from the developed model

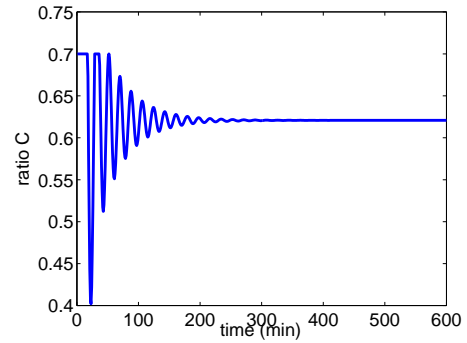


Fig. 4. The conventional PDF control input

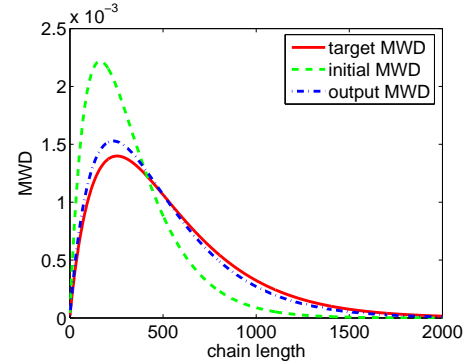


Fig. 5. The initial, final and target MWD with conventional control

The constraint for the control input is set to be  $u = C \in [0.3, 0.7]$ ; the chain length of the polymer,  $y$ , changes from 1 to 2000. The number of the B-spline basis functions used for PDF modelling is 10; the shape of each B-spline function is a parabolic curve. Fig. 2 shows the created data used for establishing the RSR B-spline PDF model. The RLS algorithm is adopted to identify the model parameters. Fig. 3 illustrates the modelling result. There's a small modelling error when the estimation is convergent. This is mainly due to the low number of B-spline functions used in PDF approximation, which is meant to avoid high computational load.

We first applied conventional output PDF control to this system. The target distribution is set corresponding to  $C = 0.65$ . Fig. 4 is the control input time profile. It can be seen that the control input is converged, but not exactly to the target control input level for the target MWD. This could be partly due to the modelling errors. Fig. 5 shows

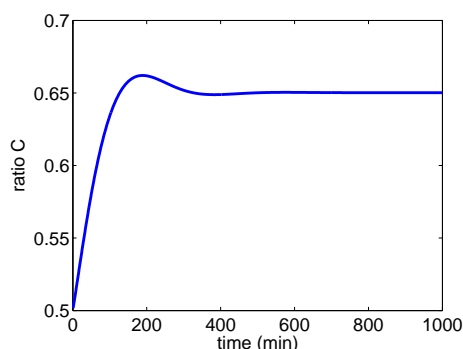


Fig. 6. The predictive PDF control input

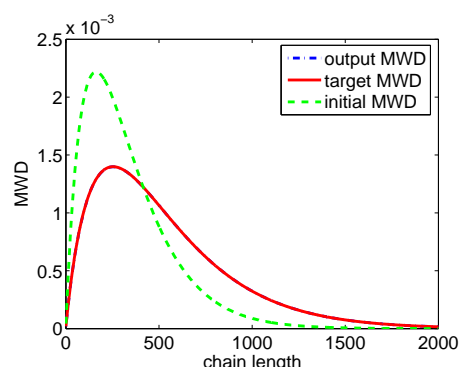


Fig. 7. The initial, final and target MWD under predictive control

the initial, final output MWDs and the target distribution, in which the final MWD gets close to the expected MWD but with a clear steady-state error.

We then applied the predictive PDF control to the same model. The simulation results are demonstrated in Fig. 6-7. It can be seen from Fig. 6 that the control input converges to the expected input level of  $C = 0.65$ . Fig. 7 illustrates that the final output MWD reaches the target distribution (two curves overlap with each other). Comparing this result with that of the conventional PDF control, a clear improvement can be seen in the predictive control strategy which eliminates tracking error in output MWD even though there is a small modelling error.

## 6. CONCLUSION

In this paper, an alternative RSR B-spline model is proposed for output PDF modelling, in which the *actual weights* are used instead of the *pseudo weights*. This largely simplifies the modelling procedure for the parameter estimation of the RSR B-spline model. Based on the new modelling of output PDF, the conventional PDF controller and the predictive PDF controller are employed to drive the output PDF getting close to the target PDF. The integrated modelling and control algorithm is applied to a simulation study of an exemplar styrene polymerization process for the purpose of closed-loop MWD control. The simulation results verify the effectiveness of the proposed algorithm and shows the strength of predictive PDF control strategy.

## REFERENCES

- Clarke-Pingle, T. and MacGregor, J. (1998). Optimization of molecular weight distribution using batch-to-batch adjustments. *Ind. Eng. Chem. Res.*, 37, 3660–3669.
- Crowley, T. and Choi, K. (1997). Discrete optimal control of molecular weight distribution in a batch free radical polymerization process. *Ind. Eng. Chem. Res.*, 36, 3676–3684.
- Crowley, T. and Choi, K. (1998). Experimental studies on optimal molecular weight distribution control in a batch-free radical polymerization process. *Chem. Eng. Sci.*, 53, 2769–2790.
- Echevarria, A., Leiza, J., de la Cal, J., and Asua, J. (1998). Molecular weight distribution control in emulsion polymerization. *AIChE J.*, 44, 1667–1679.
- Takamatsu, T., Shioya, S., and Okada, Y. (1988). Molecular weight distribution control in a batch polymerization reactor. *Ind. Eng. Chem. Res.*, 27, 93–99.
- Wang, H. (2000). *Bounded Dynamic Stochastic Systems: Modelling and Control*. Springer-Verlag, London.
- Wang, H., Baki, H., and Kabore, P. (2001). Control of bounded dynamic dynamic stochastic distributions using square root models: an applicability study in papermaking system. *Trans. Inst. Meas. Contr.*, 23, 51–68.
- Wang, H. and Yue, H. (2003). A rational spline model approximation and control of output probability density functions for dynamic stochastic systems. *Trans. Inst. Meas. Contr.*, 25, 93–105.
- Wang, J., Cao, L., Wu, H., Li, X., and Jin, Q. (2011). Dynamic modelling and optimal control of batch reactors based on structure approaching hybrid neural networks. *Ind. Eng. Chem. Res.*, 50, 6174–6186.
- Wu, H., Cao, L., and Wang, J. (2012). Gray-box modelling and control of polymer molecular weight distribution using orthogonal polynomial neural networks. *J. Proc. Contr.*, 22, 1624–1636.
- Wu, H., Hu, J., and Xie, Y. (2007). Characteristic model-based all-coefficient adaptive control method and its applications. *IEEE Trans. Syst., Man, Cybern., pt C: Appl. Rev.*, 37, 213–221.
- Yue, H., Wang, H., and Cao, L. (2006). Control orientated b-spline modelling of a dynamic mwd system. In *Prepr. Int. Symp. Adv. Contr. Chem. Proc.*, 719–724. Gramado, Brazil.
- Yue, H., Wang, H., and Zhang, J. (2008). Shaping of molecular weight distribution by iterative learning probability density function control strategies. *Proc. IMechE Pt I: J. Syst. Contr. Eng.*, 222, 639–653.
- Yue, H., Zhang, J., Wang, H., and Cao, L. (2004). Shaping of molecular weight distribution using b-spline based predictive probability density function control. In *Proc. 2004 Am. Contr. Conf.*, 3587–3592. 2004 AACC, Boston, USA.
- Zhang, J. and Yue, H. (2007). Steady-state modelling and control of molecular weight distributions in a styrene polymerization process based on b-spline neural networks. In D. Liu, S. Fei, Z. Hou, H. Zhang, and C. Sun (eds.), *Advances in Neural Networks - ISNN2007, LNCS*, volume 4491, 329–338. Springer.
- Zhou, J., Yue, H., and Wang, H. (2005). Shaping of output pdf based on the rational square-root b-spline model. *Acta Automatic Sinica*, 31, 343–351.