Optimal Operation of an Energy Integrated Batch Reactor - Feed Effluent Heat Exchanger System *

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Abstract: Energy integration in batch reactors offers significant savings but at the cost of additional operational constraints. In this paper, optimal operation of a batch reactor-feed effluent heat exchanger system is pursued for a production campaign. The coupling between subsequent batches due to energy integration is exploited to predict and thus plan future batches to achieve desired product purity at the end of the production campaign in the presence of disturbances and time-dependent energy prices. The proposed solution leads to better operation compared to a controller with disturbance rejection.

Keywords: Optimization, Batch Process Modeling and Control, Energy Processes and Control

1. MOTIVATION

Energy integration in batch process systems is achieved by (simultaneous or sequential) optimization of batch schedule and energy consumption (Kemp and Deakin, 1989; Zhao et al., 1998; Majozi, 2006; Halim and Srinivasan, 2008). While such designs promise economic benefits, their operation is challenging compared to their continuous counterparts. Due to the dynamic nature of batch systems, energy integration is constrained by temperature (thermal equilibrium) as well as time (availability of cold and hot streams) constraints (Wang and Smith, 1995). This has resulted in two major integration strategies for batch process systems - direct energy integration and indirect energy integration (Fernandez et al., 2012).

The strong dependence between energy integration and batch schedule means that economic benefits are highly sensitive to any disturbances. Such disturbances, especially the ones changing batch processing times, can reduce the effectiveness of energy integration, and in some cases, can render such integration infeasible.

In previous work (Jogwar and Daoutidis, 2014), we have shown that the coupling between subsequent batches due to energy integration in batch process systems results in slow network-level dynamics. This slow dynamics captures the batch-to-batch evolution of process variables. Such slow dynamics can be triggered by a local (to a batch) disturbance. Furthermore, it has been shown that simple rejection of such a local disturbance may not lead to optimal operation over a production campaign. In this paper, we address the problem of optimal operation of energy integrated batch systems with the help of a batch reactor-feed effluent heat exchanger (BR-FEHE) system as a representative example. Control and optimization of repetitive batch systems, in the absence of any energy integration, has been pursued within the framework of adaptive control (Flores-Cerrillo and MacGregor, 2003), iterative learning control (Lee and Lee, 2007) and optimal control (Srinivasan et al., 2003). The novelty of this work lies in the efficient utilization of the natural inter-batch coupling resulting from energy integration. Specifically, we explicitly utilize a model of the slow batch-to-batch dynamics for the solution of the optimization problem that determines the optimal operating conditions for the production campaign.

The rest of the paper is organized as follows. Section 2 provides a brief description of the system. Section 3 presents a prediction model to capture the slow interbatch dynamics. This model is then used in Section 4 for the optimization of energy consumption in the BR-FEHE system for two sets of disturbance studies.

2. ENERGY INTEGRATED BR-FEHE SYSTEM

One of the frequently used strategy employed in energy integrated reactors, especially the ones operating at elevated temperature, is to utilize the energy available with the reactor effluent (hot stream) to preheat the feed (cold stream). This is achieved by installing a process-to-process heat exchanger (FEHE) as shown in Figure 1. This system uses direct energy integration strategy (direct transfer of energy from the hot stream to the cold stream). This requires the hot stream (reactor effluent) to be available

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Fig. 1. BR-FEHE system with direct energy integration



Fig. 2. Gantt chart representing schedule for the BR-FEHE system (L: loading, O: operating, U: unloading)

at the same time as the cold stream (reactor feed). Thus, such a direct strategy cannot be employed within a batch and typically integration is pursued between hot and cold streams of successive batches. Figure 2 shows the Gantt chart for this system. The FEHE, which is a counter-current exchanger, operates continuously over specific time intervals. Additional details about the system can be found in Jogwar et al. (2014).

Detailed dynamic model of the BR-FEHE system can be obtained via unsteady state material and energy balance equations. A consecutive reaction system (A \rightarrow B \rightarrow) is considered wherein the intermediate component is the main product. For such a system, the trade-off between product yield and energy consumption becomes a key issue. We are specifically interested in developing an optimal operation strategy which will allow for (energy) efficient operation in an event of a local disturbance (increased/reduced heating capacity) and/or time-dependent energy price. For reference, the detailed dynamic model is presented in the Appendix section. Table 1 gives definitions and the nominal values for the major process variables.

3. PREDICTION MODEL FOR SLOW BATCH-TO-BATCH DYNAMICS

In Jogwar and Daoutidis (2014), it was shown that the BR-FEHE in Figure 1 exhibits dynamics over two time scales. For example, Figure 3 depicts the evolution of the reactor temperature for a disturbance of -20% in the heater duty over the production campaign. The fast time scale captures the dynamics of the process variables in a batch whereas the slow time scale captures the batch-

Variable/	Description	Value
Parameter		
Fin	Furnace feed rate	$5.77 \times 10^{-4} m^3/s$
F_{heater}	Furnace unloading rate	$2.31 \times 10^{-3} m^3/s$
Freactor	Reactor unloading rate	$5.77 \times 10^{-4} m^3/s$
T_{in}	Feed inlet temperature	300.00 K
$T_{Cout,FEHE}$	FEHE cold side	$837.84 \ K$
	exit temperature	
$T_{Hout,FEHE}$	FEHE cold side	$302.01 \ K$
,	exit temperature	
T _{heater,end}	Heater exit temperature	878.57 K
T _{reactor,end}	Reactor exit temperature	889.96 K
C_{A0}	Feed concentration, A	$1000 \ mol/m^{3}$
C_{B0}	Feed concentration, B	$0 \ mol/m^3$
$C_{A,reactor,end}$	Reactor concentration, A	$21.66 \ mol/m^3$
$C_{B,reactor,end}$	Reactor concentration, B	$913.29 \ mol/m^3$
$C_{B,out}$	Product concentration, B	$913.29 \ mol/m^3$
Q_{heater}	Heater duty	$393.05 \ kW$
α	FEHE bypass ratio	0.1000
k_{10}	Kinetic Pre-exponent	$5.35 \times 10^5 \ s^{-1}$
	for reaction $A \to B$	
k_{20}	Kinetic Pre-exponent	$9.22 \times 10^{12} s^{-1}$
	for reaction $\mathbf{B} \to \mathbf{C}$	
E_1	Activation energy	$150.72 \ kJ/mol$
	for reaction $A \to B$	
E_2	Activation energy	$301.44 \ kJ/mol$
	for reaction $\mathbf{B} \to \mathbf{C}$	
ΔH_1	Heat of reaction	-44307 J/mol
	for reaction $A \to B$	
ΔH_1	Heat of reaction	-65938 J/mol
	for reaction $\mathbf{B} \to \mathbf{C}$	
U	Heat transfer coefficient	$209.2 \ kW/m^2/K$
A	Hear transfer area	$0.4 \ m^2$

Table 1. Nominal values of the process parameters for the BR-FEHE system

to-batch evolution of the process variables. This interbatch dynamics can be effectively used to predict the effect of a local disturbance on the system outputs over a production campaign. Furthermore, it can also be used for efficient utilization of costly resources by manipulating the batches of a production campaign. In this section, we develop a simplified model to capture the batch-to-batch dynamics. The main objective of the model is to capture the effect of the heater duty in a batch ($Q_{heater,k}$) which is considered the main disturbance on the purity of the desired product in the tank ($C_{B,out,k}$) in the presence of inter-batch coupling through the FEHE. The subscript krepresents the batch number. It is assumed that the batch processing times are kept constant.



Fig. 3. Response of the reactor temperature over the production campaign for a -20% disturbance in heater duty for batch # 2

Fired heater

Given the heater temperature at the beginning of the operating phase $(T_{heater,0,k})$, the temperature at the end of the operating phase $(T_{heater,end,k})$ can be obtained by integrating Eq. (11) in Appendix with $F_{in} = F_{heater} = 0$ and $V_{heater,0,k} = V_{heater,min} + F_{in} \times \text{FEHE}$ runtime:

$$T_{heater,end,k} = T_{heater,0,k} + \frac{Q_{heater,k} \times \text{Heater runtime}}{V_{heater,end,k}\rho C_p}$$
(1)

where the subscript 0 represents the value at the beginning of the operating phase.

Reactor

The hot reactant is completely transferred from the fired heater to the reactor. This gives $V_{reactor,0,k} = V_{heater,0,k}$ and $T_{reactor,0,k} = T_{heater,end,k}$. For the operating phase of the reactor, Eq. (14) and (15) cannot be integrated analytically. To this end, Eq. (14) is numerically integrated for a variety of $T_{reactor,0,k}$ values in the range of 800-1000K. The resulting values of $T_{reactor,end,k}$ and $C_{B,reactor,end,k}$ are fitted in the following Gaussian functions:

$$T_{reactor,end,k} = \sum_{i=1}^{3} a_{T,i} * exp \left(-1 * \left((T_{reactor,0,k} - b_{T,i})/c_{T,i} \right)^2 \right) + T_0$$

$$C_{B,reactor,end,k} = \sum_{i=1}^{4} a_{C,i} * exp \left(-1 * \left((T_{reactor,0,k} - b_{C,i})/c_{C,i} \right)^2 \right) + C_0$$
(2)

with

 $a_T = \begin{bmatrix} 328.1 & 5.063 & 856.3 \end{bmatrix}^T, a_C = \begin{bmatrix} 385 & 570.8 & 182.5 & 468.9 \end{bmatrix}^T,$ $b_T = \begin{bmatrix} 1135 & 948.8 & 930.7 \end{bmatrix}^T, b_C = \begin{bmatrix} 902.2 & 870.8 & 924.6 & 829.4 \end{bmatrix}^T,$ $c_T = \begin{bmatrix} 180.6 & 28.94 & 470.6 \end{bmatrix}^T, c_C = \begin{bmatrix} 27.2 & 37.61 & 20.35 & 50.86 \end{bmatrix}^T,$ $T_0 = 0.366 \text{ and } C_0 = 0.$

Figure 4 shows the comparison between the actual and the fitted data.

FEHE

The reactor effluent stream and the cold feed are the two inputs to the FEHE. Assuming constant feed conditions,

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Fig. 4. Comparison between the actual and fitted data for the batch reactor

the FEHE Eq. (8) and (9) were numerically integrated. During the operating phase of the FEHE, the fired heater is loaded with the heated feed. For the various values of the reactor effluent temperature $T_{reactor,end,k}$, the corresponding temperature of the heater at the end of the loading phase was fitted in the following form:

$$T_{heater,0,k+1} = 0.8847 \times T_{reactor,end,k} + 50.91$$
 (3)

Product tank

The product formed in the reactor in the k^{th} batch is added to the product tank where it mixes with the product formed in the earlier batches. The overall and component material balance gives the following evolution equations:

$$V_{productTank,k} = V_{productTank,k-1} + F_{reactor} \times \text{FEHE runtime} \\ C_{B,out,k} = \frac{F_{reactor} \times \text{FEHE runtime}}{V_{productTank,k}} C_{B,reactor,end,k} + \frac{V_{productTank,k-1}}{V_{productTank,k}} C_{B,out,k-1}$$
(4)

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Table 2. Values of parameters used for optimization

Parameter	Value
p_1 to p_{20}	$80 \ units/kWh$
p_{21} to p_{50}	$40 \ units/kWh$
$C_{B,out,desired}$	913.3 mol/m^3
$Q_{heater,min}$	$275.13 \ kW$
$Q_{heater,max}$	$510.96 \ kW$

Eq. (1), (2), (3) and (4) together capture the evolution of process variables over multiple batches. Specifically, they can predict the effect of a local disturbance in $Q_{heater,k}$ on the purity of the product B ($C_{B,out,k}$) over the production campaign.

4. OPTIMAL OPERATION OF THE BR-FEHE SYSTEM

Let us now consider optimal operation of this BR-FEHE system in the presence of unanticipated disturbances. Optimal operation for this system is achieved by meeting the desired product purity in the product tank at the end of the campaign (batch # 50) by consuming minimum external energy. It is considered that there is a disturbance in the heater duty during batch # 2 (which triggers the batch-to-batch dynamics). Additionally, it is considered that energy price is time-dependent. The following optimal operation problem is set up:

$$\begin{array}{ll} \underset{Q_{heater,k}(2 < k \leq 50)}{\text{minimize}} & J = \sum_{i=1}^{50} p_i Q_{heater,i} \\ \text{subject to} & C_{B,out,k} = f\left(C_{B,out,k-1}, Q_{heater,k}\right) \\ & C_{B,out,50} \geq C_{B,out,desired} \\ & Q_{heater,min} \leq Q_{heater,k} \leq Q_{heater,max} \\ \end{array} \right.$$
(5)

where the objective function J represents the total cost of utilities, p_i represents the cost of utility during the i^{th} batch, $C_{B,out,desired}$ is the desired product purity at the end of the campaign, and $Q_{heater,min}$ and $Q_{heater,max}$ represent the minimum and maximum duty possible for the fired heater. The function $f(\cdot)$ captures the evolution of $C_{B,out,k}$ over multiple batches and is a combination of Eq. (1), (2), (3) and (4). The values of the various parameters used are tabulated in Table 2.

In the first simulation case study, the disturbance in $Q_{heater,2}$ is -20% of the nominal value. The optimization problem in Eq. (5) is solved using the NLPSQP solver in gPROMS. After 97 iterations, an optimal profile of heater duty is found for batches 3 through 50. The CPU time taken is only 6.9895s. The BR-FEHE dynamic model in Appendix is then simulated with this optimal input profile for the considered local disturbance. Additionally, this performance is compared with a case where the local disturbance is regulated using a controller of the following form:

$$Q_{heater,k} = \frac{V_{heater,0,k}C_p}{\text{heater runtime}} \left(T_{heater,end,set} - T_{heater,0,k}\right)$$
(6)

wherein $T_{heater,end,set}$ is the desired set point. Figure 5 depicts the responses of the uncontrolled, controlled and optimal cases. The values of the objective function for

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the uncontrolled case, the controlled case and the optimal case are 273.56, 275.10 and 269.09 units respectively. The uncontrolled case, which represents the openloop response, shows the propagation of the local disturbance over the production campaign. It can be seen that this case leads to the highest product purity which can be attributed to the constructive nature of the disturbance. However, energy consumption in this case (as highlighted by the objective function) is higher than the optimal case. The controlled case tends to compensate for the disturbance in the batches following the local disturbance (without considering time-dependent energy prices) and thus performs less efficiently even compared to the uncontrolled case. The optimal solution defers the use of external energy until it is available at a cheaper rate (see p_i values in Table 2). The optimizer does not react to the local disturbance directly but keeps the heater duty close to the nominal value for most of the time. Only when the energy is available at a cheaper rate, extra energy is utilized. Furthermore, less energy is consumed towards the end of the campaign as the purity deviations at that time are not going to significantly change the overall composition of the tank. The optimal case presents a 2.2% reduction in the objective function over the controlled case. Note that the final product purity in the optimal case is slightly lower than the desired value. This can be attributed to the mismatch between the detailed hybrid (continuous + discrete) dynamic model used for simulation and the simplified discrete prediction model used for optimization. One way to handle this is by increasing the product purity specification during optimization. For example, if we set the desired product purity as 914.0 during optimization, Figure 6 shows the corresponding responses. In this case, the savings reduce to 2.0% but the final product purity obtained is greater than the desired value.

In the next simulation case, the disturbance in $Q_{heater,2}$ is +20% of the nominal value. In this case, the optimizer took 108 iterations with CPU time of 7.301s. Figure 7 depicts the response of the BR-FEHE system under this local disturbance for the controlled, uncontrolled and optimal case. The values of the objective function for the uncontrolled case, the controlled case and the optimal case are 276.71, 275.15 and 269.52 units respectively. For the uncontrolled case, the disturbance adversely affects the reactor operation and the final product purity is lower than the desired value. The nature of the openloop responses to disturbances of the same magnitude but different directions ($\pm 20\%$) highlights the nonlinear nature of the batch-to-batch dynamics. Due to this nonlinearity, simple rejection of the local disturbance in the controlled case does not lead to the desired product purity for this local disturbance. The optimal case presents a 2.0%reduction in the objective function over the controlled case.

5. CONCLUDING REMARKS

In this paper, we have considered the optimal operation of an energy integrated batch process system. It was shown that the inter-batch coupling introduced due to energy integration provides an opportunity to pursue campaignlevel optimization of energy consumption through the manipulation of individual batches. To capture the interbatch dynamics, a simplified model was developed based



Fig. 5. Product purity and heater duty profile for a -20% disturbance in $Q_{heater,2}$

on the solution of the material and energy balance equations, and mathematical regression. The effectiveness of the proposed framework was demonstrated with the help of case studies on an energy integrated batch reactorfeed effluent heat exchanger network. Specifically, energy savings of the order of 2% were documented over a (controlled) case without optimization. It can be noted that the case considered here tries to achieve the desired product purity at the end of the campaign with upper/lower bounds on the purity of the product formed during the intermediate batches. The operational strategy considered here does not discard the below-par batch (obtained during the local disturbance) but adjusts the remaining batches (as per slow batch-to-batch dynamics) in the campaign to achieve the desired product purity at the end of the campaign. Such a strategy has additional time and energy savings compared to conventional policy of discarding the below-par batch obtained in the case of such local disturbances. The results in this paper highlight opportunities for campaign-wide run-time optimization for energy integrated batch process systems.

The framework presented in this paper has general applicability. The challenge remains to systematically derive



Fig. 6. Product purity and heater duty profile for a -20% disturbance in $Q_{heater,2}$ with updated desired purity constraint

the mathematical description of the slow batch-to-batch dynamics, and is currently being pursued in our research.

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Fig. 7. Product purity and heater duty profile for a +20% disturbance in $Q_{heater,2}$

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APPENDIX

Dynamic model for the BR-FEHE system as given in Jogwar et al. (2014)

$$\frac{dV_{sourceTank}}{dt} = -F_{in} \tag{7}$$

$$\frac{\partial T_H}{\partial t} = -v_H \frac{\partial T_H}{\partial z} - \frac{UA\left(T_H - T_C\right)}{\rho C_p V_H} \tag{8}$$

$$\frac{\partial T_C}{\partial t} = v_C \frac{\partial T_C}{\partial z} + \frac{UA(T_H - T_C)}{\rho C_p V_C} \tag{9}$$

$$T_{H,z=0} = T_{reactor,end}$$

$$T_{C,z=L} = T_{in}$$

$$\frac{dV_{heater}}{dt} = F_{in} - F_{heater}$$
(10)

$$\frac{dT_{heater}}{dt} = \frac{F_{in}\left(T_{Cout,FEHE} - T_{heater}\right)}{V_{heater}} + \frac{Q_{heater}}{V_{heater}\rho C_p} \tag{11}$$

$$\frac{dV_{reactor}}{dt} = F_{heater} - F_{reactor} \tag{12}$$

$$\frac{dC_{A,reactor}}{dt} = \frac{F_{heater}}{V_{reactor}} \left(C_{A0} - C_{A,reactor} \right) -k_{10}exp \left(\frac{-E_1}{RT_{reactor}} \right) C_{A,reactor}$$
(13)

$$\frac{dC_{B,reactor}}{dt} = \frac{F_{heater}}{V_{reactor}} \left(C_{B0} - C_{B,reactor} \right) + k_{10} exp \left(\frac{-E_1}{RT_{reactor}} \right) C_{A,reactor} - k_{20} exp \left(\frac{-E_2}{RT_{reactor}} \right) C_{B,reactor}$$
(14)
$$\frac{dT_{reactor}}{F_{heater}} = \frac{T_{heater}}{T_{heater}} \left(T_{heater} - T_{heater} \right)$$

$$\frac{dT}{dt} = \frac{1}{V_{reactor}} \left(T_{heater} - T_{reactor} \right) + \left(\frac{-\Delta H_1}{\rho C_p} \right) k_{10} exp \left(\frac{-E_1}{RT_{reactor}} \right) C_{A,reactor} + \left(\frac{-\Delta H_2}{\rho C_p} \right) k_{20} exp \left(\frac{-E_2}{RT_{reactor}} \right) C_{B,reactor}$$
(15)

$$\frac{dV_{productTank}}{dt} = F_{reactor} \tag{16}$$

$$\frac{dC_{B,out}}{dt} = \frac{F_{reactor}}{V_{productTank}} \left(C_{B,reactor} - C_{B,out} \right)$$
(17)
$$\frac{dT_{out}}{dT_{out}} = \frac{(1-\alpha)F_{reactor}}{(1-\alpha)F_{reactor}} \left(T_{H_{reactor}} + T_{reactor} - T_{reactor} \right)$$

$$\frac{T_{out}}{dt} = \frac{(1-\alpha)F_{reactor}}{V_{productTank}} \left(T_{Hout,FEHE} - T_{out} \right) \\
+ \frac{\alpha F_{reactor}}{V_{productTank}} \left(T_{reactor} - T_{out} \right)$$
(18)

Note that these equations capture all the three (L, O and U) phases of these equipment.

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