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PROCESS DESIGN AND CONTROL

Optimizing the Initial Conditions To Improve the Dynamic Flexibility of Batch Processes

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It is shown in this paper that by changing the initial operation condition of batch processes, the dynamic performance of the system can be varied largely. The initial operation conditions are often ignored in design of batch processes for flexibility against disturbances or parameter variations. When the initial conditions are not rigid, as in the case of a batch reactor where the initial reaction temperature is quite arbitrary, optimization can also be applied to determine the "best" initial condition to be used. Problems for dynamic flexibility analysis, including initial conditions and process operation, can be formulated as dynamic optimization problems. If the initial conditions are considered, the conditions can be transferred into control variables in the first step of optimization. The solution of the dynamic optimization is based on the Runge-Kutta integration algorithm and decomposition search algorithm. This method, as illustrated and tested with two highly nonlinear chemical engineering problems, enables the optimal solution to be determined.

Introduction

The problems with running of chemical plants are often related to the uncertainty of the parameters. The uncertainties can correspond to variation either in the values of external parameters, such as quality of the feed streams, product demand, or environmental conditions, or the values of internal parameters, such as transfer coefficients, reaction constants, physical properties of the materials, uncertainties in model parameters, and so forth. The chemical plants must have the satisfactory level of flexibility to achieve a feasible operation over the given range of the above stated uncertain conditions. The systematic incorporation of flexibility in the synthesis and design of chemical processes has received increasing attention in the literature.[1−8]

As discussed by Swaney and Grossmann,[7,8] the physical performance of a chemical process can be described by the following constraints

$$\mathbf{h}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0 \tag{1}$$

$$\mathbf{g}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0 \tag{2}$$

where $\dim\{\mathbf{h}\} = \dim\{\mathbf{x}\}$. In eqs 1 and 2, $\mathbf{h}$ is the vector of equations (e.g., mass and energy balances or equilibrium relations) which hold for steady−steady operation of the processes, and $\mathbf{g}$ is the vector of inequalities (e.g., design specifications or physical operating limits) which must be satisfied if operation is to be feasible. The variable $\mathbf{d}$ is the vector of design variables, $\mathbf{x}$ is the vector of the state variable, $\mathbf{z}$ is the vector of the control variables, and $\boldsymbol{\theta}$ is the vector of the uncertain parameters. The state variables can be implicitly eliminated between eqs 1 and 2, so that the process system may be described by the following simplified inequality constraints:

$$\mathbf{g}(\mathbf{d}, \mathbf{x}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}), \mathbf{z}, \boldsymbol{\theta}) = \mathbf{f}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta} \leq 0 \tag{3}$$

Given a nominal parameter value $\boldsymbol{\theta}^{\mathrm{N}}$ and expected deviations $\Delta\boldsymbol{\theta}^{+}$, $\Delta\boldsymbol{\theta}^{-}$ in the positive and negative directions, the specified set of uncertain parameters $\mathbf{T}$ will be given by

$$\mathbf{T} = (\boldsymbol{\theta}|\boldsymbol{\theta}^{\mathrm{N}} - \Delta\boldsymbol{\theta}^{-} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^{\mathrm{N}} + \Delta\boldsymbol{\theta}^{+}) \tag{4}$$

According to the parameter set $\mathbf{T}$, the feasibility test for a design can be formulated mathematically as the max−min−max problem

$$\chi(d) = \max_{\boldsymbol{\theta}\in\mathbf{T}} \min_{\mathbf{z}} \max_{j\in\mathbf{J}} f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \tag{5}$$

where $\chi(d)$ can be regarded as a feasibility measure for a given design $\mathbf{d}$. If $\chi(d) \leq 0$, the design is feasible in $\boldsymbol{T}$. If $\chi(d) > 0$, the solution will identify a critical point $\boldsymbol{\theta}^{\mathrm{c}} \in \mathbf{T}$ for which the greatest violation in the constraints occurs.

In order to quantify the ability of such processes to operate at points other than the nominal point of operation, a scalar flexibility index, F, can be formulated as the problem

$$F = \max \delta \tag{6}$$

$$s.t. \max_{\boldsymbol{\theta}\in\mathbf{T}(\delta)} \min_{\mathbf{z}} \max_{j\in\mathbf{J}} f_j(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}) \leq 0$$

$$T(\delta) = (\boldsymbol{\theta}|\boldsymbol{\theta}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}^{-} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}^{+}), \quad \delta \geq 0$$

This flexibility index F represents the largest scaled deviation that the design can accommodate, while remaining feasible. A value of $F \geq 1$ indicates that the flexibility target is clearly satisfied; $F < 1$ index indicates that at least one parameter variation causes failure.

There are different approaches proposed to handle the steady-state flexibility analysis problem.[7−13] On the basis of the solution of the steady-state flexibility analysis, researchers redesigned the continuous processes to improve the flexibility.[14−18] However, the feasibility and flexibility of operation for a dynamic system is different from the steady system. This was proven by

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Dimitriadis and Pistikopoulos[3] in an example of a simple storage tank dynamic system. On the basis of the steady state approach, a formulation for dynamic feasibility of operation was presented in the literature.[3] The problem was equivalent to the optimization problem of the algebraic equations as their initial condition was fixed.

$$\chi(d) = \max_{\boldsymbol{\theta}(t)\in \mathbf{T}(\delta(t))} \min_{\mathbf{z}(t)\in \mathbf{Z}(t)} \max_{t\in[0,H]} \mathbf{g}(\mathbf{d}, \mathbf{x}(t), \mathbf{z}(t), \boldsymbol{\theta}(t), \boldsymbol{t}) \quad (7)$$

$$s.t.\ \mathbf{h}(\mathbf{d}, \mathbf{z}(t), \dot{\mathbf{x}}(t), \mathbf{x}(t), \boldsymbol{\theta}(t)) = 0; \quad \mathbf{x}(0) = \mathbf{x}^0 \quad (8)$$

$$T(\delta(t)) = \{\boldsymbol{\theta}(t) | \boldsymbol{\theta}^{\mathrm{L}} - \delta(t)\Delta\boldsymbol{\theta}^{-} \le \boldsymbol{\theta}(t) \le \boldsymbol{\theta}^{\mathrm{U}} + \delta(t)\Delta\boldsymbol{\theta}^{+}\} \quad (9)$$

$$\mathbf{z}(t) = \{\mathbf{z}(t) | \mathbf{z}^{\mathrm{L}}(t) \le \mathbf{z}(t) \le \mathbf{z}^{\mathrm{U}}(t)\} \quad (10)$$

To solve the problem of flexibility analysis of a dynamic system in the form of eqs 7−10, the orthogonal collocation techniques were applied.

Clearly, the flexibility analysis for a dynamic system is more important than the steady state system. The processes' flexibility cannot actually be described without accounting for the processes' control dynamics. Brengel and Seider[19] also advocated the need for design and control integration. The flexibility design and controllability integration were identified and discussed by several groups.[20−25] In the batch processing, there is no inflow or outflow of reactants or products while the reaction is being carried out. The reactants are initially charged into a vessel, mixed, and left to react for a certain period. The resultant mixture is then discharged. This is an inherently unsteady-state operation, where composition and temperature change with time.[26] In fact, except in the work by Dimitriadis and Pistikopoulos,[3] the flexibility analysis for the dynamic system is mainly applied to the continuous processes. The flexibility issue of batch processes has not been yet extensively studied. So batch processes offer some of the most interesting and challenging problems in flexibility analysis because of their inherent dynamic nature often dependent on their initial conditions. Modeling of batch reactors results in differential and algebraic equations (DAEs), and optimization of such reactors requires the use of dynamic optimization technique.

To obtain the solution of the flexibility analysis in dynamic system, the orthogonal collocation techniques[27] with a polynominal approximation were applied in the work.[3] Nevertheless, the method relies on the assumption that the initial conditions are fixed for the batch process. It is important to note that the regions of the feasible operation for batch processes are affected by their initial condition as shown in Example 1. This implies that it is meaningful for the dynamic flexibility analysis of batch processes that the initial condition should be considered. Neglecting this fact can lead to serious overestimation of the flexibility of batch processes. Therefore, the main question that will be addressed in this paper is about the dynamic flexibility analysis for the batch process including the initial condition as well as operation condition constraints.

In this paper, a new approach is presented for the problem of dynamic flexibility analysis of batch processes including the initial conditions. When the initial condition is not rigid as in the case of a batch reactor, where the initial volume is quite freely varied, optimization can also be applied to determine the "best" initial condition to be used.

The formulation of the flexibility analysis for batch processes is scaled by its flexibility index. The solution procedures are presented for the cases of point and path constraints. For instance, the requirement that the volume of liquid in a batch reactor should lie between certain bounds during operation is a path constraint. The former involves the initial condition and end point constraint which are often required for batch processes. The solution procedures are based on the Runge-Kutta integration algorithm and decomposition search algorithm. For the initial condition point constraint, the solution strategy consists of transformation of initial condition into control variable in the first solution step. The solution procedures are implemented on the MATLAB platform, and the application of the formulations is illustrated in two examples.

Search and Integration Method in Dynamic Flexibility Analysis

It will be shown in this section that the dynamic flexibility analysis problem is extended for batch processes including the initial condition constraints. The formulation can be expressed as the following

$$\chi(\mathbf{d}) = \max_{\boldsymbol{\theta}(t)\in \mathbf{T}(\delta(t))} \min_{\mathbf{z}(t)\in \mathbf{Z}(t)} \max_{t\in[0,H]} \mathbf{g}(\mathbf{d}, \mathbf{x}(t), \mathbf{z}(t), \mathbf{x}(0), \boldsymbol{\theta}(t), t) \quad (11)$$

$$s.t.\ \mathbf{h}(\mathbf{d}, \mathbf{z}(t), \dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{x}(0), \boldsymbol{\theta}(t)) = 0 \quad (12)$$

$$\mathbf{x}(0) = \mathbf{z}_{\mathbf{x}} = \{z_{x(i)} | z^{\mathrm{L}}_{x(i)} \le z_{x(i)} \le z^{\mathrm{U}}_{x(i)}\} \quad (13)$$

$$\mathbf{z}(t) = \{\mathbf{z}(t) | \mathbf{z}^{\mathrm{L}}(t) \le \mathbf{z}(t) \le \mathbf{z}^{\mathrm{U}}(t)\} \quad (14)$$

$$\mathbf{T}(\delta(t)) = \{\boldsymbol{\theta}(t) | \boldsymbol{\theta}^{\mathrm{L}} - \delta(t)\Delta\boldsymbol{\theta}^{-} \le \boldsymbol{\theta}(t) \le \boldsymbol{\theta}^{\mathrm{U}} + \delta(t)\Delta\boldsymbol{\theta}^{+}\} \quad (15)$$

where the initial conditions of the system are described as eq 13. It means that the initial conditions can be handled as a constraint in the optimal problem. If eqs 11−15 are applied to batch processes, the optimal solution will determine the "best" initial value of the system. For the optimal problem, it is difficult to handle the initial values of some of the state variables using orthogonal techniques. Because the initial point of each element is required to take into account in the approximation in the orthogonal techniques, some initial values of the state variables are unknown at first. In fact, the control variables should be optimized in the dynamic optimal problem. To solve the optimal problem with initial condition, the optimal initial values of certain state variables can be regarded as control variables.

To effectively solve the problem of eqs 11−15, some simplification should be introduced. For example, the design variables **d** are fixed for the existing process system. So eq 12 can be written as follows:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, \mathbf{z}, \boldsymbol{\theta}) \quad (16)$$

To ensure the product quality and process safety, path and point constraints must be satisfied:

$$\mathbf{x}(t_f) \ge \mathbf{x}^{t_f} \quad (17)$$

$$\mathbf{x}^{\mathrm{L}} \le \mathbf{x} \le \mathbf{x}^{\mathrm{U}} \quad (18)$$

Equation 17 is the point constraint, and eq 18 is the path constraint. For example, the final reactant conversion must exceed the specified value which can be expressed as eq 17. For the batch process system, a time horizon H can be defined which corresponds to a whole batch reaction time. The optimal problem is to find the maximum of the value of the δ of eq 15, the suitable $\mathbf{Z}(t)$ and the "best" initial value of the state vector for which the path and point constraints are satisfied in the time

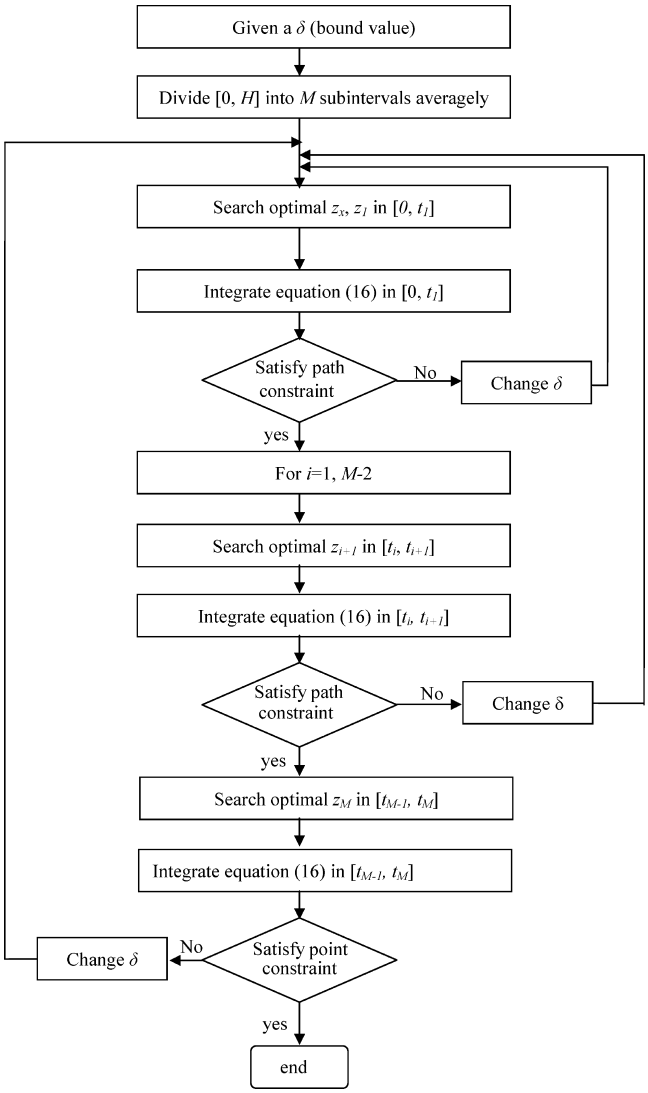

Figure 1. Algorithm of the proposed method.

interval [0, H]. The above problem can be solved by decomposition and integration to obtain an optimal result as presented by Luus and Hennessy.[28] However, the initial region size should be chosen in the method of ref 28 at first. In the later search steps, the contraction factor η is used, and the region size was stored to η times the initial region size. If the value of η is unsuitable, the region will be collapsed. So the algorithm of the optimal problem used here is based on the golden section search and Runge−Kutta integration method.[29] The algorithm is presented in Figure 1, and it involves 10 steps:

S.1. Assign an initial value to the flexibility index δ in the expected range of uncertainty parameters. First the boundary value of the uncertain parameter corresponding to the flexibility index is assigned to the δ.

S.2, Divide the time interval [0, H] into M subintervals [0, t_1], [t_1, t_2],..., [t_{k-1}, t_k],..., [t_{M-1}, t_M], each of an equal length $L = H/M$. In general, the interval L of the subinterval is 5 s for the selection of the M.

S.3. For the differential eq 16, the initial value of the state vector is chosen according eq 13. Then the control variables are chosen in the range of eq 14 for integration of the differential eq 16 in the first subinterval [0, t_1] using the Runge−Kutta method. If the result of the integration is out of the range of path constraints of eq 18, then the control variables are chosen again. If the result of the integration is out of the range of the path constraint of eq 18 for all the control variables in the range of eq 14, then the initial value of the state vector should be given again. If the result of the state vector integration is satisfied for the path constraint, then it is stored for use in S.4 and all the control variables are stored as $\mathbf{Z}_1$.

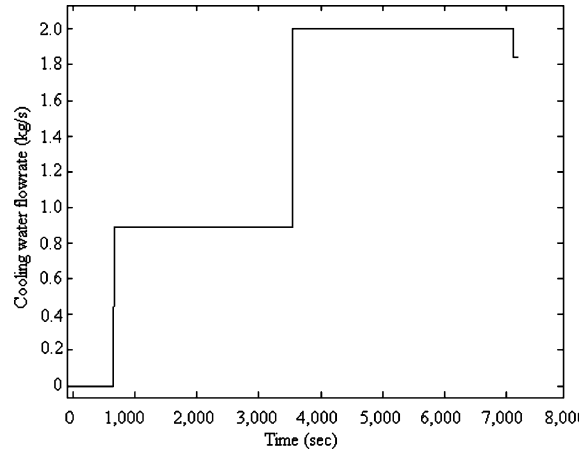

Figure 2. Cooling water flow rate vs time at the critical point in Example 1.

S.4. In the interval [t_1, t_2], the initial value of the state vector is given by the result of S.3, and the control variables are chosen for the differential eq 16; then eq 16 is integrated by the Runge−Kutta method. If the result of the integration for the state vector is out of the path constraints, the control variables are chosen again. If the result is in the range of the path constraints, the result of the integration is stored for use in S.5 and all the control variables are stored as $\mathbf{Z}_2$; then S.5 is next.

S.5. Repeat S.4 for the interval [t_2, t_3], [t_3, t_4], and so forth until the interval [t_{M-2}, t_{M-1}].

S.6. To integrate in the interval [t_{M-2}, t_M] for the differential eq 16, the result of the integration in the interval [t_{M-2}, t_{M-1}] is used for its initial value. The control variables should be selected in the variation scale [$\mathbf{Z}^L$, $\mathbf{Z}^U$] to satisfy the end point constraints. The value of the control variables is stored as $\mathbf{Z}_M$.

At first, to simplify the calculations, the flexibility index is assigned as the value of the permission bound time. For instance, the flexibility index δ is initialized as the value 1 at the beginning of the optimization.

Examples

Two examples are presented to illustrate the importance of the initial conditions for the dynamic flexibility of the batch process.

Example 1. A highly exothermic, first-order reaction (A → B) is carried out in a jacketed batch reactor that is described in ref 3. The mathematical model that is used to describe the system is given as eqs 19−24 and the parameters of the model are $k_0 = 6\ s^{-1}$, $E = 28\ 750$ J/mol, $R = 8.314$ J/ (mol·K), $\Delta T_{cw} = 30$ K, $C_p = 250$ J/(mol·K), $C_{p,cw} = 4200$ J/(kg·K), and $0 \le F_{cw} \le 2$ kg/s. The heat of reaction, ΔH_r, is not known exactly, but it is considered to vary between −72 500 and −82 500 J/mol with an expected nominal value of −77 500 J/mol. The cooling water flow rate, F_{cw}, can be adjusted during the operation of the reactor to satisfy operational constraints and end-time specifications and can therefore be regarded as an available control variable.

$$\frac{dN_A}{dt} = -kN_A; \quad N_A(0) = 20000\ \text{mol} \tag{19}$$

$$\frac{dN_B}{dt} = kN_A; \quad N_B(0) = 0 \tag{20}$$

$$C_P(N_A + N_B)\frac{dT}{dt} = kN_A(-\Delta H_r) - Q_{cw} \tag{21}$$

where

$$Q_{cw} = F_{cw}C_{p,cw}\Delta T_{cw}$$

$$k = k_0 e^{-E/RT}$$

The following requirements must be satisfied:
(i) The final reactant conversion must exceed 95%,

$$\frac{N_A(t = H)}{N_A(t = 0)} \leq 0.05 \tag{22}$$

(ii) Because of safety considerations, the temperature in the reactor can not exceed a maximum of 400 K at any time during operation,

$$T(t) \leq 400 \text{ K}, \quad 0 \leq t \leq H \tag{23}$$

(iii) The temperature of the reacting mixture at the end of the operation must not exceed 308 K so that discharge and cleaning operations can take place,

$$T(t = H) \leq 308 \text{ K} \tag{24}$$

Given that duration of each batch cycle is 2 h, it is required to determine if the reactor can operate under uncertainty and simultaneously satisfy the constraints.

According to ref 3, the dynamic flexibility index evaluation problem was solved for the two vertex directions from the nominal point of operation. The time horizon was divided into six intervals of variable length, and the profile of the cooling water flow rate, F_{cw}, was assumed to be piecewise constant over these intervals. Along the positive vertex direction, it was found that the system was able to handle 78% of the expected uncertainty range ($\delta^+ = 0.7788$, $\Delta H_r^{crit,+} = 81\,394$ J/mol); similarly, along the negative vertex direction, $\delta^- = 7.2384$ and $\Delta H_r^{crit,-} = 41\,308$ J/mol. The dynamic flexibility index of the system was therefore $\delta = 0.7788$, and the critical point of operation corresponded to a value of $\Delta H_r^{crit} = 81\,394$ J/mol. However, the result provided in this paper by the novel method is better than the result given in ref 3. The system can handle 100% of the expected uncertainty range ($\delta^+ = 1$, $\Delta H_r^{crit,+} = 82\,500$ J/mol) by the method presented in this paper. So the dynamic flexibility index of the system is $\delta = 1$, and the critical point of operation corresponds to a value of $\Delta H_r^{crit} = 82\,500$ J/mol. For this value of dynamic flexibility index, the initial reaction temperature is 308 K. The required profile of the cooling water flow rate for the system to operate feasibly at this critical point is shown in Figure 2. In this case the process constraints on final conversion and final reactor temperature are marginally satisfied as shown in Figure 3. For different initial reaction temperature, not the optimal temperature, $T(0) = 309$ K and $T(0) = 307$ K; the results of batch run are also shown in Figure 3.

To obtain the dynamic flexibility index in the fixed initial conditions, the presented optimization method is used. As shown in ref 3, the initial reaction temperature is fixed as $T(0) = 298$ K. The results are presented in Figure 3. The critical dynamic flexibility index δ is 0.7788, and the critical value of the uncertain parameter is $\Delta H_r^{crit} = 81\,394$ J/mol.

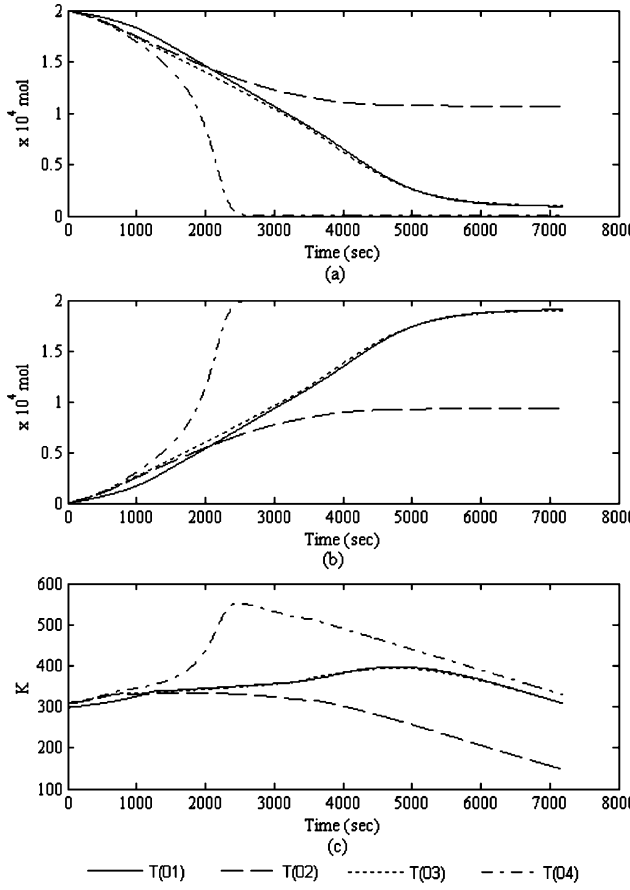

Figure 3. Reactant and product holdup and reaction temperature vs time at the critical point for Example 1. (a) The holdup of the reactant, (b) the product, and (c) the temperature of the reactor. The different initial temperatures are expressed as $T(01)$, $T(02)$, $T(03)$, and $T(04)$. $T(01) = 298$ K, $T(02) = 307$ K, $T(03) = 308$ K, and $T(04) = 309$ K.

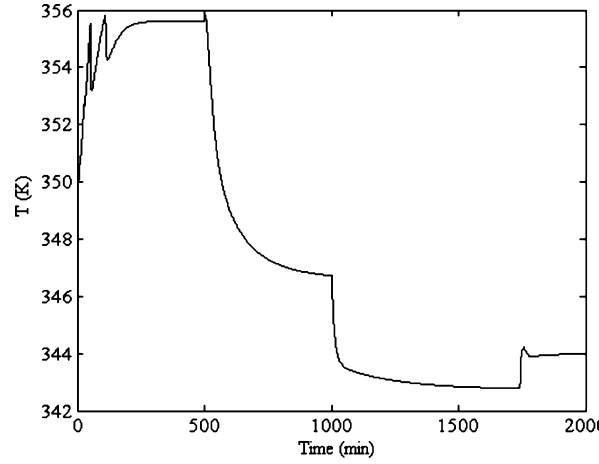

Figure 4. Temperature in the reactor. Flexibility index $\delta = 0.8$ for Example 2 at the fixed initial condition.

When the initial condition is fixed, the obtained result is the same as in ref 9.

In Figure 3, the constraint of the reaction temperature is satisfied, but the constraint of the final conversion cannot reach 95% under the initial reaction temperature $T(02) = 307$ K. When the initial reaction temperature is $T(04) = 309$ K, the constraint of the final conversion is satisfied but the path constraint of the reaction temperature is not satisfied as shown in Figure 3. The reason for these phenomena is that the initial reaction temperature is not optimal, so the critical uncertainty parameter is not

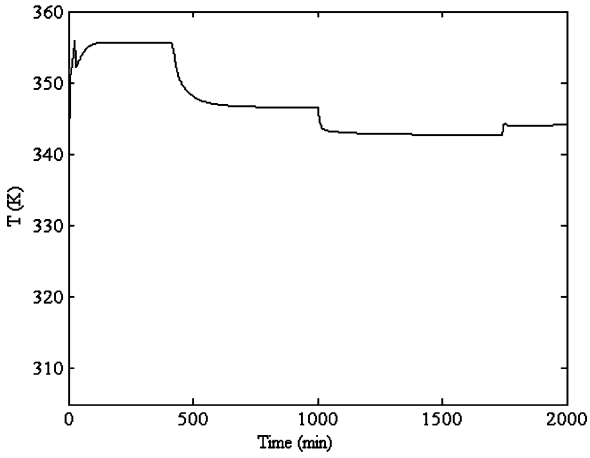

Figure 5. Temperature in the reactor. Flexibility index $\delta = 1.0$ for Example 2 at the optimal initial condition.

satisfied. For the critical uncertainty parameter $\Delta H_r^{crit} = 81\,394$ J/mol, the optimal initial reaction temperature is $T(03) = 308$ K.

Example 2. There is a highly studied exothermic polymerization reaction that produces a polyol lubricant starting from *n*-butanol and propylene oxide

$$C_4H_9OH + (n+1)C_3H_6O \rightarrow C_4H_9(OC_3H_6)_nOCH_2CHOHCH_3 + \text{heat}$$

The reactor initially contains a certain amount of catalyzed reactant, and the next oxide is fed. A typical batch operation takes 33.3 h. The case is a practical polymerization reaction. The problem was originally introduced by Kneale and Forster[30] and recently was studied by Shacham et al.[31] and Uygun and Huang.[32] The system is described by the set of equations:

$$\frac{dM}{dt} = F - V$$

$$C\frac{dM}{dt} + M\frac{dC}{dt} = F - V - r$$

$$\frac{dX}{dt} = r$$

$$MC_p\frac{dT}{dt} = FC_p(T_0 - T) - V\lambda - r(-\Delta H_{rxn}) - Q$$

where

$$r = kcM$$

$$k = A\exp\left(-\frac{E}{RT}\right)$$

$$\text{Mw} = \frac{M_0 + X}{N}$$

The values of the parameter in the model are used as in refs 30−32. To consider the effect of the uncertain parameters, the 10% uncertainty in the activation energy is introduced as it is assumed that the activation energy is inaccurately measured.

When the initial temperature is fixed $T(0) = 353$ K, the dynamic flexibility is $\delta^+ = 1$, $\delta^- = 0.8$. So the dynamic flexibility index is $\delta = 0.8$. The reaction temperature for the flexibility index $\delta = 0.8$ is shown in Figure 4. If the initial reaction temperature is free in the range of [274, 400] K, then the dynamic flexibility index can be improved to $\delta = \delta^+ = \delta^- = 1.0$. Correspondingly, the reaction temperature is shown in Figure 5, and the initial temperature $T(0) = 305$ K when the flexibility index is $\delta = 1.0$.

Summary

A systematic framework is proposed for improving the performance of dynamic systems. On the basis of the novel method, the initial condition of the dynamic systems can be incorporated into the optimization algorithm. The presented approach is an especially useful method for the optimization of batch processes including the initial condition and operation condition. The proposed approach is illustrated by two examples. The method can be applied in the optimization of the existing batch reactor as well as a new design.

In Example 1, the uncertain parameter is included in the model of the batch process. The dynamic flexibility index of the batch process is obtained by a new formulation of the problem. It was reported in ref 3 that dynamic flexibility index $\delta = 0.7788$ and the initial reaction temperature is fixed at $T(0) = 298$ K. Using the method presented in this paper, the dynamic flexibility index of the batch process is $\delta = 1$ and the initial reaction temperature is optimized at $T(0) = 308$ K. The initial condition of the batch process is an important factor influencing the reactor performance. When the initial reaction temperature is set as $T(0) = 309$ K or $T(0) = 307$ K, the dynamic flexibility index $\delta = 1$ cannot be satisfied.

In Example 2, the uncertain parameter is the activation energy of the reaction taking place in the semibatch process. By optimizing the initial condition and the operation of the semibatch process, the dynamic performance is improved as the optimal initial condition is obtained. When the initial reaction temperature is fixed at 353 K, the dynamic flexibility index is $\delta = 0.8$. If the initial reaction temperature is adjusted to $T(0) = 305$ K, the dynamic index can be arrived at $\delta = 1.0$.

The result of the two examples shows that the optimization of batch processes should consider the initial condition of the system. Integrating the optimization of the initial condition and process operation will improve the dynamic flexibility of batch processes.

Acknowledgment

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Nomenclature

$\mathbf{d}$ = vector of design variables
$\mathbf{z}$ = vector of control variables
$\boldsymbol{\delta}$ = flexibility index variables
R = gas constant
C = concentration
C_p = heat capacity
$C_{p,cw}$ = heat capacity of cooling water
V = vapor discharge rate
M_w = polymer molecular weight
k = reaction rate constant
t = time

ΔT_{cw} = temperature difference of cooling water between inlet and outlet
$\mathbf{x}$ = vector of state variables
$\boldsymbol{\theta}$ = vector of uncertain parameters
F = flexibility index
T = temperature
ΔH_r = heat of reaction
F_{cw} = flow rate of cooling water
$T(0)$ = initial temperature
M = mass in reactor
N = initial alcohol charge
E = activation energy
k_0 = reaction rate constant

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