

Partial Differential Equation Model Based Control: Application to a Bleaching Reactor

Stéphane Renou* and Michel Perrier

Département de génie chimique

École Polytechnique de Montréal

C.P. 6079, succ. Centre-ville Montréal, H3C 3A7, Canada

Denis Dochain

CESAME, Université Catholique de Louvain

Av. G. Lemaître 4-6, 1348 Louvain-La-Neuve, Belgium

Sylvain Gendron

PAPRICAN, 570 Blvd St-Jean

Pointe-Claire, H9R 3J9, Canada

Abstract

Reactor engineering generally uses distributed parameter models for design purpose. These models are not often used for process control design. May the use of this kind of complex models improve control performance? This paper compares different control strategies based on a distributed parameter model to a time-scaled DMC that only uses a simple input-output model for the control of a bleaching reactor.

Keywords

Distributed parameter systems, Late-lumping control, Early-lumping control, DMC, Bleaching reactor

Introduction

The design of tubular reactors is usually performed by using mass and energy balances on a thin slice of the reactor. This modelling approach leads to partial differential equation models. However, process control practice for this type of reactor often uses lumped models such as first order plus delay transfer functions. Could there be some advantage to use the distributed parameter model for control purposes? On one hand, answering this question is easier when actuators and sensors are also distributed like in furnace heat control. Using a distributed parameter model then allows to use all the information in a structured manner. On the other hand, when sensors and actuators are only present at boundaries, performance enhancement using a distributed parameter model is not obvious. This question will be explored in this paper on a bleaching reactor application.

The bleaching process is the last step of pulp preparation. Its purpose is to improve the brightness of the pulp to a specified level which fulfills customers needs. The control objective for a bleaching reactor is then to obtain the desired brightness with a minimum output brightness variance at the lowest chemical cost. Traditional approaches to this control problem include variations around compensated brightness and scheduling, but the increase of computer power and the introduction of on-line analyzers offer new possibilities for model-based control such as directly using the PDE model.

Different models for the bleaching are presented in the literature for control purposes. Traditionally transfer function or other input-output models are used. But the need for more complex models is pointed out with the use of mixed model. Barrette and Perrier (1995) use multiple CSTR and Wang et al. (1995) use a combina-

tion of CSTR and PFR. Recently, a PDE model have been proposed by Renou et al. (2000b).

Various approaches have been considered to use a PDE phenomenological model directly. Ray (1981) proposed to divide control approaches on PDEs in two groups. The first group is composed of early lumping methods where a preliminary discretization of the PDE model is used to obtain a set of ODEs. This lumping is often realized by numerical techniques such as finite difference, orthogonal collocation or finite elements. Christofides (1996) has used the Galerkin method for the control of parabolic PDE. Early lumping techniques also includes the use of global differentiation proposed by Dochain (1994) as an approximation of partial derivative. This approach have been applied to hyperbolic PDE on a bioreactor by Bourrel (1996) and on a bleaching reactor model by the authors (Renou et al., 2000b). The second group of techniques is based on late lumping methods where the controller design problem is solved directly with the PDE model. When necessary, lumping may be applied for controller implementation. Christofides (1996) has used this approach in the case of hyperbolic system with a distributed control action. The control of parabolic PDE has been previously addressed by Hong and Bentsman (1994). They provide a design solution for systems in which the control action appears explicitly in the PDE system. For the boundary control problem, the authors have proposed a direct adaptive control strategy in Renou et al. (2000a) for the linear case.

The objective of this study is to present some results on the use of more complex models to enhance control performance. For this purpose, an early lumping and a late lumping strategy are compared to a simple time-scaled Dynamic Matrix Control (DMC) algorithm. The first section of the paper presents the PDE model development for a ClO_2 bleaching reactor. The second section briefly show the design ideas for each controller. The fol-

*Now with GE Corporate Research & Development, General Electric Company, Building KW Room D-211, P.O. Box 8 Schenectady NY 12301. Email: renou@crd.ge.com.

lowing section presents the main comparative results in terms of response to flow variations, step point changes and kinetic parameter mismatch.

Bleaching Reactor Model

The bleaching process for chemical pulp consists of extracting lignin from wood fibre. This brownish colored complex polymer is responsible for wood fiber coloration. It could be degraded by using a strong oxidant like ClO_2 . A PDE model for this process reactor can be obtained by mass balances on lignin (L) and ClO_2 (C) on a thin section of the reactor. The following space axial dispersion model is then obtained:

$$\frac{\partial L(z, t)}{\partial t} = -v \frac{\partial L(z, t)}{\partial z} + D \frac{\partial^2 L(z, t)}{\partial z^2} - r_L(L(z, t), C(z, t)) \quad (1)$$

$$\frac{\partial C(z, t)}{\partial t} = -v \frac{\partial C(z, t)}{\partial z} + D \frac{\partial^2 C(z, t)}{\partial z^2} - r_C(L(z, t), C(z, t)) \quad (2)$$

$$\begin{aligned} \left. \frac{\partial L(z, t)}{\partial z} \right|_{z=0} &= \frac{v}{D} (L(0, t) - L_{in}(t)) \\ \left. \frac{\partial C(z, t)}{\partial z} \right|_{z=0} &= \frac{v}{D} (C(0, t) - C_{in}(t)) \\ \left. \frac{\partial C(z, t)}{\partial z} \right|_{z=l} &= \frac{\partial C_{out}}{\partial z} = 0 \\ \left. \frac{\partial L(z, t)}{\partial z} \right|_{z=l} &= \frac{\partial L_{out}}{\partial z} = 0 \end{aligned} \quad (3)$$

In this model, reaction kinetics explicitly appears and can be identified by laboratory batch experiments. Hydrodynamical parameters v and D can be determined by tracer analysis. Here the kinetic data obtained by Savoie and Tessier (1997) have been considered and hydrodynamical parameters were deduced from Pudlas et al. (1999) as shown in Renou et al. (2000b). The following kinetics model and hydrodynamical parameters are used:

$$r_{L1}(L, C) = -k_L C^2 L^2 = -0.0065 C^2 L^2 \quad (4)$$

$$r_{C1}(L, C) = -k_C C^2 L^2 = -0.0010 C^2 L^2 \quad (5)$$

$$v = 1 \text{ m/s}, D = 0.001 \text{ m}^2/\text{s} \quad (6)$$

for a 30 meter tower. Finally we consider the inlet concentration of ClO_2 , C_{in} , and the lignine concentration at the outlet, L_{out} , as the manipulated variable and the controlled variable, respectively. Lignine and ClO_2 measurement are assumed to be available at the both ends of the reactor.

Time-Scaled DMC

The DMC controller is designed using two dynamic matrices: β_{CL} for ClO_2 input to lignin output response and

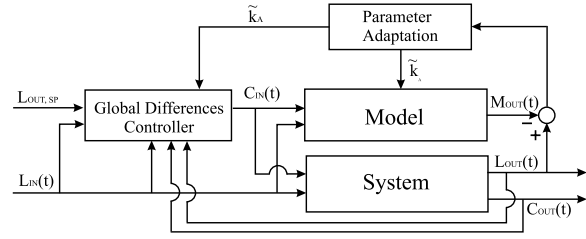


Figure 1: Global differences controller.

β_{LL} for lignin input to lignin output response. At each control step, the following criterion is applied:

$$\begin{aligned} \min_{\Delta u(k)} \phi &= [e(k+1) - \beta_{CL} + K^2 \Delta u(k)^T \Delta u(k)^T]^T \\ & [e(k+1) - \beta_{CL} + K^2 \Delta u(k)^T \Delta u(k)^T] \quad (7) \end{aligned}$$

The prediction error takes the input lignin disturbances into account such as:

$$\begin{aligned} e(k+1) &\equiv y^*(k+1) \\ &\quad - [\hat{y}^0(k) + w(k+1) + \beta_{LL} \Delta L(k)] \quad (8) \end{aligned}$$

In the preceding equation, y^* is the set point, \hat{y}^0 is the prediction if no further control action is taken, w is the estimation of disturbance and ΔL is the variation of lignin at the inlet. Traditional DMC is sensitive to flow rate variations since they represent, in fact, a variation of dead-time from an input-output point of view. To overcome this problem efficiently, information about the flow rate has to be transmitted to the controller. To reach this goal, the prediction time span is scaled by the variation of flow rate. Thus, the Δt between each calculation of the control action is scaled by the ratio between the new flow rate and the old flow rate. This approach can be practically implemented by using oversampling or interpolating dynamic matrices and prediction.

Early Lumping Approach

One of the problems with the PDE model described by Equations 1–3 is that the control action does not appear explicitly in the PDE equations. Dochain (1994) have proposed to use global differences as an approximation for space partial derivatives. This early lumping approach introduces ClO_2 input and lignin output in an approximate model. An exact linearization approach of this model can then be considered. The following approximation are used for both species:

$$\frac{\partial L(1, t)}{\partial z} = \frac{L(1, t) - L(0, t)}{\Delta z} = L_{out}(t) - L_{in}(t) \quad (9)$$

$$\begin{aligned} \frac{\partial^2 L(1, t)}{\partial z^2} &= \frac{L(2, t) - L(1, t) - L(0, t)}{\Delta z^2} \\ &= L_{in}(t) - L_{out}(t) \quad (10) \end{aligned}$$

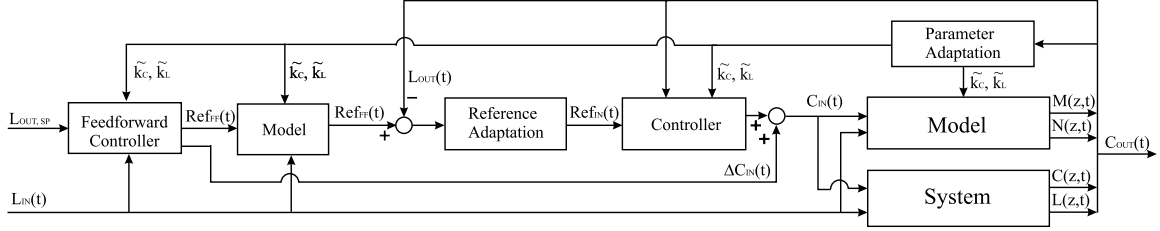


Figure 2: Late lumping internal model controller.

To obtain the approximate model, system mass balances are expressed at the reactor outlet, global differences are introduced and both equations are combined by their kinetic term. These operations give the following result:

$$\begin{aligned} \frac{dL_{out}(t)}{dt} &= -v(L_{out}(t) - L_{in}(t)) + D(L_{in}(t) - L_{out}(t)) \\ &+ \frac{k_{L1}}{k_{C1}} \left(\frac{dC_{out}(t)}{dt} + v(C_{out}(t) - C_{in}(t)) \right. \\ &\left. - D(C_{in}(t) - C_{out}(t)) \right) \end{aligned} \quad (11)$$

Using a backward finite difference to approximate the ClO_2 time derivative, an input-output relation between ClO_2 input and lignin output can be obtained. Exact linearization principle can be applied on this equation to obtain the following control law in which λ and γ are external loop tuning parameters:

$$\begin{aligned} C_{in}(t) &= \frac{1}{v + D} \left(vC_{out}(t) + DC_{out} \right. \\ &+ \frac{C_{out}(t) - C_{out}(t-1)}{\Delta t} + \frac{k_{C1}}{k_{L1}} \left[u \right. \\ &\left. + v(L_{out}(t) - L_{in}(t)) + D(L_{in} - L_{out}) \right] \end{aligned} \quad (12)$$

$$\begin{aligned} u(t) &= \lambda \left[(L_{sp} - L_{out}(t)) \right. \\ &\left. + \gamma \int_0^t (L_{sp} - L_{out}(t)) dt \right] \end{aligned} \quad (13)$$

To insure more robustness to this algorithm, an adaptation mechanism is added for the reaction rate ratio as shown in Figure 1. A model is simulated in parallel with a variable k_{L1} , noted k_A , which is modified according to the error between the adaptation model and the system model on lignin using a linear first order filter.

Late Lumping Approach

To use the whole information of the PDEs model an internal model approach is considered. The error between the model and the system is then used in direct adaptive control scheme. To account for lignin inlet variation a feedforward compensation is added to this controller. The feedforward controller action is divided in two parts. The first part uses an internal model of the process to give an estimation of the reference output to the controller. The second part directly gives a correction of

ClO_2 needed to compensate for the deviation of lignin from the nominal operating point. Those calculation are based on a relaxation algorithm. Figure 2 shows the proposed control structure.

The controller design is performed using the Lyapunov second method following the approach presented in Renou et al. (2000a). The controller and adaptation laws are defined by:

$$\dot{\tilde{C}}_{in} = \frac{(C_{in} - Ref_{in})^2}{w + (C_{in} - Ref_{in})^2} \tilde{C}_{in} \quad (14)$$

$$\begin{aligned} &+ \frac{(C_{in} - Ref_{in})}{w + (C_{in} - Ref_{in})^2} f_c \\ \dot{\tilde{C}}_{in} &= \tilde{C}_{in} \end{aligned} \quad (15)$$

$$\begin{aligned} f_c &= \langle e_C, -v \frac{\partial e_C}{\partial z} \rangle + \langle e_L, -v \frac{\partial e_L}{\partial z} \rangle \\ &+ \langle e_C, \tilde{k}_C Q \rangle + \langle e_L, \tilde{k}_L Q \rangle \\ &+ \frac{\theta}{\epsilon} (C_{in} - Ref_{in}) \dot{Ref}_{in} \end{aligned} \quad (16)$$

$$\dot{Ref}_{in} = -\theta(L_{out}(t) - Ref_{ff}(t)) \quad (17)$$

$$\dot{\tilde{k}}_L = -a \langle e_L, Q \rangle \quad (18)$$

$$\dot{\tilde{k}}_C = -b \langle e_C, Q \rangle \quad (19)$$

using the following error functions:

$$e_L(z, t) = L(z, t) - M(z, t) \quad (20)$$

$$e_C(z, t) = C(z, t) - N(z, t) \quad (21)$$

$$Q(z, t) = L^2 C^2 - M^2 N^2 \quad (22)$$

In those equations, $M(z, t)$ and $N(z, t)$ are the lignin and chlorine dioxide model profiles, respectively. The controller law uses, for implementation purposes, only information from sensors at both ends of the reactor. Overall this control structure will behave as a feedforward controller if the model match the system. Otherwise the feedback part will account for model mismatch.

Simulation Results

Numerical simulation of the control algorithm applied to the system has been performed using a sequencing algorithm with a 100 node mesh (Renou et al., 2000c). In this algorithm, convection, dispersion and reaction

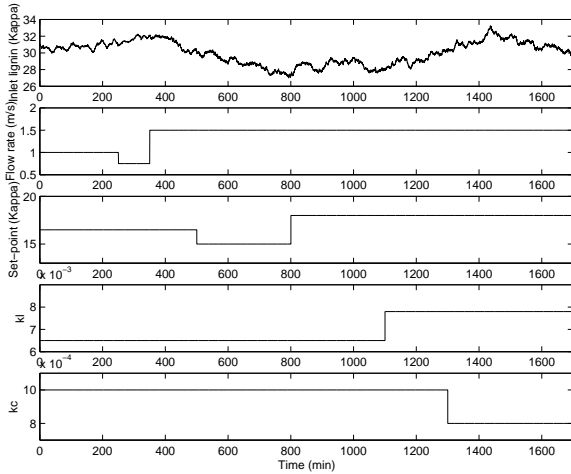


Figure 3: Operating conditions variations.

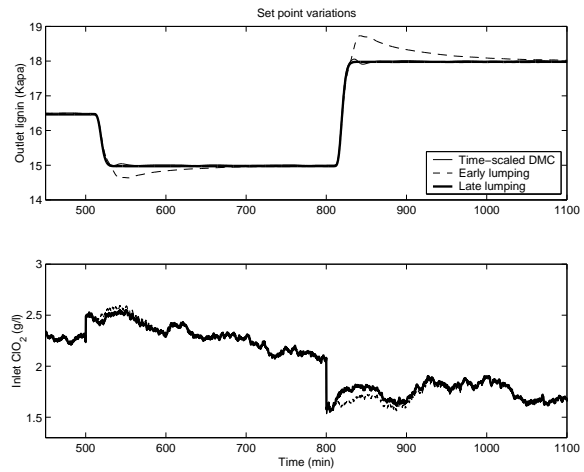


Figure 5: Set-point variations.

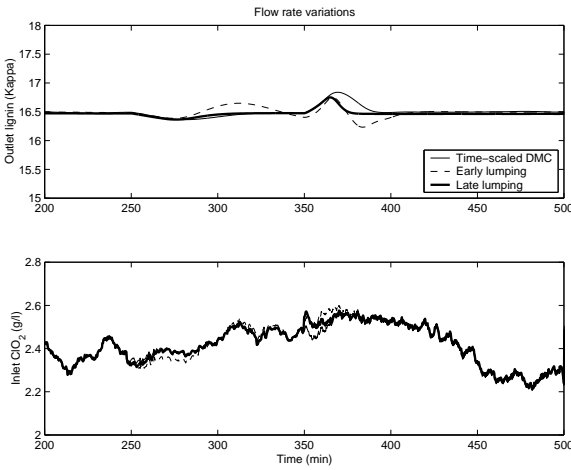


Figure 4: Flow rate variations.

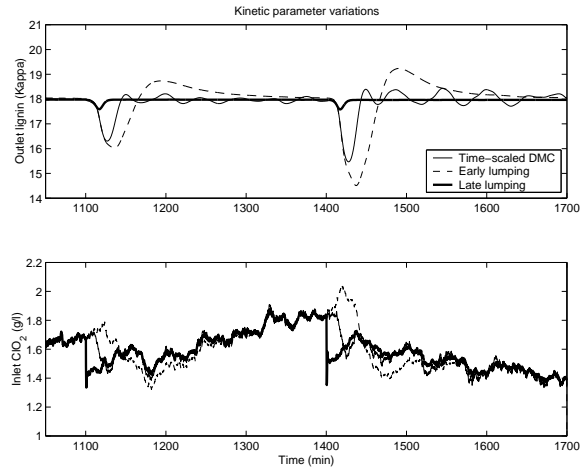


Figure 6: Model perturbations.

phenomena are successively considered at each time step. The controller parameters have been chosen to minimize overshoot and oscillations. Simulations are started at steady state with $L_{in} = 31 \text{ Kappa}$ and $C_{in} = 2.35 \text{ g/l}$. The Kappa index is a measure of pulp whiteness. A sequence of events is applied to deviate the process from its nominal operating point as shown in in Figure 3.

Figure 4 shows the response of the system to flow rate variations. In each case the response of the controller to the variation of the delay is adequate. This result is guaranteed in the DMC case by the time-scaling of the model. In PDE based models, the time delay is implicit, and therefore, including flow rate variation directly in the control law accounts for time delay variation. The late lumping controller gives the less important deviation from set point in transient.

Figure 5 shows the response of the system to set-point variations. In this simulation, time-scaled DMC and late lumping controller give similar results that match open-loop dynamics of the reactor. The early lumping con-

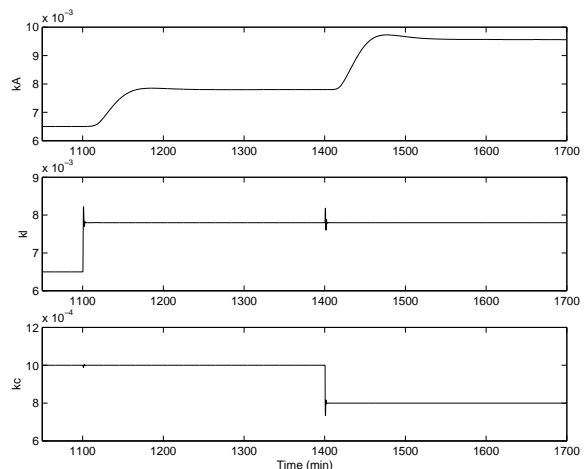


Figure 7: Kinetic parameter estimations.

troller exhibits an overshoot in case of set-point variation : this is due to the use of important simplifications in the PDE model. This overshoot can be reduced at the cost of a slower response time. Figure 6 shows the response of the system to kinetic parameter disturbances and parameter adaptations in PDE-based controller are shown in Figure 7. In this simulation time-scaled DMC exhibits oscillations. The linear model use in this controller is showing its limits to the successive deviations from the nominal operating point. The early lumping controller induces a large deviation from the set point as for the set-point variation, but the transient is still smooth. The late lumping controller provides a fast response to kinetic parameter variation.

Conclusion

A comparison between three levels of modeling for control have been presented: time-scaled DMC, a early lumping approach based on global differentiation of partial derivatives and a late lumping approach based on Lyapunov second method with feedforward action. The simulation results show the improvement by using a PDE model for tubular reactors. This improvement is particularly important when the process moves away from its nominal operating point where the nonlinearities in the kinetics cannot be followed adequately by a simple linear model.

References

- Barrette, M. and M. Perrier, Modelling and Control of a Hypochlorite Bleaching Stage for Dissolving Pulp, In *Process Control 1995*, pages 11–22 (1995).
- Bourrel, S., *Estimation et commande d'un procédé paramtres répartis utilisé pour le traitement biologique de l'eau à potabiliser*, Ph.D. Thesis, Université Paul Sabatier (1996).
- Christofides, P. D., *Nonlinear Control of Two-Time-Scale and Distributed Parameter Systems*, Ph.D. Thesis, University of Minnesota (1996).
- Dochain, D., *Contribution to the Analysis and Control of Distributed Parameter Systems with Application to (Bio)Chemical Processes and Robotics*, Agrégation Thesis, Université catholique de Louvain (1994).
- Hong, K. S. and J. Bentsman, "Direct Adaptive Control of Parabolic Systems: Algorithm Synthesis and Convergence and Stability Analysis," *IEEE Trans. Auto. Cont.*, **39**(10), 2018–2033 (1994).
- Pudlas, M., P. Tessier, and M. Savoie, Implementation of a Bleach Plant Supervisory Control System at Northwood Inc., In *Papfac Western Conference* (1999).
- Ray, W. H., *Advanced Process Control*. McGraw-Hill, New York (1981).
- Renou, S., M. Perrier, D. Dochain, and S. Gendron, Direct Adaptive Control of a Linear Parabolic System, In *IFAC SYSID 2000*, pages ThMD1–1, Santa-Barbara (2000a).
- Renou, S., M. Perrier, D. Dochain, and S. Gendron, Nonlinear Control Design for Pulp Bleaching, In *Control System 2000*, pages 351–354, Victoria (2000b).
- Renou, S., M. Perrier, D. Dochain, and S. Gendron, "Solution of the Convection-Dispersion-Reaction Equation by a Sequencing Method," *Submit to Comp. & Chem. Eng.* (2000c).

Savoie, M. and P. Tessier, "A Mathematical Model for Chlorine Dioxide Delignification," *Tappi J.*, **80**(6), 145–152 (1997).

Wang, R. X., J.-C. Tessier, and C. P. J. Bennington, "Modeling and Dynamic Simulation of a Bleach Plant," *AIChE J.*, **41**(12), 2603–2613 (1995).