

Transient Temperature Control of Exothermic Fixed-Bed Reactors

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Abstract

The transient temperature control of a fixed-bed, catalytic, hydrodealkylation reactor is approached from the LQG/LTR (linear quadratic Gaussian/loop transfer recovery) control perspective. The LTR method is a systematic procedure to guarantee the robustness of the LQG controller. Applying this technique to the hydrodealkylation reactor, we expect to extract its robust properties. In this paper, the proposed controller solves the surprising temperature excursion problem, that is, transient temperature peaks rising when a drop in feed temperature, by injection of quench gases into the reactor system. Simulation results of the proposed method have exhibited satisfactory capability of attenuating the transient temperature peaks, thus preventing deactivation of catalyst solid, initiation of undesired side reactions and structural damage to the reactor.

1. Introduction

During the past years many efforts have been made to extend the knowledge of the dynamic behavior of fixed-bed reactor with exothermic chemical reactions. The problems included in describing the dynamic behavior of exothermic fixed-bed reactors are complicated enough, because the temperature and concentration gradients in the reactant gas field must be considered simultaneously with the influence of diffusion accompanied by chemical reaction inside the catalyst solid. The dynamic behavior of fixed-bed reactor systems, however, is much complex. One of surprising dynamic features is that when the temperature of the feed to a fixed-bed reactor is suddenly decreased, a transient temperature rise may occur. This unexpected dynamic is caused by the difference in the speed of propagation of the concentration and temperature disturbances. It is referred to as the wrong-way behavior. If such a temperature rise is too high, this behavior may damage the catalyst solid and the mechanical structure of the reactor system.

The wrong-way phenomenon was discovered first by Boreskov and Slinko (1965), and Crider and Foss (1966). Hoiberg et al. (1971) observed this behavior during the experiments of a laboratory reactor in which the exothermic reaction occur between hydrogen and oxygen catalyzed by platinum on granules of silica gel. Van Doesberg and DeJong (1976) studied experimentally and theoretically the transient behavior of an adiabatic fixed-bed methanator and measured the wrong-way responses. Sharma and Hughies (1979) investigated the effect of perturbations on the performance of an adiabatic reactor used for processing the exothermic catalytic oxidation of carbon monoxide and also observed this phenomenon of temperature waves. Sampath et al. (1975) predicted theoretically the wrong-way behavior for a non-catalytic gas-solid fixed-bed reactor. Mcgreavy and Naim (1977) observed a similar response by simulating catalytic processes. Mehta et al. (1981) proposed a simple algebraic expression for single reaction to predict the maximal transient temperature rise during the wrong-way behavior. Liou and Chou

(1983) discovered that the physical constants of inter-phase and intra-phase heat and mass diffusion play important roles in temperature peaks of transient behavior. Pinjala et al. (1988) studied the conditions, under which the wrong-way behavior occurs. Menzinger et al. (2004) reviewed the generic physical reasons why and how a fixed-bed reactor responds dynamically to perturbations and examined when or under which operating conditions the dynamic response becomes pronounced and, hence, dangerous to safe or to economic reactor operation.

Pavlica (1970) investigated various control schemes for the control of temperature peaks of the wrong-way behavior and the best was shown to be one in which the inlet concentration is reduced. Glger et al. (1980) studied several control strategies for the same problem and the best method of feeding a fraction of the reactants at an intermediate point along the reactor bed was recommended. Panfilov and Sheintuch (2001) employed linear stability analysis combined with the Galerkin method to stabilize the front pattern in a homogeneous fixed-bed reactor.

From the brief review of wrong-way behavior within fixed-bed reactors, suffice it to say that very seldom in the literature on the control of wrong-way behavior, have the control scheme been designed to account explicitly for model uncertainty. Basically, these techniques almost fail in explicitly treating the fundamental aspect of robust control, which is vitally important for fixed-bed reactors. Since the control design of reactor systems poses problems involving model uncertainties originating from various sources, i.e., linearization from non-linear process dynamics, model reduction for design, and variation of the process parameters in the process of the operation. Thus, the design of any satisfactory chemical process control scheme requires the consideration of stability, performance and robustness.

The above observations lead us to adopt the LQG/LTR technique as a regulatory controller of fixed-bed reactor for its robustness and the systematic design procedure. LQG/LTR is an extension of the well-known Linear-Quadratic Gaussian (LQG) approach to optimal control of linear, multivariable systems with measurement and model uncertainty. The loop transfer recovery (LTR) method attempts to guarantee the robustness of the LQG controller. This paper employs an LQG/LTR controller design procedure to reflect the above considerations. Al-

though the control schemes derived under this approach have several advantages, the main limitation for the methodology applicability is the requirement of some kind of linear control design model. The fact is that the fixed-bed reactor is a non-linear distributed parameter system. Applying this technique to problem of the control of transient temperature waves within the reactor, however, requires some cares.

The scope of this paper is to elucidate the benefits of quench gas use as a tool to optimize heat transfer and reduce the transient temperature peaks. In this paper, a mechanistic dynamic model that describes the wrong-way behavior of the fixed-bed reactor with quench gas is provided, and a suitable lumped model is developed by the orthogonal collocation method. Then, the control of transient temperature peaks during wrong-way behavior is approached from a LQG/LTR perspective. The proposed controller states a novel application in the field since it solves the temperature wave problem by considering the practically operational constraints in reactor temperature. The operational fact that must be considered in the design of a control algorithm for such a reactor is that sudden changes in manipulated variables, which may cause a rapid decrease in temperature within the reactor, should be avoided. Model order reduction for the controller design is achieved by means of keeping principal eigenvalues on nominal model. The system robustness is recovered by adjusting the design parameter of a Kalman filter. Time domain nonlinear fixed-bed reactor system simulations are performed for the verification of the designed controller.

2. The Hydrodealkylation Reactor

The case of chemical process is considered here in the study of the hydrodealkylation reactor system. The process parameters for such a reactor, which are partially taken from Pavlica (1970), are summarized in Table 1. The reaction rate equations are summarized in Table 2. Reaction 1 is typical of a hydrocracking reaction and reaction 2 is the hydrodealkylation of toluene. In catalytic toluene hydrodealkylation, several reactions may take place, but for the purpose of simulation of temperature profile, the simplified two reactions are considered (Pavlica, 1970, Glger et al., 1980). The mathematical model is described with the following assumptions:

1. negligible axial dispersion,
2. negligible intraphase temperature gradients,
3. negligible interphase and intraphase concentration gradients,
4. constant physical and chemical data including gas density, heat capacity, reaction heat and overall heat transfer coefficient, and
5. no reaction in the vapor phase.

The mass and heat balances for the adiabatic reactor model are (Glger et al., 1980):

$$\begin{aligned} \hat{\rho}^s C_p^s \frac{\partial T^s}{\partial t} &= U_o \hat{a}(T^G - T^s) + k_1 \\ &\times \exp(-E_1/RT^s) C_1^{1.5} (-\Delta H_1) \\ &+ k_2 \exp(-E_2/RT^s) \\ &\times C_{H_2}^{0.5} C_2 (-\Delta H_2) \end{aligned} \quad (1)$$

$$f \bar{C} C_p^G \left\{ \frac{v}{L} \frac{\partial T^G}{\partial z} + \frac{\partial T^G}{\partial t} \right\} = U_o \hat{a}(T^s - T^G) \quad (2)$$

$$f \frac{v}{L} \frac{\partial C_1}{\partial z} + f \frac{\partial C_1}{\partial t} = -k_1 \exp(-E_1/RT^s) C_1^{1.5} \quad (3)$$

$$f \frac{v}{L} \frac{\partial C_2}{\partial z} + f \frac{\partial C_2}{\partial t} = -k_2 \exp(-E_2/RT^s) C_{H_2}^{0.5} C_2 \quad (4)$$

where the superscript *s* refers to the solid phase and superscript *G* refers to the gas phase. The associated initial and boundary conditions are expressed as:

$$\begin{aligned} z \geq 0, \quad t = 0: \quad T^s &= T_{ss}^s(z) \\ z = 0, \quad t \geq 0: \quad T^G &= T_0^G \\ z = 0, \quad t \geq 0: \quad C_1 &= C_{10} \\ z = 0, \quad t \geq 0: \quad C_2 &= C_{20} \end{aligned} \quad (5)$$

The chemical reaction of toluene hydrodealkylation is highly exothermic. Adiabatic operation is considered since this will maximize the thermal excursions. Industrial reactors often control hot spot formation by using an appropriate ballast gas (Papavassiliou and Wagner, 1999). Here we consider that the temperature is adjusted by injection of quench gas. In order to decrease

the temperature in the reactor for benzene production without the adverse wrong-way effects, we propose to use a mixture of reactants as a quench gas. Quench is introduced within the bed by the inner quench tube. Therefore, the mass and heat balances for the reactor system with a direct contact quenching are:

$$\begin{aligned} \hat{\rho}^s C_p^s \frac{\partial T^s}{\partial t} &= U_o \hat{a}(T^G - T^s) + k_1 \\ &\times \exp(-E_1/RT^s) C_1^{1.5} (-\Delta H_1) \\ &+ k_2 \exp(-E_2/RT^s) \\ &\times C_{H_2}^{0.5} C_2 (-\Delta H_2) \end{aligned} \quad (6)$$

$$f \bar{C} C_p^G \left\{ \frac{v}{L} \frac{\partial T^G}{\partial z} + \frac{\partial T^G}{\partial t} \right\} = U_o \hat{a}(T^s - T^G) + U_c \hat{A}(T_c - T^G) \quad (7)$$

$$f \frac{v}{L} \frac{\partial C_1}{\partial z} + f \frac{\partial C_1}{\partial t} = -k_1 \exp(-E_1/RT^s) C_1^{1.5} \quad (8)$$

$$f \frac{v}{L} \frac{\partial C_2}{\partial z} + f \frac{\partial C_2}{\partial t} = -k_2 \exp(-E_2/RT^s) C_{H_2}^{0.5} C_2 \quad (9)$$

$$\begin{aligned} V_c \rho_c C_{pc} \left\{ \frac{v_c}{L} \frac{\partial T_c}{\partial z} + \frac{\partial T_c}{\partial t} \right\} &= U_c A(T^G - T_c) \\ &+ F_c \rho_c C_{pc}(T_{ci} - T_{c0}) \end{aligned} \quad (10)$$

The associated initial and boundary conditions are expressed as:

$$\begin{aligned} z \geq 0, \quad t = 0: \quad T^s &= T_{ss}^s(z) \\ z \geq 0, \quad t = 0: \quad T_c &= T_c(z) \\ z = 0, \quad t \geq 0: \quad T^G &= T_0^G \\ z = 0, \quad t \geq 0: \quad C_1 &= C_{10} \\ z = 0, \quad t \geq 0: \quad C_2 &= C_{20} \\ z = 0, \quad t \geq 0: \quad T_c &= T_{ci} \end{aligned} \quad (11)$$

3. Numerical Solution

The numerical solution of the coupled set of nonlinear partial differential equations describing the reactor is carried out through orthogonal collocation (Villadsen and Michelsen, 1978; Finlayson, 1980). By means of this technique the

nonlinear partial differential equations are transformed into a combined system of nonlinear ordinary differential equations on time, which is then amenable for solution as a standard initial value problem. Then the Gear's method (Hindmarsh, 1974) is used to solve these nonlinear ordinary differential equations.

In computation of system equations, the number of collocation points used was varied until the accuracy of the profiles obtained remains essentially unchanged. Finally we employ in general 12 interior axial collocation points as shown in Table 3. On the other hand, in order to insure the validity and the accuracy of the model solutions in this paper, some particular cases in earlier studies (Pavlica, 1970, Glger et al., 1980) are examined. The observations are almost in agreement with those available from the literature. We examine a situation which may occur in a fully steady state operating when a step gas temperature suddenly decreases. The possibility that such inlet temperature perturbations can lead to a transient temperature rise in the fixed-bed catalytic reactor above its initial steady state temperature is investigated. A step decrease of 27.8 K in feed temperature is observed. Figure 1 shows that the transient temperature profiles vary with time in reactant gas phase for the adiabatic operation. The fact is that the upstream section of the reactor is constantly cooled by the cold feed reactant gas. In the downstream portion of the reactor, however, a temperature peak develops above the initial steady state temperature, grows in magnitude, and moves toward the outlet of the reactor. This unexpected phenomenon can be explained as follows (Glger et al., 1980). When the feed temperature of reactant gas decreases, the catalyst solid at the entrance which is at a temperature higher than the feed, is cooled by the incoming gas, thus causing less reaction to take place in the entrance section of the reactor. As the reactant gas moves further down the reactor, they gain heat as they come in contact with the hot catalyst solid. Since the gas stream has a higher concentration of reactants, due to the fact that in the entrance section of the bed less reaction took place as compared to the initial steady state, more reactant takes place than occurred during the initial steady state. Thus, for an exothermic reaction, heat is released in an amount greater than that for the initial steady state and causes the occurrence of a temperature peak. This phenomenon is called a wrong-way

behavior.

It should be noticed that the temperature at the exit of the reactor, as shown in Figure 1, is about twice as large as the temperature depression at the inlet. This example illustrates the phenomenon of dynamic perturbation amplification (Menzinger et al., 2004): for an initial decrease of 0.032 (27.8K/867K), the highest temperature peak rise by 0.071 (60K/920K) above the steady state value. The gain is thus $G \approx 2.2$. If such a temperature peak is too high, it may deactivate the catalyst or initiate undesired side reactions or cause structure damage to the reactor. Figure 2 shows the dynamic behavior of the reactor to a step decrease of 27.8 K in feed temperature for the operation with a direct contact quenching. Obviously, the highest temperature peak, which occurs in the non-adiabatic operation, is smaller than that of the adiabatic operation. For this result, the quench gas has a strong effect on temperature excursions so it can be considered as a manipulated variable. On the other hand, the flow velocity of the reactant can also be considered here as a manipulated variable. The flow velocity input chosen as a manipulated variable was used in the treatment of the control problem of hyperbolic partial differential equation systems (Kumar et al., 1998). In the next section, the control strategy will be discussed.

4. Control Strategy

The main control objective for the reactor would typically be the regulation of the reactor temperature and exit concentration. In the hydrodealkylation reactor system, the most important control problem is that the moving hot-spot temperature has to be dealt with. Since such temperature peaks are high enough to cause structural damage to the reactor. The main disturbance considered here is a sudden change in the reactant inlet temperature. Therefore, the control problem that we consider is to suppress temperature peaks in the reactor and to prevent excessive temperature. There exists an important fact that must be considered in the design of a control scheme. Sudden changes in manipulated variables, which may cause a rapid decrease in temperature within the reactor, should be avoided. Since the sensitivity of the reactor is very high and the danger of a reactor running away possibly exists. A very reliable control sys-

tem is therefore required for this problem.

There is a simple way to avoid high temperature peaks occurring in the reactor. That is to control the feed temperature by the use of an external heat-exchanger. The temperature disturbance of the feed can be kept quite small, thus minimizing excess temperature excursions within the reactor. For a large throughput system such as the hydrodealkylation reactor that we consider, a large heat-exchanger would be needed, which may be impractical for real applications (Glger et al., 1980). On the other hand, by manipulating the inlet concentration may not be applicable in an industrial situation. From the above discussion, the volumetric flow-rate of the quench gas and the characteristic flow velocity of the reactant are first considered here as the manipulated variables. A related control problem concerning hyperbolic partial differential equation systems, where the manipulated variable is a flow velocity input, can be found in the recent paper by Kumar et al. (1998). The manipulated variables are doubted whether or not to significantly affect the reactor temperature. The related problem of controllability is considered here. The deviation profile under minor perturbation (+ 0.1 %) of flow-rate and flow velocity is given in Figure 3. For this result, the flow-rate of the quench gas and the flow velocity of the reactant have significant effects on exit temperature ($\approx 0.5K$) of the reactor so they are adequate for the manipulated variables. It should be pointed out that the highest temperature rise usually occurs at the exit of the hydrodealkylation reactor within the wrong-way behavior. The collocation points for the gas temperature and the quench gas temperature are then considered as the controlled variables. A robust controller is therefore designed here in this paper for ensuring the stability of the reactor system, for suppressing the influence of external disturbance coming from the perturbation of the reactant inlet temperature, and for controlling the operation of the reactor system without over-high temperature peaks. The proposed control configuration is briefly sketched in Figure 4.

This paper utilizes the LQG/LTR methodology to design a regulatory controller which takes advantage of the loop shaping available using LQG/LTR. This method is a development of the model-based compensator, in which a linear state estimator and a state feedback controller are developed for the system. It is found

that, by using LQG techniques to find controller gain matrices, the singular values of the closed-loop transfer function would approach the desired target loop. The objective of LTR is to shape the target loop and then attempt to recover its singular value loop shapes in the closed-loop by properly selecting the design parameters. Doyle and Stein (1981) proposed this method for the design of linear multivariable control systems. Stein and Athans (1987) gave a more detailed description about this methodology. These have been further developments and applications of this methodology by a number of researchers (Gökçek, 2001; Saberi et al., 1993; Zhou, et al., 1995; Son and Park, 2000).

5. LQG/LTR Controller

In this section we briefly introduce some results of LQG/LTR control design. A more general treatment of the LQG/LTR control system can be found in the literature (Athans, 1986; Saberi et al., 1993). The LQG/LTR method involves two design procedures. In the first step a target feedback loop, which meets the desired performance specifications without violating the stability-robustness constraints, is generated. In the second step a model-based compensator is used to approximate the performance of the target feedback loop established in step one (Athans, 1986).

Let the process to be controlled be as follows

$$\begin{aligned} \dot{x}_p(t) &= A_p x_p(t) + B_p u_p(t) \\ y(t) &= C_p x_p(t) \end{aligned} \quad (12)$$

where x_p and u_p are vectors with dimension n , m respectively. We wish to design an LQG/LTR feedback system which has the property that it has zero steady-state error to arbitrary step commands. This can be accomplished by adding one integrator in each control channel of the process. The addition of integrators is easily conducted by augmenting the nominal process model. The design process model is defined by the augmented dynamics and it is now an $(n + m)$ -dimensional system.

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ &= \begin{bmatrix} A_p & B_p \\ 0 & 0 \end{bmatrix} x(t) + \begin{bmatrix} 0 \\ I \end{bmatrix} u(t) \\ y(t) &= Cx(t) = [C_p \quad 0]x(t) \end{aligned} \quad (13)$$

With the filter loop chosen as the target feedback loop for the system, the first step in the

LQG/LTR design procedures is to synthesis a Kalman filter K_f for a system with fictitious white noise terms

$$\begin{aligned}\dot{x}(t) &= Ax(t) + Lw(t) \\ y(t) &= Cx(t) + v(t)\end{aligned}\quad (14)$$

where the matrices A and C correspond to the augmented process model. The process noise vector $w(t)$ is the white, zero mean, with identity intensity matrix I , and the measurement noise vector $v(t)$ is white, zero mean, and with intensity matrix μI . Since the noise terms do not represent real disturbances, the matrix L and the constant μ are not fixed but act as free parameters that may be chosen to meet design criteria.

With the Kalman filter theory, the relationship between the filter gain and the free parameters is given by the solution to the filter algebraic Ricatti equation.

$$\begin{aligned}P_f A^T + A P_f + L L^T - (1/\mu) P_f C^T C P_f &= 0 \\ K_f &= (1/\mu) P_f C^T\end{aligned}\quad (15)$$

It has been shown that the singular values of the Kalman filter loop are given by

$$\begin{aligned}\sigma_i [I + C(sI - A)^{-1} K_f] \\ = \sqrt{1 + \left(\frac{1}{\mu}\right) \sigma_i^2 [C(sI - A)^{-1} L]}\end{aligned}\quad (16)$$

For $\mu \ll 1$, the above equation reduces to (Zhou, et al., 1995)

$$\sigma_i [C(sI - A)^{-1} K_f] = \left(\frac{1}{\sqrt{\mu}}\right) \sigma_i [C(sI - A)^{-1} L] \quad (17)$$

The equation facilitates the choice of μ and L because these design parameters appear in the right hand side of the equation, while the frequency domain characteristics of the target feedback loop appear in the left hand side. One advantage of using the Kalman filter methodology for calculating K_f is that the target feedback loop has certain automatic performance and robustness guarantees which can be directly obtained from Eq. (17). These are

$$\begin{aligned}\sigma_{\max} S(j\omega) &\leq 1 \text{ for all } \omega \\ \sigma_{\max} T(j\omega) &\leq 2 \text{ for all } \omega\end{aligned}\quad (18)$$

where $G = C(sI - A)^{-1} K_f$, $S(s) = (I + G(s))^{-1}$, and $T(s) = (I + G(s))^{-1} G(s)$. These inequalities guarantee that the target feedback loop will

never amplify disturbances and never go unstable to model errors within some limits (Athans, 1986).

If the filter open loop matrix, $C(sI - A)^{-1} L$, approaches some multiple of the identity matrix for a given frequency, then its upper and lower singular value bounds will become equal for that frequency. From the above equation, it can be seen that identical singular value bounds of $C(sI - A)^{-1} L$ imply identical singular value bounds of $C(sI - A)^{-1} K_f$, as well. The problem, then, lies in finding the gain matrix, L , which will result in identical bounds for the filter open loop transfer matrix. The design method defines L so that $C(sI - A)^{-1} L$ approaches I/s at low and high frequencies. The resulting matrix L , composed of two sub-matrices $L_L (m \times m)$ and $L_H (n \times m)$, provides the basic form of the loop shape.

$$L = \begin{bmatrix} L_L \\ L_H \end{bmatrix} = \begin{bmatrix} -[C_p A_p^{-1} B_p]^{-1} \\ C_p^T [C_p C_p^T]^{-1} \end{bmatrix} \quad (19)$$

The other free parameter, the scalar μ , can now be selected to provide the desired crossover frequency of $C(sI - A)^{-1} K_f$.

The second step in the design procedures is to construct a model based compensator LQG/LTR for the system.

$$\begin{aligned}\dot{z}(t) &= Az(t) + Bu(t) + K_f [y - Cz(t)] \\ u(t) &= -K_c z(t)\end{aligned}\quad (20)$$

The control gain matrix K_c is given by

$$K_c = (1/\rho) B^T P_c \quad (21)$$

where P_c satisfies the control algebraic Riccati equation

$$A^T P_c + P_c A + C^T C - (1/\rho) P_c B B^T P_c = 0 \quad (22)$$

Finally, we can reduce ρ until the return ratio at the output of the compensated process has converged sufficiently closely to $C(sI - A)^{-1} K_f$ over a sufficiently large range of frequencies.

6. Linear Lumped Model

Several manipulations are required in order to convert the set of five nonlinear partial differential equations shown in Eqs. (??)-(10) to a form suitable for a linear model-based control structure. The steps are summarized as:

1. linearize about a nominal steady-state,
2. spatial discretization by orthogonal collocation, and
3. reduction of order of the linearized model for control design model.

The linearized model is obtained by means of the steady-state data as shown in Table 1. After linearization the differential equations are discretized to obtain a linear state-space representation. This process results in a 65th order model and 12 interior collocation points for the set of five nonlinear partial differential equations are selected. The linearization and discretization steps give a model of the type

$$\begin{aligned} \frac{\partial \theta_j}{\partial t} = & \frac{U_o \hat{a}}{\hat{\rho}^s C_p^s} (\phi_j - \theta_j) \\ & + [k_1 (-\Delta H_1) \left(\frac{E_1}{R(T_{ss,j}^s)^2} e^{\frac{-E_1}{RT_{ss,j}^s}} C_{1ss,j}^{1.5} \right) \\ & + k_2 C_{H_2}^{0.5} (-\Delta H_2) \\ & \times \left(\frac{E_2}{R(T_{ss,j}^s)^2} e^{\frac{-E_2}{RT_{ss,j}^s}} C_{2ss,j} \right)] \frac{1}{\hat{\rho}^s C_p^s} \theta_j \\ & + \frac{k_1 (-\Delta H_1)}{\hat{\rho}^s C_p^s} (1.5 e^{\frac{-E_1}{RT_{ss,j}^s}} C_{1ss,j}^{0.5}) \\ & \times \frac{C_{10}^G}{T_0^G} C'_{1,j} \\ & + \frac{k_2 C_{H_2}^{0.5} (-\Delta H_2)}{\hat{\rho}^s C_p^s} e^{\frac{-E_2}{RT_{ss,j}^s}} \frac{C_{20}}{T_0^G} C'_{2,j} \quad (23) \end{aligned}$$

$$\begin{aligned} \frac{\partial \phi_j}{\partial t} = & \frac{U_o \hat{a}}{f \bar{C} C_p^G} (\theta_j - \phi_j) + \frac{U_c \hat{A}}{f \bar{C} C_p^G} (\theta_{c,j} - \phi_j) \\ & - \frac{1}{LT_0^G} (A_{j1} T_{ss,1}^G + \sum_{i=2}^{N+2} A_{ji} T_{ss,i}^G) \bar{v} \\ & - \frac{v_{ss}}{L} (A_{j1} \phi_1 + \sum_{i=2}^{N+2} A_{ji} \phi_j) \quad (24) \end{aligned}$$

$$\begin{aligned} \frac{\partial C'_{1,j}}{\partial t} = & \frac{-1}{f} k_1 \left(\frac{E_1}{R(T_{ss,j}^s)^2} e^{\frac{-E_1}{RT_{ss,j}^s}} C_{1ss,j}^{1.5} \right) \frac{T_1^s}{C_{10}} \theta_j \\ & - \frac{-1}{f} k_1 (1.5 e^{\frac{-E_1}{RT_{ss,j}^s}} C_{1ss,j}^{0.5}) C'_{1,j} \\ & - \frac{1}{LC_{10}} (A_{j1} C_{1ss,1} \\ & + \sum_{i=2}^{N+2} A_{ji} C_{1ss,i}) \bar{v} - \frac{v_{ss}}{L} (A_{j1} C'_{1,1} \end{aligned}$$

$$+ \sum_{i=2}^{N+2} A_{ji} C'_{1,j}) \quad (25)$$

$$\begin{aligned} \frac{\partial C'_{2,j}}{\partial t} = & \frac{-1}{f} k_2 \left(\frac{E_2}{R(T_{ss,j}^s)^2} e^{\frac{-E_2}{RT_{ss,j}^s}} \right. \\ & \times C_{2ss,j}) C_{H_2}^{0.5} \frac{T_1^s}{C_{20}} \theta_j \\ & - \frac{-1}{f} k_2 e^{\frac{-E_2}{RT_{ss,j}^s}} C_{H_2}^{0.5} C'_{2,j} \\ & - \frac{1}{LC_{20}} (A_{j1} C_{2ss,1} \\ & + \sum_{i=2}^{N+2} A_{ji} C_{2ss,i}) \bar{v} - \frac{v_{ss}}{L} (A_{j1} C'_{2,1} \\ & + \sum_{i=2}^{N+2} A_{ji} C'_{2,j}) \quad (26) \end{aligned}$$

$$\begin{aligned} \frac{\partial \theta_{c,j}}{\partial t} = & \frac{U_c A}{V_c \rho_c C_{pc}} (\phi_j - \theta_{c,j}) \\ & + \frac{1}{V_c} \frac{T_{ci} - T_{c0}^{ss}}{T_0^G} \bar{F}_c - \frac{F_{css}}{V_c} \theta_{c0} \\ & - \frac{v_c}{L} (A_{j1} \theta_{c,1} + \sum_{i=2}^{N+2} A_{ji} \theta_{c,j}) \quad (27) \end{aligned}$$

To solve these equations in LQG/LTR we put them into state variable form

$$\begin{aligned} \dot{x}_p(t) &= A_p x_p(t) + B_p u(t) \\ y(t) &= C x_p(t) \quad (28) \end{aligned}$$

where the input is $u(t) = [\bar{v} \quad \bar{F}_c]$, represented the characteristic flow velocity of the reactant gas and the volumetric flow-rate of the quench gas. The state vector, $x_p = [\theta_j \quad \phi_j \quad C'_{1,j} \quad \theta_{c,j}]$, is composed of the collocation points for the gas concentration and temperature, and the quench gas and catalyst particle temperatures. The output, $y = [\phi_j \quad \theta_{c,j}]$, consists of the collocation points for the gas temperature and the quench gas temperature.

As the scale of the reactor dynamic model increases, the order of the corresponding LQG/LTR controller increases. Model order reduction is crucial in order to avoid the possible numerical ill-condition problem when solving the high order matrix Riccati equation in the design process. The 65th order state-space model of the reactor system was too large for control design calculations. For the hydrodealkylation reactor, it is noted that some physical insight can be used

for reducing the design model. The matching steady-state gain technique is used in getting a reduced order model for controller design. This technique consists of setting the derivative of the eliminated states to zero and solving for the remaining states (Moore, 1981). It gives the reduced order model that eliminates the states, such as solid catalyst temperatures and reactant concentrations that are not easy to be measured. This process produces a 26th order model of the same form as Eq. (28). Poles for the multivariable 26th order process model are listed in Table 4. This system is not found unstable transmission zeros. Figure 5 shows the maximum and minimum singular values of the 65th order model and the reduced order model. Notice that the set of five nonlinear partial differential equations will be used to represent the actual process in the model-based control, with the 26th order model as the design model. In this way, modeling error will be automatically built into the system resulting in more realistic design conditions.

7. Controller Design

We shall now use the LQG/LTR approach to design a compensator for the hydrodealkylation reactor system which meets the following specifications:

1. zero steady state error,
2. stable response in the presence of model errors and uncertainties, and
3. bandwidth of about 10 rad/sec.

The zero steady state error can be satisfied by augmenting the reduced process model with an integral action in each loop as described previously. The second specification can be met by applying the technique for selecting the filter gain matrix to satisfy the inequalities as Eq. (18). As for the third specification, may be achieved by manipulating the design parameter, μ . We would like to remove the transient temperature peaks as soon as possible, when the reactor system takes place the unexpected wrong-way phenomenon. The sensitivity of the reactor is very high and the danger of a reactor running away possibly exists. However, the fact, sudden changes in manipulated variables may cause a rapid decrease in temperature within the reactor, should be avoided.

The new free integrator now is placed to each loop to obtain the desired result. Figure 6 shows the maximum and minimum bounds on the singular values of the augmented system. The procedure for selecting the L matrix begins with the previously described low and high frequency components. Using Eq. (19) to compute the L matrix, and selecting various values of μ , the sensitivity function, S , and the complementary sensitivity function, T , of the target feedback loop are shown in Figure 7. It should be noted that this system results in $\mu \leq 1$. Figure 8 indicates that the maximum and minimum bounds on the singular values of the target feedback loop for various values of μ . Observing the figure if we would like the bandwidth of the system to be about 10 rad/s or higher, the value of μ should be chosen as $\mu \leq 0.1$. The remaining variable which must be specified to construct the LQG/LTR compensator is the design parameter, ρ . Figure 9 presents the singular value plots of the target feedback loop and the associated recovery for the case of $\mu = 0.1$ with various values of ρ . All target loop recoveries are complete and acceptable in both cases of $\mu = 0.1, \rho = 10000$ and $\mu = 0.1, \rho = 100000$. The performance of the reactor system to a step decrease of 27.8K in feed temperature for the case of $\mu = 0.1$ and $\rho = 10000$ is shown in Figure 10. Comparison of Figures 2 and 10 clearly shows that the maximum peak temperature is reduced about from 900 K to 884 K with this control action. Figure 11 shows the temperature responses of the reactor for a feed temperature increase of 27.8 K. Notice that the feed gas temperature undergoes a positive step change, the response of the reactor shows almost no overshoot temperature excursions than that of the final steady-state profile. It is obvious that this control action improves the transient response. The temperature peaks should be further reduced if the control action is tuned by a larger value of ρ . Figure 12 plots the simulation results. As we might expect, the maximum temperature in the reactor is much smaller compared to the response shown in Figure 10. In Figure 12, the temperature excursions are suppressed. It can be seen that the proposed control scheme is effective in controlling temperature excursions.

8. Conclusions

When the temperature of the feed to a fixed-bed hydrodealkylation reactor suddenly drops, a transient temperature rise may occur. This surprising dynamic behavior is caused by the difference in the speed of propagation of the concentration and temperature disturbances and is referred to as the wrong-way behavior. This paper presents a procedure to design LQG/LTR control of the hydrodealkylation reactor when the system encounters the unexpected wrong-way phenomenon. Although the control laws derived under the LQG/LTR approach have several advantages, the main limitation for the methodology applicability is the requirement of linear ordinary differential systems. Since the hydrodealkylation reactor is a distributed parameter system which consists of the set of five nonlinear partial differential equations. Applying this LQG/LTR technique to temperature control of the reactor system, however, requires some cares. Primary importance is given to the crucial issue of controller design in the face of model uncertainty and model error arising from model reductions and linearization. The matching DC gain and Schur computation techniques are used in getting suitable model order reductions for the controller design. A practical strategy, the temperature controlled by injection of quench gas into the reactor, is employed. It has been shown that the designed control scheme is effective in controlling temperature excursions. The results of this work would hopefully contribute towards the improvement of problems involving wrong-way behavior and hot spot phenomenon.

9. Nomenclature

\hat{a} surface area of the packing per unit reactor volume
 \hat{A} surface area of the quench tube per unit reactor volume
 A surface area of quench tube
 C_p^s specific heat of solid
 C_p^G specific heat of gas
 C_{pc} specific heat of quench gas
 \bar{C} average molar density of gas phase
 C_i molar concentration of species i per unit volume
 C'_1 deviation variable, $C'_1 = \frac{C_1 - C_{1ss}}{C_{10}}$
 C'_2 deviation variable, $C'_2 = \frac{C_2 - C_{2ss}}{C_{20}}$
 E_i activation energy of i th reaction

f bed void fraction
 F_c volumetric flow-rate of quench gas
 \bar{F}_c deviation variable, $\bar{F}_c = F_c - F_{c,ss}$
 k_i rate constant of i th reaction
 L reactor length
 \hat{r}_i rate of the i th reaction per unit reactor volume
 R gas constant
 t time
 T_c quench gas temperature
 T_{ci} inlet temperature of quench gas
 T_{co} outlet temperature of quench gas
 T^G gas temperature
 T_0^G inlet gas temperature
 T^s solid temperature
 U_o overall heat transfer coefficient based on catalyst surface area
 U_c overall heat transfer coefficient based on quench tube area
 v gas velocity
 v_c quench gas velocity
 \bar{v} deviation variable, $\bar{v} = v - v_{ss}$
 V_c volume of quench tube
 z^* distance along the reactor
 z dimensionless distance $z = \frac{z^*}{L}$

Greek Letters

$(-\Delta H_i)$ heat of reaction associated with reaction i
 θ deviation variable, $\theta = \frac{T^G - T_{ss}^G}{T_0^G}$
 θ_c deviation variable, $\theta_c = \frac{T_c - T_{c,ss}}{T_0^G}$
 θ_{c0} deviation variable, $\theta_{c0} = \frac{T_{c0} - T_{c0,ss}}{T_0^G}$
 $\hat{\rho}^s$ bulk density of the catalyst
 ϕ deviation variable, $\phi = \frac{T^s - T_{ss}^s}{T_0^G}$

Subscripts

0 initial
 ss steady state

10. References

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Figures

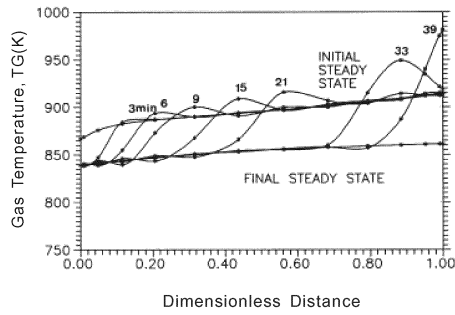


Figure 1

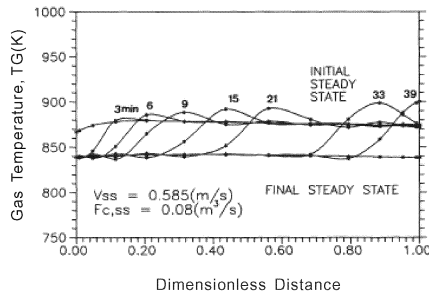


Figure 2

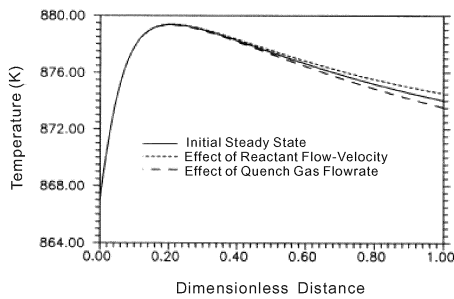


Figure 3

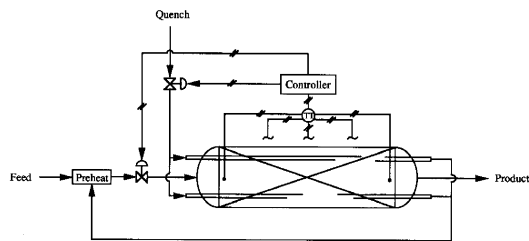


Figure 4

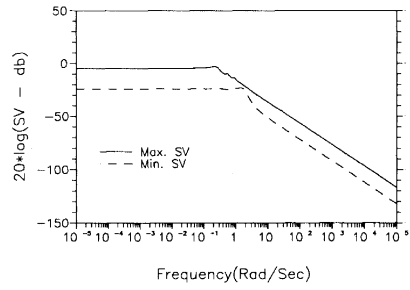
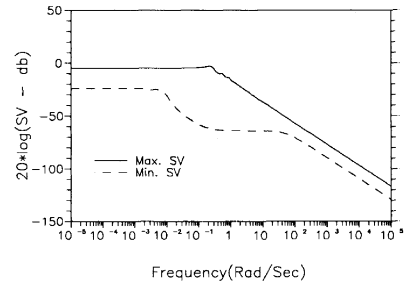


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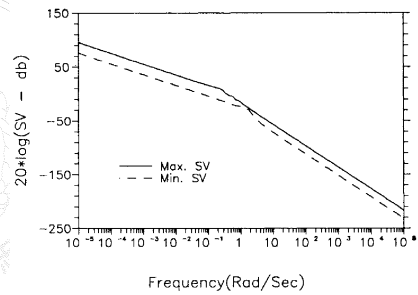


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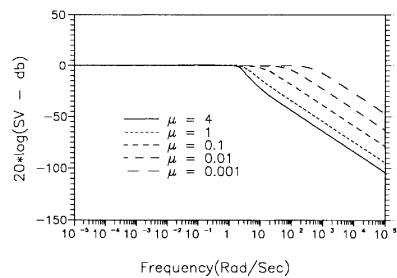
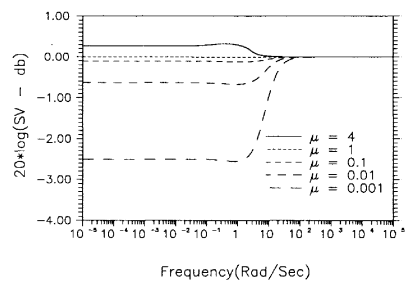


Figure 7

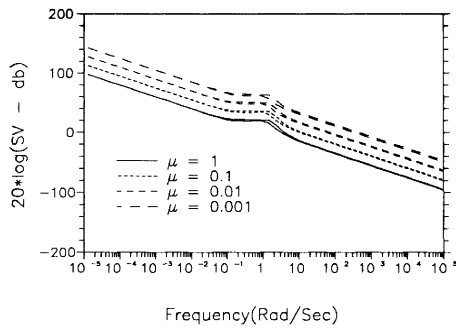


Figure 8

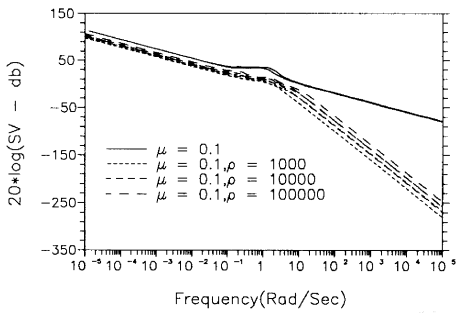


Figure 9

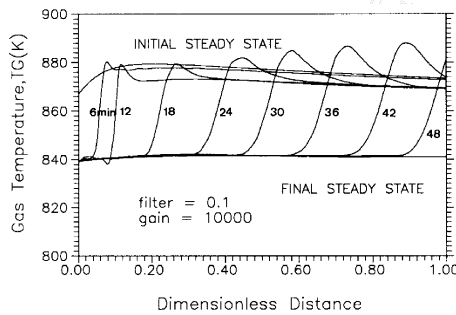


Figure 10

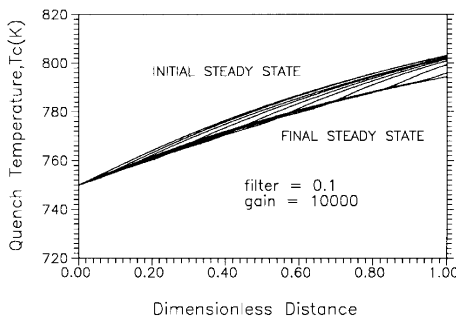
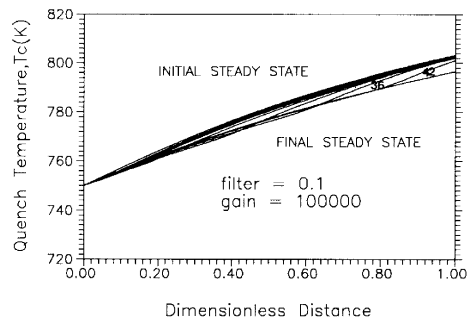
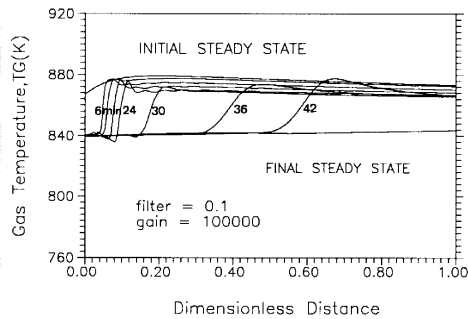
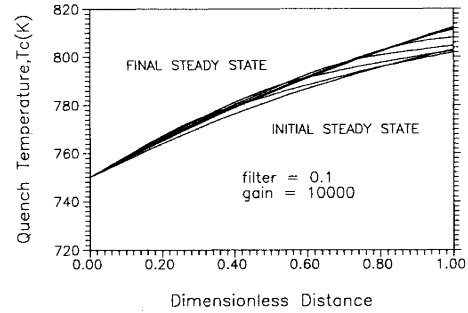
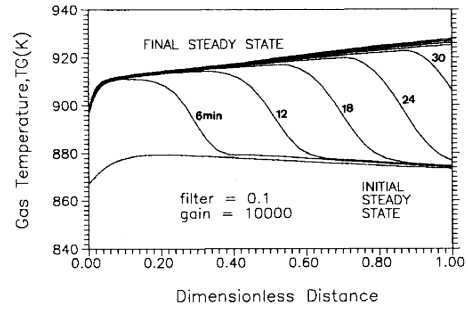


Figure 11



Tables

Table 1. Values of process and design parameters for the hydrodealkylation reactor

$L = 7.01 \text{ m}$	$\bar{C} = 0.794 \text{ kmol} / \text{m}^3$
$v = 0.585 \text{ m} / \text{s}$	$C_{H_2} = 0.564 \text{ kmol} / \text{m}^3$
$f = 0.4$	$\hat{\rho}^s C_p^s = 4.020 \times 10^6 \text{ J} / (\text{K m}^3)$
$U_o \hat{a} = 1.005 \times 10^6 \text{ W} / (\text{K m}^3)$	$T_o^G = 867 \text{ K}$
$C_p^G = 6.237 \times 10^4 \text{ J} / (\text{kmol K})$	$V_c = 3.962 \text{ m}^3$
$F_c = 0.08 \text{ m}^3 / \text{s}$	$U_c \hat{A} = 12693.68 \text{ W} / (\text{K m}^3)$
$U_c A = 50292.361 \text{ W} / \text{K}$	$T_{ci} = 750 \text{ K}$

Table 2. Values of reaction rates and parameters for the hydrodealkylation reactor

	reaction 1	reaction 2	units
k_i	3.629×10^{22}	1.112×10^{13}	$\text{m}^{1.5} / \text{s} (\text{kmol})^{0.5}$
E_i	3.604×10^8	2.523×10^8	J / kmol
$(-\Delta H)$	9.202×10^7	1.394×10^8	J / kmol
\hat{r}_i	$k_1 \exp(-E_1 / RT^s) C_1^{1.5}$	$k_2 \exp(-E_2 / RT^s) C_{H_2}^{0.5} C_2$	$\text{kmol} / (\text{s m}^3)$
C_{i0}	9.337×10^{-3}	4.004×10^{-2}	kmol / m^3

Table 3. Collocation points

0.009220	0.562616
0.047941	0.683916
0.115049	0.793659
0.206341	0.884951
0.316084	0.952058
0.437383	0.990780

Table 4. Poles of 26th order reactor model

-2.718	-0.740 ± 1.575j
-1.202	-0.699 ± 1.532j
-1.866 ± 1.605j	-0.415 ± 1.750j
-1.121 ± 0.271j	-0.221 ± 1.239j
-1.077 ± 0.590j	-0.165 ± 0.933j
-0.975 ± 0.889j	-0.141 ± 0.596j
-0.827 ± 1.226j	-0.097 ± 0.263j