

CASCADE OPTIMIZATION AND CONTROL OF BATCH REACTORS

Xiangming Hua, Sohrab Rohani and Arthur Jutan*
Department of Chemical and Biochemical Engineering
University of Western Ontario, London, Canada N6A 5B9

* ajutan@uwo.ca

Abstract: In this study, a cascade closed-loop optimization and control strategy for batch reactors is proposed. A simple physical conservation model is used to describe the dynamics of the batch reactor. Using model reduction a cascade system is developed, which can effectively combine optimization and control to achieve good on-line optimization and tracking performance, with limited information on the reaction system. A two-tier estimation scheme using a nonlinear observer for the heat production rate and the reaction rates is developed. A closed-loop optimization strategy is proposed, which uses a descending horizon dynamic optimization algorithm based on nonlinear programming (NLP), and an additive disturbance is used for feedback. An adaptive nonlinear tracking system is designed based on the generic model control (GMC) algorithm. The efficiency of this strategy is demonstrated through simulations on a batch reactor under various operations conditions.

Keywords: Batch reactors; Closed-loop dynamic optimization; adaptive nonlinear control; calorimetric state estimation; nonlinear observer.

1. INTRODUCTION

Batch reactors provide flexible means of producing high value-added products in specialty chemical, biotechnical, and pharmaceutical industries. To realize the production objectives, the batch reactors have to be operated optimally in a precise fashion; the optimization and control of batch reactors present some of the most interesting and challenging problems for both academia and industry in process control (Berber, 1995).

A traditional approach to the batch reactor optimization and control problem has been off-line optimization and open-loop control. Since there was no feedback from the process output, this scheme is very sensitive to uncertainties in initial conditions, process dynamics and disturbances occurring during the batch operation.

We propose an optimization scheme which avoids the traditional singularities and high computational burden, and is combined with a control strategy which is able to accommodate the non linearities of the system. Furthermore, we take into account the practical problem of limited reaction kinetics information, by using a nonlinear observer.

In this work, a simple physical conservation model with limited reaction kinetic information is used. The model is then decomposed into two parts: a reduced mass balances model (RMBM) and reduced energy balances model (REBM). The RMBM is used to design the on-line optimizer, and the REBM to design the controller. As is usual in practice, the reactor temperature is used as the decision variable for the optimization problem. This allows a cascade implementation, which can effectively combine optimization and control. Using this approach, the singularity problem in dynamic optimization is avoided (Palanki, et.al.,1998) and the computational burden is decreased. The system can then be decoupled, which allows independent design of the optimizer and the controller.

In previous studies some techniques have been successfully developed for estimating the heat production rate (Jutan and Uppal, 1984; Farza, *et al.*, 1999). These so-called "calorimetric state estimation" techniques are used for on-line estimation of the heat production rate.

Here, a descending horizon dynamic optimization algorithm based on nonlinear programming (NLP) is

proposed which implements an on-line open-loop optimization strategy, using calorimetric measurement information. The effect of modeling error and unmeasured disturbances are treated as additive unknown disturbances. This is similar to the Model Predictive Control strategy and allows feedback to be introduced into the open-loop optimization algorithm.

To ensure good tracking performance, it is necessary to apply a nonlinear controller due to the complex characteristics of the batch reactor. The Generic Model Controller (GMC) (Lee and Sullivan, 1988) has some attractive advantages (Cott and Macchietto, 1989; Hua and Jutan, 2000), and is used here.

In addition, an on-line, two-tier, estimation scheme is developed for the heat production rate and the reaction rates, using a specialized nonlinear observer developed by Farza, *et al.* (1999) which is both easy to tune and implement.

2. REACTOR MODEL AND CASCADE IMPLEMENTATION

A typical batch chemical reactor is considered here, and it is assumed that there are m reactions taking place with n different components (reactants and products) participating in the reactor (usually $m < n$). For heating and cooling the reactor contents, a heat exchanger can be used before the jacket inlet stream, in addition to a single-pass jacket system around the reactor vessel. Without loss of generality, it is also assumed that the jacket temperature is perfectly regulated by PID temperature controller(s). Thus, the dynamics of the heat exchanger with the control system will not be modeled.

2.1 Batch reactor model

The following $n + 1$ differential equations can be derived for the reactor.
Mass balances (n equations):

$$\dot{\mathbf{M}} = \mathbf{S}_c \mathbf{R} \quad (1)$$

Energy balances (one equation):

$$\dot{T}_r = \frac{1}{WC_p} Q + \frac{UA_h}{WC_p} (T_j - T_r) \quad (2)$$

where, $\mathbf{M} = [M_1 \ M_2 \ \dots \ M_n]^T$ is a $n \times 1$ vector of the mass or the number of mole of n components, \mathbf{S}_c is a $n \times m$ stoichiometric coefficient matrix, $\mathbf{R} = [R_1 \ R_2 \ \dots \ R_m]^T$ is a $m \times 1$ vector of m reaction rates, which are nonlinear functions with respect to the component mass and the reaction temperature, T_r

and T_j are the temperatures inside the reactor and the jacket, respectively. Q is the heat production rate:

$$Q = \Delta \mathbf{H}^T \mathbf{R} \quad (3)$$

where $\Delta \mathbf{H}^T = [(\pm \Delta H_1) \ (\pm \Delta H_2) \ \dots \ (\pm \Delta H_m)]$ is a $1 \times m$ vector of the heat of reaction, W and C_p are total mass of the reactor contents and heat capacity, respectively. U is the heat-transfer coefficient, and A_h is the heat-transfer area. It is assumed that all physical parameters in the model are constant. In this work, no knowledge of the reaction kinetics is required for the estimation of the heat production rate and the reaction rate, as well as for the design of the tracking system. In designing the optimizer, however, we need to perform end point calculations, and thus need to, initially, make use of some approximate reaction rate expressions obtained from *prior* knowledge and experimental studies. All temperature and flowrate measurements are available.

2.2 Model reduction and cascade system

Instead of using the full model (Eq's 1-3) (which implies full kinetic information) directly, the dynamic model (Eqs. 1-2) is decoupled into an RBM that consists of the n equations (Eq. 1), and an REBM that consists of the Eq. 2. The RBM is used to design the optimizer, and the REBM to design the controller. The controller design is based only on the REBM and requires just temperature measurements. Since the reactor temperature is the input of the RBM, it is selected as the decision variable for the optimization subsystem. However, the reactor temperature is the controlled variable in the tracking subsystem. A cascade optimization and tracking system is then used (Figure 1)

2.3 Formulation of closed-loop optimization problem

The on-line closed-loop optimization of the batch reactor is formulated as:

$$\min_{T_r(t)} J = \mathbf{f}(\mathbf{M}(t_f)) \quad (4)$$

subject to satisfying:

$$\dot{\mathbf{M}}(t) = \mathbf{S}_c \mathbf{R}, \quad \mathbf{R} = \mathbf{R}(\mathbf{M}, T_r) \quad (5)$$

$$t_k \leq t \leq t_f, \quad k = 0, 1, \dots, N-1 \quad (6)$$

$$\mathbf{M}(t_k) = \mathbf{M}_k \quad (7)$$

$$T_{r\min} \leq T_r(t) \leq T_{r\max} \quad (8)$$

\mathbf{M}_k is the initial state vector of the component mass at the time t_k . The effect of modelling error and unknown disturbances is treated as an additive, unmeasured disturbances d_1 and d_2 .

This approach allows the introduction of feedback into the algorithm.

3. ADAPTIVE NONLINEAR TRACKING

An adaptive nonlinear controller is developed using the REBM. The manipulated input of this tracking system is the jacket temperature T_{jd} and the tracked variable is the reactor temperature T_r . The REBM can be rewritten as:

$$\dot{T}_r = a\hat{Q} + b(T_{jd} - T_r) \quad (9)$$

where \hat{Q} is the estimate of heat production rate.

The GMC control algorithm (Lee and Sullivan, 1988) can then be represented as

$$T_{jd} = T_r - \frac{a}{b}\hat{Q} + \frac{1}{b}\left(K_1(T_{r,sp} - T_r) + K_2\int_0^t (T_{r,sp} - T_r)dt\right) \quad (10)$$

4. ON-LINE ESTIMATION

An on-line two-tier estimation approach is developed: firstly to estimate the heat production rate based on the REBM and temperature measurements, using calorimetric state estimation, and then to estimate m reaction rates based on the ‘‘measured’’ (inferred) heat production rate and a subset of component mass or concentration measurements. Following Farza, *et al.* (1999), we obtain the following heat production rate estimator:

$$\dot{\hat{T}}_r = a\hat{Q} + b(T_j - T_r) - 2\mathbf{q}_Q(\hat{T}_r - T_r) \quad (11)$$

$$\dot{\hat{Q}} = -\mathbf{q}_Q^2 a^{-1}(\hat{T}_r - T_r) \quad (12)$$

where, \mathbf{q}_Q is a tuning parameter, and a and b are constants defined by Equation 9.

We can also obtain the following reaction rate estimator:

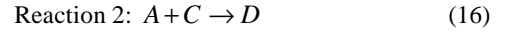
$$\dot{\hat{\mathbf{M}}} = \bar{\mathbf{S}}_c \hat{\mathbf{R}} - 2\mathbf{q}_R(\hat{\mathbf{M}} - \bar{\mathbf{M}}) \quad (13)$$

$$\dot{\hat{\mathbf{R}}} = -\mathbf{q}_R^2 \bar{\mathbf{S}}_c^{-1}(\hat{\mathbf{M}} - \bar{\mathbf{M}}) \quad (14)$$

where, \mathbf{q}_R is a tuning parameter.

5. CASE STUDY

In order to demonstrate the efficiency of the proposed optimization and control strategy, the batch chemical reactor, used by Cott and Macchietto (1989), is considered. This is a well-mixed, liquid-phase reaction system, with two reactions taking place:



where, component A and B are reactants. Component C is the desired product while D is an unwanted byproduct.

5.1 Simulation studies

The batch reactor was simulated using a detailed physical model. Gaussian noise was added to the measurements. The sampling rate Δt_{opt} for the online optimization and Δt_{ctrl} for the control were selected as 4~6 *min* and 12 *sec*, respectively.

Under the constraint of the jacket inlet temperature $0 \leq T_{jin,sp} \leq 128$ °C, it was found that reasonable choices of the GMC controller parameters were $K_1 = 0.0417 \text{ sec}^{-1}$ and $K_2 = 7.7161 \times 10^{-8} \text{ sec}^{-2}$. The resulting closed-loop control system, with estimated heat production rate achieved excellent set-point tracking.

Figures 2-3 show on-line estimation and cascade closed-loop optimization and control performance of the batch reactor operating under a nominal operating condition, respectively. Figure 2 illustrates the transient behavior of the real and estimated heat production rates, and two reaction rates, respectively. From this figure, we see that all estimators have good dynamic tracking performance. The closed-loop optimal temperature profile T_{opt} is shown in Figure 3. The reactor temperature T_r is shown to satisfactorily track the T_{opt} trajectory. The change in the set-point of the jacket inlet temperature is also shown in this figure. The optimal objective value under this nominal operating condition is $MC(t_f) = 6.3963 \text{ kmol}$. The molar profiles of all the components under closed loop control are shown in Figure 4.

To verify the optimization performance of the cascade closed-loop optimization and control system, the standard end-point dynamic optimization of this batch reactor (Palanki, *et al.*, 1998) was carried out off-line under the nominal operating conditions. The open-loop optimal temperature profile is shown in Figure 5 and is seen too be very similar to the closed loop profile. The predicted

optimal objective value is $M_C(t_f) = 6.3949 \text{ kmol}$. Hence the optimal objective value of the resultant cascade closed-loop optimization with control system, and that of the end-point dynamic optimization are very close. Several other simulations were conducted to demonstrate the robustness of the method to measurement noise, see Figures 6 and 7.

6. CONCLUSIONS

A cascade closed loop optimisation and control strategy for batch reactors has been presented. This algorithm addresses the commonly encountered difficulty of obtaining reliable kinetic information and online concentration measurements. Reaction and concentration information is inferred from more readily available temperature measurements using a nonlinear observer which rapidly tracks the dynamics of the system. The strategy is accomplished by reducing the model into two subsystems, which allowed independent design of the optimizer and the controller.

Optimisation is accomplished with a constrained SQP algorithm, which is applied in a decending horizon fashion at each time step. Feedback is introduced indirectly by using model error associated with the unknown kinetic information. A GMC controller is effectively used to force the nonlinear system to track the optimal profile. Simulations under many different operating conditions have confirmed the performance of the strategy and showed that it compares favorably with the corresponding offline optimization results obtained via standard methods. The reduced computational burden and feedback structure make this approach suitable for online implementation.

REFERENCES

- Berber, R., "Control of Batch Reactors: A Review," *Methods of Model Based Process Control, NATO ASI Series*, Kluwer Academic Publishers, The Netherlands, **293**, 459 (1995).
- Cott, B. J. and S. Macchietto, "Temperature Control of Exothermic Batch Reactors Using Generic Model Control," *Ind. Eng. Chem. Res.*, **28**, 1177(1989).
- Farza, M., H. Hammouri, C. Jallut and J. Lieto, "State Observation of a Nonlinear System: Application to (Bio) chemical Processes," *AIChE J.*, **45**, 93 (1999).
- Hua, X. and A. Jutan, "Nonlinear Inferential Cascade Control of Exothermic Fixed-bed Reactors," *AIChE J.*, **46**, 980 (2000).
- Jutan, A. and A. Uppal, "Combined Feedforward-Feedback Servo Control Scheme for an Exothermic Batch Reactor," *Ind. Eng. Chem. Process Des. Dev.* **23**, 597 (1984).
- Lee, P. L., and G. R. Sullivan, "Generic Model Control (GMC)," *Comptu. Chem. Eng.*, **12**, 573 (1988).

Palanki, S. and M. Krothapally, "On-line Optimization of Batch Processes," *Trends in Chem. Eng.*, **5**, 45 (1998).

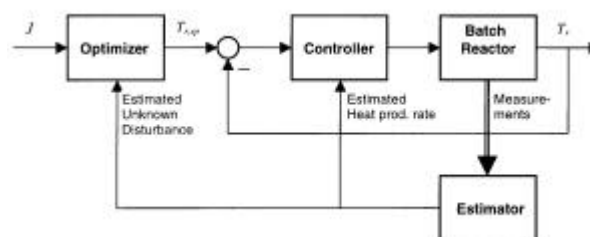


Fig. 1: Cascade optimization and tracking system

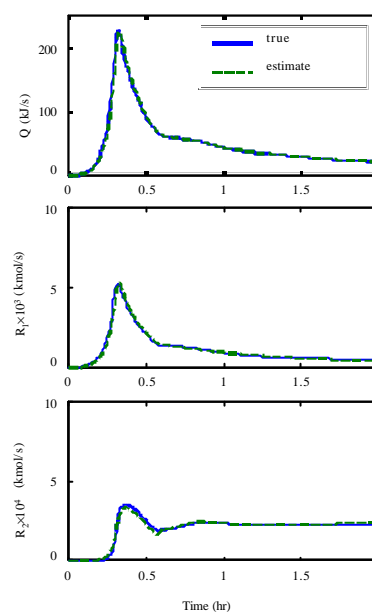


Fig 2: On-line estimation performance under the nominal condition.

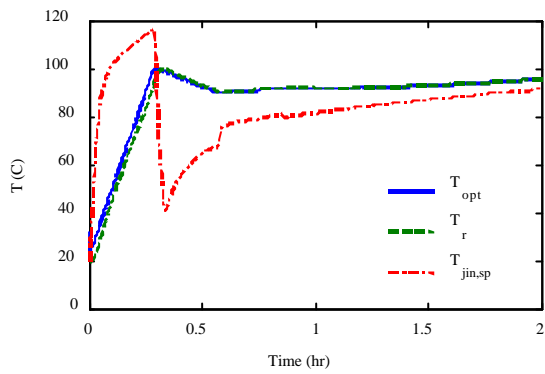


Fig. 3: Closed-loop optimisation and control performance under the nominal condition.

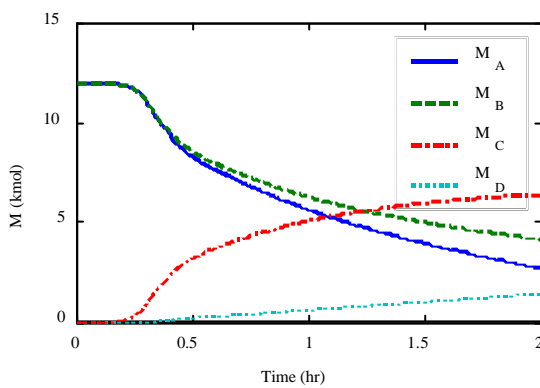


Fig. 4: Mole profiles of all components with closed-loop optimisation and control.

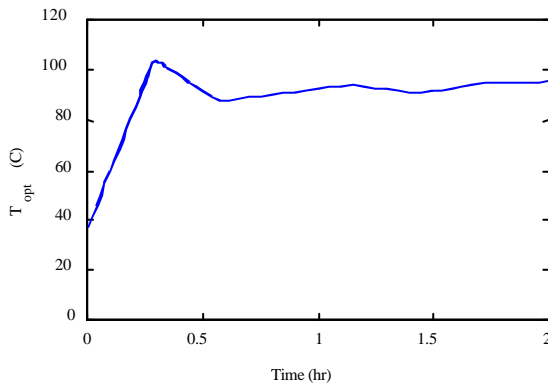


Fig. 5: Open loop optimal temperature profile calculated off-line using end-point optimisation algorithm under the nominal condition.

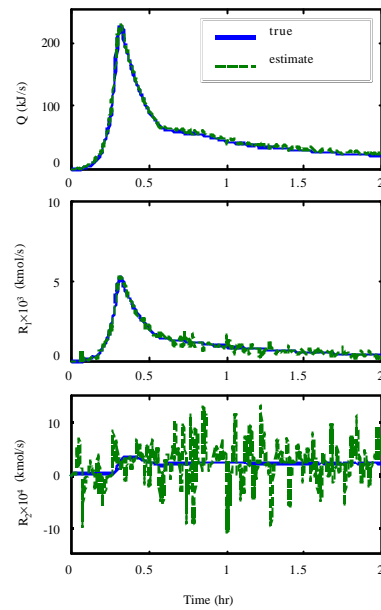


Fig. 6: On-line estimation performance with the same condition as in Figures 2-3, but with noisy measurements.

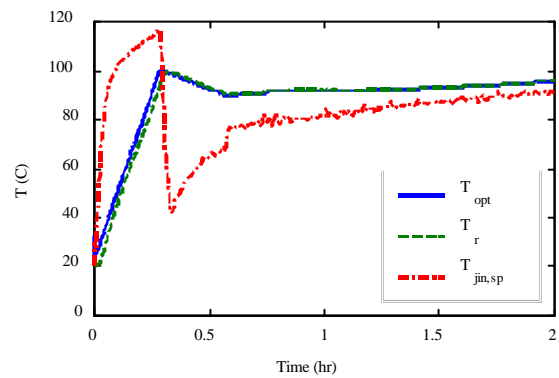


Fig. 7: Closed-loop optimization and control performance with the same condition as in Figs. 2-3, but with noisy measurements.