Integration of design and control by nonlinear analysis

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Chapter 5 Interaction between Design and Control of Heat-Integrated PFR

Abstract

The interaction between design and control of a heat-integrated plug-flow reactor (PFR) is analysed. Four design alternatives and three control structures are considered. Linear controllability analysis shows that designs with small steam-generator and large feed-effluent heat exchanger (FEHE) cannot be stabilised. At steady-state, control structures using furnace duty as manipulated variable can reject disturbances in feed flow rate, steam-generator duty and FEHE fouling. However, fast control cannot be achieved. Moreover, there is no incentive to add a bypass around the FEHE. The nonlinear behaviour of the controlled system is analyzed using bifurcation theory. The points in the design parameter space are classified according to their position relative to the cusp and Hopf-and-pitchfork varieties. The range of design parameters for which the system cannot be stabilised is detected. The results of linear and nonlinear analysis are confirmed by dynamic simulation.
Chapter 5. Interaction between Design and Control of Heat-Integrated PFR

**Introduction**

In industrial processes where an exothermic reaction takes place, heat exchange between the effluent of adiabatic reactor and the feed stream may be used for energy saving. There are several reasons to include additional units in the system:

- A heater (furnace) is required for startup. Moreover, positive feedback due to heat integration may lead to state multiplicity or instability. In this case, furnace duty can be the manipulated variable in a temperature control loop, in order to achieve stable operation.
- The heat excess must be removed in a cooler (steam-generator). Placing the steam-generator before the FEHE allows heat recovery at higher temperature and is therefore preferable in view of exergetic considerations.
- Rapid quench of the reactor effluent may be necessary to minimize coking and to avoid the fouling of heat-exchange units.

The resulting structure, presented in Figure 5.1, will be called heat-integrated PFR.

![Diagram of heat-integrated plug-flow reactor](image)

**Figure 5.1. Heat-integrated plug-flow reactor.**

The feed is preheated by the reactor effluent in feed-effluent heat exchanger (FEHE). Start-up, control or plant energy balance may require additional units: furnace, quench, steam-generator.
Although this structure is attractive from the viewpoint of energy saving, state multiplicity, isolated solution branches and oscillatory behaviour are possible. Hence, control problems are expected. A design procedure was proposed to ensure a desired multiplicity pattern and a stable point of operation, and to avoid high sensitivity (Bildea and Dimian, 1998).

Silverstein and Shinnar (1982) evaluated the stability of a very similar system, using the frequency response of the individual equipment components. They considered the multiplicity region and concentrated on the intermediate, open-loop unstable operating point. A control loop, maintaining the furnace exit temperature by adjusting the fuel rate to the furnace, could stabilise the system. The authors pointed out that industrial furnaces are normally sluggish and a bypass around FEHE could provide a manipulated variable to achieve quick control.

Tyreus and Luyben (1993) analyzed a reactor / preheater process. Reactor dynamics (dead-time and inverse response) was captured by a transfer function containing a gain, a positive zero, dead-time and two first-order lags. The dynamics of the FEHE was neglected. The coupled system was unstable for loop gain greater than unity. Bypass around the FEHE was used to stabilise the system. The authors pointed out that, contrary to conventional wisdom, the addition of integral action in the control loop improved closed loop stability.

Luyben et al. (1998) considered the control of a heat-integrated PFR, without steam-generator. Using nonlinear dynamic simulation, they showed that systems with a large furnace (and low heat integration) are easier to control.

This work studies the interaction between design and control of a heat-integrated PFR. In the next section, the nonlinear, dynamic model is presented. It is shown that two design parameters have to be set during conceptual design: FEHE efficiency and steam-generator duty. Four different design alternatives, for which controllability problems are expected, are investigated. Three different control structures are considered. Linear controllability analysis shows that systems with small steam-generator and large FEHE are difficult to stabilise. Bypass around the FEHE can not be used to reject disturbances and there is no incentive to control both FEHE and furnace outlet temperatures. Next, the nonlinear behaviour of the controlled system is analyzed by bifurcation theory. The range of design parameters for which the system can not be stabilised is detected. The operating points are classified according to
their position relative to different bifurcation varieties. Doing this, the meaning of “small” or “large” units becomes clear. The results are confirmed by nonlinear dynamic simulation.

**Design considerations and model equations**

During conceptual design, the reactor volume, FEHE efficiency, furnace and steam-generator duties are of interest. Moreover, detailed equipment sizing is not necessary.

Feed flow rate \( (F) \), reactor inlet temperature \( (T_2) \) and the conversion \( (X) \) are typical initial data. Consequently, the reactor may be designed if reaction kinetics and thermodynamics (adiabatic temperature rise, \( \Delta T_{ad} \)) are known.

The first design decision refers to FEHE efficiency \( (\varepsilon) \). The size of FEHE determines the multiplicity pattern, the stability of the operating point and the sensitivity to energy disturbances. Bildea and Dimian (1998) discuss this issue in detail.

When the FEHE efficiency is known, the net energy requirement \( (q) \) can be calculated:

\[
q = (1-\varepsilon) \cdot Fc_p T_0 + (q_h - \varepsilon \cdot q_c) = (1-\varepsilon) \cdot Fc_p T_2 - \varepsilon \cdot Fc_p \Delta T_{ad} X
\]  

(5.1)

However, it must be split between feed enthalpy \( (T_0) \), furnace and steam-generator duties \( (q_h, q_c) \). Considering fixed feed temperature, the second decision concerns the steam-generator duty. Note that the furnace duty can be calculated from the overall energy balance.

In this article, we consider a case where moderate conversion is required. Table 5.1 presents the kinetic, thermodynamic and design parameters. They correspond to the toluene hydrodealkylation (Douglas, 1988). First-order kinetics can be assumed because of the large hydrogen excess. For this reaction, the boundary between unicity and multiplicity regions is located at a rather low value of FEHE efficiency \( (\varepsilon^* = 0.32) \). Four design alternatives are presented in Table 5.2.

Design 1 has a small FEHE \( (A_s = 130 \text{ m}^2, \varepsilon = 0.28) \). The operating point is in the unicity region, but close to the unicity-multiplicity boundary. Design 2 has a large FEHE \( (A_s = 1500 \text{ m}^2, \varepsilon = 0.745) \). Hence, the operating point is in the multiplicity region. In Designs 1A and 2A, a large quantity of energy is used to generate steam, and a large amount of energy is provided in the furnace. Conversely, less steam is generated in Designs 1B and 2B, a smaller furnace being necessary. Note that energy recovered in the FEHE increases from Design 1A to Design 2B.
Table 5.1. Kinetic, thermodynamic and design parameters

<table>
<thead>
<tr>
<th>Feed</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>flowrate, $F$ (kg/s)</td>
<td>8</td>
</tr>
<tr>
<td>temperature, $T_0$ (°C)</td>
<td>30</td>
</tr>
<tr>
<td>pressure, $p$ (atm)</td>
<td>35</td>
</tr>
<tr>
<td>reactant mole fraction, $y$</td>
<td>0.09</td>
</tr>
<tr>
<td>specific heat, $c_p$ (J/(kg K))</td>
<td>4000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reactor</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>reaction enthalpy, $\Delta H_r$ (J/mol)</td>
<td>-48000</td>
</tr>
<tr>
<td>pre-exponential factor, $k_0$ (s$^{-1}$)</td>
<td>2.65 $10^{14}$</td>
</tr>
<tr>
<td>activation energy, $E_a$ (J/(mol K))</td>
<td>282876</td>
</tr>
<tr>
<td>conversion, $X$</td>
<td>0.75</td>
</tr>
<tr>
<td>inlet temperature, $T_2$ (°C)</td>
<td>637</td>
</tr>
</tbody>
</table>

FEHE

| heat transfer coefficient, $K_{at}$ (W/(m$^2$ K)) | 100.0 |
| bypass, 1-$\alpha$ | 0.2 |

<table>
<thead>
<tr>
<th>Furnace</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>tube diameter, $d_w$ (m)</td>
<td>0.05</td>
</tr>
<tr>
<td>tube wall thickness, $\delta_w$ (m)</td>
<td>0.005</td>
</tr>
<tr>
<td>tube density, $\rho_w$ (kg/m)</td>
<td>7800</td>
</tr>
<tr>
<td>tube specific heat, $c_{p,w}$ (J/(kg K))</td>
<td>2000</td>
</tr>
<tr>
<td>heat transfer coefficient, $K_{wt}$ (W/(m$^2$K))</td>
<td>200</td>
</tr>
<tr>
<td>tube temperature, $T_w$ (°C)</td>
<td>800</td>
</tr>
</tbody>
</table>

Table 5.2. Design alternatives of the HDA heat-integrated reactor.

<table>
<thead>
<tr>
<th></th>
<th>Design 1A</th>
<th>Design 1B</th>
<th>Design 2A</th>
<th>Design 2B</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Furnace</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>duty, $q_h/10^3$ (W)</td>
<td>16436</td>
<td>13969</td>
<td>12665</td>
<td>6011.2</td>
</tr>
<tr>
<td>area, $A_{wt}$ (m$^2$)</td>
<td>223.9</td>
<td>205.3</td>
<td>194.48</td>
<td>121.9</td>
</tr>
<tr>
<td><strong>Steam-generator</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>duty, $q_c/10^3$ (W)</td>
<td>10576.3</td>
<td>1047</td>
<td>10577.5</td>
<td>1048.96</td>
</tr>
<tr>
<td>$T_s$ (°C)</td>
<td>297</td>
<td>588</td>
<td>297</td>
<td>588</td>
</tr>
<tr>
<td><strong>FEHE</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>efficiency, $\varepsilon$</td>
<td>0.28</td>
<td>0.28</td>
<td>0.745</td>
<td>0.745</td>
</tr>
<tr>
<td>area, $A_{at}$ (m$^2$)</td>
<td>130.0</td>
<td>130</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>hot side outlet temperature, $T_1$ (°C)</td>
<td>104.7</td>
<td>186</td>
<td>228.8</td>
<td>445.5</td>
</tr>
<tr>
<td>cold side outlet temperature $T_6$ (°C)</td>
<td>223.85</td>
<td>435.6</td>
<td>102.7</td>
<td>181.9</td>
</tr>
<tr>
<td>duty / $10^3$ (W)</td>
<td>2390.8</td>
<td>4992</td>
<td>6362</td>
<td>13295.8</td>
</tr>
</tbody>
</table>
The assumptions made to develop the dynamic model are:

1. Reactor dynamics may be described by a plug-flow, pseudo-homogeneous model.
2. A detailed model of the steam-generator is not necessary, since we regard its duty as a disturbance.
3. For FEHE, an efficiency model is adequate because of fast dynamics.
4. A fast fuel flow rate – flue-gas temperature control loop is used to set the furnace duty at the prescribed value (Shinskey, 1988). Consequently, the heat transfer from burner to tubes (hot-side) is not included in the model. Moreover, temperature variation along the tubes is neglected and the cold-side heat-transfer coefficient is assumed to be constant. These assumptions allow an approximate furnace design (number of tubes, diameter, length, and thickness) and development of a model describing the essential dynamic behaviour.

The model equations are presented below:

**FEHE:**

\[ T_i = (1 - \varepsilon) \cdot T_0 + \varepsilon \cdot T_s \]  
(5.2a)

**Furnace (fluid, and tubes wall)**

\[
\frac{\partial T_b}{\partial t} = -w \cdot \frac{\partial T_b}{\partial z} + 4 \cdot \frac{K_{wf} \cdot (T_w - T_h)}{d_w \cdot \rho \cdot c_p} 
\]  
(5.2b)

\[
\frac{\partial T_w}{\partial t} = \frac{1}{\rho_w \cdot c_{pw} \cdot V} \left( q_b - \pi \cdot d_w \cdot K_{wf} \cdot \int (T_w - T_h) \, dz \right) 
\]  
(5.2c)

**Reactor**

\[
\frac{\partial C}{\partial t} = -w_r \cdot \frac{\partial C}{\partial z} - r(C, T_r) 
\]  
(5.2d)

\[
\frac{\partial T_r}{\partial t} = -w_r \cdot \frac{\partial T_r}{\partial z} + \frac{(-\Delta H_r)}{\rho \cdot c_p} \cdot r(C, T_r) 
\]  
(5.2e)

**Steam-generator**

\[ T_s = T_4 - \frac{q_e}{F \cdot c_p} \]  
(5.2f)

Additionally, first-order lags of 30 seconds were considered for temperature measurements, FEHE bypass flow rate, and furnace duty.
Chapter 5. Interaction between Design and Control of Heat-Integrated PFR

Controllability analysis

The main control objective is to keep the reaction conversion and selectivity within acceptable limits. Their control demands composition analysers that are expensive, require maintenance and have unfavourable dynamics. However, both variables depend on the reaction temperature. Hence, we consider control structures that include the reactor inlet temperature as the main controlled variable.

Our analysis will evaluate stability and disturbance rejection properties of different design alternatives. We consider the furnace duty and bypass around FEHE as potential manipulated variables, and feed flow rate, steam-generator duty and FEHE heat transfer coefficient as disturbances.

Three different control structures are investigated (Table 5.3). First (CS 1), furnace duty is used to control the reactor inlet temperature. Secondly (CS 2), FEHE bypass and furnace inlet temperature are the manipulated and controlled variables, respectively. The setpoint of this loop can be used, in a cascade manner, to control reactor inlet temperature. Both furnace duty - reactor inlet temperature and FEHE bypass - furnace inlet temperature loops are used in the third control structure.

<table>
<thead>
<tr>
<th>Table 5.3. Control structures</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>Outputs</td>
</tr>
<tr>
<td>$y_1$</td>
</tr>
<tr>
<td>$y_2$</td>
</tr>
<tr>
<td>Inputs</td>
</tr>
<tr>
<td>$u_1$</td>
</tr>
<tr>
<td>$u_2$</td>
</tr>
<tr>
<td>Disturbances</td>
</tr>
<tr>
<td>$d_1$</td>
</tr>
<tr>
<td>$d_2$</td>
</tr>
<tr>
<td>$d_3$</td>
</tr>
</tbody>
</table>
Chapter 5. Interaction between Design and Control of Heat-Integrated PFR

Linear analysis

The axial coordinate in Eqs. 5.2 was discretized by finite differences and the model was linearized around steady-state. The following state-space representation was obtained:

\[
\frac{dx(t)}{dt} = A \cdot x(t) + B \cdot u(t) + B_d \cdot d(t) \tag{5.3a}
\]

\[
y(t) = C \cdot x(t) + D \cdot u(t) + D_d \cdot d(t) \tag{5.3b}
\]

\[
e(t) = r(t) - y(t) \tag{5.3c}
\]

\(x\), \(u\), \(d\), \(y\), \(e\) and \(r\) are the vectors of the state variables, manipulated inputs, disturbances, controlled outputs, control errors and setpoints, respectively. \(A\), \(B\), \(B_d\), \(C\), \(D\) and \(D_d\) are matrices of appropriate dimensions.

In order to obtain meaningful controllability results, the inputs, disturbances and outputs were scaled. In terms of scaled variables, the control objective is to keep the control error \(|e(t)|<1\), using manipulated inputs \(|u(t)|<1\), when disturbances \(|d(t)|<1\) affect the process. The scaling factors are 1 K for temperatures and 25% of the nominal value for other variables.

In terms of transfer functions, the linear model of the process is given by:

\[
y(s) = G(s) \cdot u(s) + G_d(s) \cdot d(s) \tag{5.4}
\]

where:

\[
G(s) = C \cdot (sI - A)^{-1} \cdot B + D \tag{5.5a}
\]

\[
G_d(s) = C \cdot (sI - A)^{-1} \cdot B_d + D_d \tag{5.5b}
\]

Skogestad and Postlewaite (1996) review the linear controllability indices. Linear models were used only for controllability analysis. The full nonlinear model was used to evaluate the performance of the control system.

Stability

Computation of the eigenvalues of the \(A\) matrix shows that the operating points are stable for Designs 1A and 1B, but unstable for Designs 2A and 2B.

Figure 5.2 presents a part of the root-locus plot for Design 2A and CS1 (similar results are obtained with CS2). Two eigenvalues located near the imaginary axis are of interest. They are denoted by \(\lambda_+\) and \(\lambda_-\), according to their sign if the controller gain is zero.
There is a limited range of controller gain that ensures stability.

When the controller gain is increased, λ⁺ is shifted towards the left half plane and crosses the imaginary axes. Hence, there is a minimum controller gain for stability. In the same time, λ⁻ moves to the right. When λ⁺ and λ⁻ meet, a pair of complex conjugate eigenvalues emerges and moves to the right half plane. Hence, there is also a maximum controller gain for stability.

For Design 2B, λ⁺ and λ⁻ meet in the right half plane, near the imaginary axis. Hence, for all controller gains, there is at least one eigenvalue located in the right half plane. Consequently, linear analysis predicts that Design 2B can not be stabilised by a P-controller.

For the heat-integrated PFR, integral controller action has the usual, destabilising effect. This is in contrast with the catalytic reactor / preheater process (Tyree and Luyben, 1993), where integral action improved closed loop stability.

**Interactions**

For CS3 we compute the Relative Gain Array in order to evaluate the input-output pairing under decentralised control:

\[ \Lambda = G \otimes (G^{-1})^T \]  

\[(5.6)\]
The diagonal RGA elements for designs 1A, 1B, 2A and 2B are 4.274, 4.289, -0.954 and -0.964, respectively. Decentralised integral controllability requires positive values for stable systems, but negative values for unstable systems with one RHP pole. This condition is fulfilled in all cases.

Close-to-one diagonal elements denote little interaction. Small values in the RGA matrix also indicate that model uncertainty is not a problem.

The RGA_number, defined as:

\[
RGA\_number = \| I - \Lambda(j\omega) \| \text{sum}
\]

has small value and falls to zero for high frequency (Figure 5.3), showing that good control performance is possible.

![Figure 5.3. CS 3: RGA_number.](image)

- Design 1A; ■ - Design 1B; ▲ - Design 2A; × - Design 2B

RGA_number has small values and drops to zero at high frequency.

**Disturbance rejection**

To analyse the disturbance rejection properties, we calculate the Closed Loop Disturbance Gain (CLDG), defined by:

\[
\tilde{G}_d = \tilde{G} \cdot G^{-1} \cdot G_d
\]

where \( \tilde{G} \) is a matrix consisting of diagonal elements of \( G \).
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Its elements, $\tilde{g}_{dk}$, give the apparent gain of the $k^{th}$ disturbance on the $i^{th}$ output under decentralised control. For SISO systems, disturbance gain and CLDG are equivalent. The necessary condition to avoid inputs saturation is:

$$|g_i| > |\tilde{g}_{dk}|, \quad \forall k$$  \hspace{1cm} (5.9)

Figure 5.4 presents loop and disturbance gains when furnace duty is the manipulated variable (CS1). At low frequency, condition 5.9 is fulfilled for Design 1A and 2A. Hence, disturbances can be rejected. For Design 1B and 2B, it is necessary to slightly increase the maximum allowed control action, in order to avoid input saturation. It all cases, fast disturbances cannot be rejected because condition 5.9 is not satisfied at high frequencies. Feed flow rate is the worst disturbance. Large steam-generator duty (Design 1A and 2A), is the second demanding disturbance. Note that fast change of FEHE heat transfer coefficient is not expected, so we are only concerned with low frequency response.

![Graphs showing gain and disturbance gains for different designs.](image)

**Figure 5.4.** CS1: Frequency-dependent (rad/s) loop and disturbance gains.

- $g$: ●, ▲, X, $g_{dk}$, k=1,2,3.
- Slow disturbances can be rejected, but fast control cannot be achieved.
Diagrams in Figure 5.5 present the loop and disturbance gains when bypass around FEHE is the manipulated variable (CS2). Changes of the feed flow rate can not be handled. Disturbances in steam-generator duty can be rejected only if the steam-generator duty is small (Design 1B, 2B). Only Designs 2A and 2B can cope with FEHE fouling. On the whole, Design 2B (large FEHE, small steam-generator) performs the best.

\[
\begin{align*}
\text{Figure 5.5. CS2: Frequency-dependent (rad/s) loop and disturbance gains.} \\
\& g; n, \Delta, \times, g_{dk}, k=1,2,3. \\
\text{Feed flow rate disturbances can not be rejected.} \\
\text{Designs 1A and 2A can not handle change of steam-generator duty.} \\
\text{Only Design 2A can cope with FEHE fouling.}
\end{align*}
\]

In CS3, a second controller is added to CS1. It regulates the furnace inlet temperature using a bypass around FEHE. RGA elements show that, compared to CS1, the gain of main loop (furnace duty - reactor inlet temperature) is lower for Design 1A and 1B, and is practically unchanged for Designs 2A and 2B.

The change in the effect of the $k^{th}$ disturbances on $i^{th}$ output, caused by decentralised control, is given by the relative disturbance gain (RDG) defined as $\beta_{ik} = \tilde{g}_{ik} / g_{ik}$. Figure 5.6 presents the RDG of the feed flow rate disturbance. Interactions increase the gain from
disturbance to reactor inlet temperature; Hence, there is little incentive to add the second control loop. Moreover, except Design 2B, bypass around FEHE is not powerful enough to control furnace inlet temperature when the system is affected by disturbances.

Figure 5.6. CS3: Frequency-dependent (rad/s) RDG of feed flow rate disturbance. ♦ - \( \beta_{12} \), ■ - \( \beta_{22} \). Interactions increase the gain from disturbance to reactor inlet temperature.

Nonlinear analysis

The control of the heat-integrated reactor in the toluene hydrodealkylation (HDA) plant has been considered by Luyben et al. (1998). They pointed out that is difficult to stabilise systems with large FEHE and small furnace. In this section, we identify the region in the design parameter space leading to designs that can not be stabilised. To achieve this goal, we use elements of the bifurcation theory (Guckenheimer and Holmes, 1983). The model equations can be written in the following dimensionless form:
Chapter 5. Interaction between Design and Control of Heat-Integrated PFR

Furnace:

\[
H_i \cdot M_b \frac{\partial \theta_b}{\partial \tau} = -\frac{\partial \theta_b}{\partial \xi} + Da \cdot H_t \cdot (\theta_w - \theta_b)
\]  
(5.10a)

\[
H_i \cdot M_w \frac{\partial \theta_w}{\partial \tau} = Da \cdot H_b - Da \cdot H_c \cdot \int_0^1 (\theta_w - \theta_b) \cdot d\xi
\]  
(5.10b)

Reactor:

\[
\frac{\partial X}{\partial \tau} = -\frac{\partial X}{\partial \xi} + Da \cdot \exp\left(\frac{\gamma \cdot \theta_x}{1+\theta_x}\right) \cdot (1-X)
\]  
(5.10c)

\[
Le \frac{\partial \theta_x}{\partial \tau} = -\frac{\partial \theta_x}{\partial \xi} + B \cdot Da \cdot \exp\left(\frac{\gamma \cdot \theta_x}{1+\theta_x}\right) \cdot (1-X)
\]  
(5.10d)

Temperature sensor:

\[
M_s \frac{d\theta_s}{d\tau} = Da \cdot (\theta_s(1) - \theta_s)
\]  
(5.10e)

P-controller (SP=0) and duty valve:

\[
M_v \frac{dH_b}{d\tau} = Da \cdot (H_b^* - K_c \cdot \theta_s - H_b)
\]  
(5.10f)

Boundary conditions:

\[
\theta_b(0) = (1-\epsilon) \cdot \theta_0 + \epsilon \cdot (\theta_s(1) - Da \cdot H_c)
\]  
(5.10g)

\[
\theta_s(0) = \theta_s(1)
\]  
(5.10h)

Figure 5.7 presents, qualitatively, the conversion vs. controller gain and Damkohler number for two sets (FEHE efficiency, steam-generator duty). The first diagram corresponds to design 2A (large FEHE, large steam-generator). Model equations are used to compute the controller bias (the value of the manipulated variable when the controlled variable equals its set point). This is denoted as the nominal case and is represented by the dark lines. The system exhibits three steady-states for small controller gain. The middle state is of interest, but is unstable. Increasing the controller gain, the branches become closer. They coalesce for a critical value of the controller gain. This is a pitchfork bifurcation point. For higher values of the controller gain, only one steady-state is possible. When the controller gain is further increased, the system loses stability due to a Hopf bifurcation. Hence, the pitchfork and Hopf points bound the range of controller gain that ensures state unicity and stability.

The extent of the unicity and stability region decreases when the FEHE efficiency increases or the steam-generator duty decreases. For a critical value of FEHE efficiency,
Pitchfork and Hopf bifurcations occur at the same value of the controller gain. Incidentally, the Design 2B is very close to this limit. This situation is presented in the second diagram of Figure 5.7. If FEHE efficiency is further increased, the design can no longer be stabilised.

![Design 2A](image)

![Design 2B](image)

**Figure 5.7. Conversion vs. controller gain and Damköhler number.**

Pitchfork and Hopf bifurcation points bound the range of controller gain that ensures state unicity and stability. Middle steady-state can not be stabilised for large FEHE efficiency and small steam-generator duty.

The correct value for the controller bias can not be calculated when design parameters are uncertain. This is denoted as the perturbed case and is presented in Figure 5.7 by the light lines. The Hopf point is one limit of the stability region. Depending on the model parameter uncertainty, the other limit is the fold point located on the lower or the upper solution branch. Note that the region of state unicity and stability is larger. However, zero control error can not by achieved by proportional control.

In order to classify the steady-state and dynamic behaviour of the controlled system, we choose the controller gain as bifurcation parameter. The Hopf and fold points are 1-codimensional, which means that the value of one parameter is fixed (Guckenheimer and
Holmes, 1983). In the general case, a pitchfork point has codimension 3. However, the assumption that the parameters used for bias calculation are exactly known introduces $Z_2$-symmetry. Consequently, the pitchfork point becomes also 1-codimensional (Golubitsky and Schaeffer, 1985).

Consider a fixed, large FEHE efficiency. Then, there is a particular value of the steam-generator duty for which the pitchfork and Hopf bifurcation occur at the same value of the controller gain, like in the second diagram of Figure 5.7. This point has codimension 2. We call it “Hopf-and-pitchfork”. Computing its locus in the space of the design parameters (FEHE efficiency, steam-generator duty), we trace the boundary between the designs can be stabilised, and designs that can not. Similarly, computing the locus of the cusp variety (Guckenheimer and Holmes, 1983), we trace the boundary between state unicity and multiplicity.

The results are presented in Figure 5.8. The cusp and Hopf-and-pitchfork varieties divide the design parameter space into three regions. In region I, the unique steady-state is stable for low controller gain, but unstable for high controller gain. State multiplicity appears when the cusp variety is crossed to region II, but it is possible to find a controller gain that gives a unique stable steady-state. When the Hopf locus is crossed to region III, it is impossible to get both state unicity and stability.

![Figure 5.8. Phase diagram in the space of design parameters.](image)

Cusp and Hopf-and-pitchfork varieties divide the parameters space into regions with different conversion vs. controller gain bifurcation diagrams.
Dynamic simulation

We verify first that design 2B can not be stabilised. Figure 9 presents the results of dynamic simulation, when CS1 is used. Initially, the system is at steady-state. After 2000 s., the feed flow rate is changed by 0.1%, for 100 s. In the first simulation, the controller gain is lower than the gain at the pitchfork point. For this reason, there are multiple steady-states and the operating point is unstable. Hence, the disturbance drives the system to the extinguished state. In the second simulation, the controller gain is slightly increased past the pitchfork point. Consequently, only one steady-state exists. However, it is unstable and surrounded by a limit cycle.

![Dynamic simulation results](image)

**Figure 5.9. Dynamic simulation results.**

For large FEHE and small steam-generator duty, it is impossible to get both state unicity and stability.

A question that naturally arises is: “The results of linear controllability analysis are applicable to such nonlinear systems?” To answer this question, we apply feed flow rate and steam-generator duty disturbances to Designs 1A, 1B and 2A. CS1 with Tyreus - Luyben controller settings (Table 5.4) is used. The results are presented in Figure 5.10.
Table 5.4. Controller tuning

<table>
<thead>
<tr>
<th>Design</th>
<th>$K_c$ ($10^3$ W/K)</th>
<th>$T_i$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>160</td>
<td>1100</td>
</tr>
<tr>
<td>1B</td>
<td>160</td>
<td>1000</td>
</tr>
<tr>
<td>2A</td>
<td>50</td>
<td>1800</td>
</tr>
</tbody>
</table>

In all cases, the manipulated variable is strong enough to reject disturbances. However, disturbance rejection is slow and the control error is initially large. For Designs 1A and 1B, feed flow rate is the worst disturbance and input saturation occurs. For design 2A, the disturbances considered are almost equally difficult. These results agree with linear controllability analysis.

Figure 5.10. Dynamic simulation
Results of linear controllability analysis are confirmed.
Conclusions

In this article, we analyzed the interaction between design and control of a heat-integrated PFR. The following conclusions are drawn:

- The controllability of the heat-integrated PFR is determined by two design decisions: FEHE efficiency and steam-generator duty.
- Systems with small steam-generator and large FEHE can not be stabilized. The Hopf-and-pitchfork variety bounds the range of design parameters for which the system can be stabilized.
- At steady-state, control structures using furnace duty as manipulated variable can reject disturbances in feed flow rate, steam-generator duty and FEHE fouling. However, fast control can not be achieved. There is no incentive to add a bypass around FEHE because it enhances the effect of disturbances.
- Designs with small FEHE are also difficult to control if the operating point is close to the cusp variety.
- The results of linear and nonlinear analysis are confirmed by dynamic simulation.

The approach presented here may be extended to similar problems, where state multiplicity and instability limits the range of controllable designs.

Notation

\[ A = \text{area, m}^2 \]
\[ c_p = \text{specific heat, J/(kg K)} \]
\[ C = \text{concentration, mol/m}^3 \]
\[ Da = \text{Damkohler number, dimensionless} \]
\[ Da = \frac{V_r \cdot \rho}{F} \cdot k(T) \]
\[ d = \text{diameter, m} \]
\[ F = \text{mass flowrate, kg/s} \]
\[ \Delta H_r = \text{heat of reaction, J/mol} \]
\[ H_h = \text{furnace duty, dimensionless} \]
\[ H_h = \frac{q_h}{\rho \cdot c_p \cdot \bar{T} \cdot V_r \cdot k(T)} \]
\[ H_c = \text{steam-generator duty, dimensionless} \]
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\[
Q_c = \frac{\rho \cdot c_p \cdot \bar{T} \cdot V_r \cdot k(\bar{T})}{K_{st} \cdot A_{st}}
\]

\(H_t\) = furnace heat transfer area, dimensionless

\[
H_f = \frac{K_{st} \cdot A_{st}}{\rho \cdot c_p \cdot V_r \cdot k(\bar{T})}
\]

\(K\) = heat transfer coefficient, \(W/(m^2 K)\)

\(Le\) = Lewis number, dimensionless \((Le=1)\)

\(m\) = mass, kg

\(M_w\) = furnace, mass of the tube walls, dimensionless

\[
M_h = \frac{\rho_w \cdot c_{pw} \cdot \delta_w \cdot k(\bar{T})}{K_{st}}
\]

\(NTU\) = number of transfer units, dimensionless,

\[
NTU = \frac{K_{st} \cdot A_{st}}{F \cdot c_p}
\]

\(q\) = duty, \(W\)

\(t\) = time, \(s\)

\(\bar{t}\) = reference time, \(s\)

\[
\bar{t} = \frac{V_r \cdot \rho}{F}
\]

\(T\) = temperature, \(K\)

\(\bar{T}\) = reference temperature \((\bar{T} = T_2)\), \(K\)

\(V\) = volume, \(m^3\)

\(w\) = velocity, \(m/s\)

\(z\) = axial coordinate, \(m\)

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Greek letters

\( I - \alpha \) = bypass around FEHE
\( \rho \) = mass density, kg/m\(^3\)
\( \xi \) = thickness of furnace tube walls, m
\( \varepsilon \) = FEHE efficiency, dimensionless

\[
\varepsilon = \frac{1 - e^{-r_{t-u}(I-\alpha)}}{1 - \alpha \cdot e^{-r_{t-u}(I-\alpha)}}
\]

Subscripts

\( c \) = steam-generator
\( f \) = furnace, fluid phase
\( h \) = furnace
\( r \) = reactor
\( s \) = FEHE, shell-side
\( t \) = FEHE, tube-side
\( w \) = furnace, tube wall

Literature cited


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