Appendix H

Dynamic Models and Parameters Used for Plantwide Control Chapters

H.1 ENERGY BALANCE AND PARAMETERS FOR THE REACTOR/ DISTILLATION COLUMN MODEL (APPENDIX F)

Energy Balance for the Reactor

Assumptions made in developing the balance:

1. Cooling temperature $T_C$ is constant.
2. There is no vapor phase in the reactor.
3. There are no heat losses to the environment.
4. All streams and reactor contents have the constant heat capacity $C_P$.

\[
\frac{dT_R}{dt} = \frac{1}{C_P H_R} \left[ F_0 C_P(T_0 - T_R) + D C_P(T_D - T_R) - U A(T_R - T_C) - H_R \lambda k_R z \right] \quad \text{(H-1)}
\]

Parameters in Table H.1 and controller settings in Table H.2 were used in the simulations shown in Figs. F.9a and F.9b.

H.2 CORE REACTOR/FLASH UNIT MODEL AND PARAMETERS (APPENDIX G)

H.2.1 Simulation Models

In developing a simulation model that corresponds to the core elements of the reactor/flash unit plant, we first state the general modeling assumptions, then develop the model equations in several forms. The first model is based on the methods of Chapter 2. The second model is a simplified version. The third is developed specifically to use with a symbolic equation manipulator such as Mathematica for calculating the RGA. An evaluation of the three models, including comparison of their degrees of freedom, is considered in Exercise G.1. Figure G.5 illustrates the process units and stream numbering conventions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor feed rate</td>
<td>$F_0$</td>
<td>460</td>
<td>lb-mol/h</td>
</tr>
<tr>
<td>Feed temperature</td>
<td>$T_0$</td>
<td>530.0</td>
<td>°R</td>
</tr>
<tr>
<td>Distillate (recycle) rate</td>
<td>$D$</td>
<td>500</td>
<td>lb-mol/h</td>
</tr>
<tr>
<td>Distillate temperature</td>
<td>$T_D$</td>
<td>587.2</td>
<td>°R</td>
</tr>
<tr>
<td>Reactor holdup</td>
<td>$H_R$</td>
<td>2400</td>
<td>lb-mol</td>
</tr>
<tr>
<td>Reactor composition</td>
<td>$z$</td>
<td>0.5</td>
<td>mass fraction</td>
</tr>
<tr>
<td>Reactor temperature</td>
<td>$T_R$</td>
<td>616.4</td>
<td>°R</td>
</tr>
<tr>
<td>Cooling coil temperature</td>
<td>$T_C$</td>
<td>596.1</td>
<td>°R</td>
</tr>
<tr>
<td>Heat capacity</td>
<td>$C_P$</td>
<td>0.75</td>
<td>Btu/lb-mol °R</td>
</tr>
<tr>
<td>Overall heat transfer coeff.</td>
<td>$U$</td>
<td>150.5</td>
<td>Btu/h ft$^2$ °R</td>
</tr>
<tr>
<td>Area for heat exchange</td>
<td>$A$</td>
<td>3630</td>
<td>ft$^2$</td>
</tr>
<tr>
<td>Specific reaction rate</td>
<td>$k_R$</td>
<td>0.33</td>
<td>h$^{-1}$</td>
</tr>
<tr>
<td>Heat of reaction</td>
<td>$\lambda$</td>
<td>$-30,000$</td>
<td>Btu/lb-mol</td>
</tr>
</tbody>
</table>

Parameters in Tables H.1 and H.2 reported by Wu and Yu (1996).
Modeling Assumptions:

1. Mixing is perfect in each vessel.
2. Volume $V_R$ is controlled by $w_3$ and assumed to be constant.
3. Temperature in each vessel is constant.
4. Volume $V_F$ is controlled and assumed to be constant. It is small compared to Volume $V_R$.
5. Volume $V_T$ varies to provide surge capacity between the flash unit and reactor.
6. Density $\rho$ is constant.
7. Stream 1 is pure A ($x_{1A} = 1$).
8. Stream 2 is a mixture of B and D.
9. The holdup in the piping is negligible; materials move from vessel to vessel in zero time.

Material Balances:

**Reactor:**

Ordinarily, reaction rate is expressed in terms of reactant concentrations—for example, in units of kg-mol/m$^3$:

$$r_c = k' [c_{R,A}] [c_{R,B}]$$

where subscript $R$ denotes reactor. This expression can be converted to compositions expressed in mass fraction by rewriting the molar concentration terms as follows:

$$r_c = k' \left( \frac{\rho x_{R,A}}{MW_A} \right) \left( \frac{\rho x_{R,B}}{MW_B} \right)$$

where $x$ denotes mass fraction; the mass density $\rho$, with units of kg/m$^3$, is assumed to be constant; and $MW_A$ and $MW_B$ are the molecular weights for A and B, respectively.

$$K_c \text{ normally is dimensionless. For simulation purposes, the controller is assumed to contain the gains of both the measurement transmitter and the control valve.}$$

<table>
<thead>
<tr>
<th>Alternative</th>
<th>Control Loop</th>
<th>CV - MV</th>
<th>$K_c$</th>
<th>$\tau_c$, min</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Composition</td>
<td>$x_B - V$</td>
<td>$-2.4 \times 10^4$ lb-mol/h</td>
<td>57.6</td>
</tr>
<tr>
<td></td>
<td>Composition</td>
<td>$x_D - R$</td>
<td>$6.82 \times 10^3$ lb-mol/h</td>
<td>76.7</td>
</tr>
<tr>
<td></td>
<td>Level</td>
<td>$H_R - F$</td>
<td>$-2.26$ hr$^{-1}$</td>
<td>21.2</td>
</tr>
<tr>
<td>2</td>
<td>Composition</td>
<td>$x_B - V$</td>
<td>$-1.7 \times 10^4$ lb-mol/h</td>
<td>76.7</td>
</tr>
<tr>
<td></td>
<td>Composition</td>
<td>$x_D - R$</td>
<td>$5.33 \times 10^3$ lb-mol/h</td>
<td>86.4</td>
</tr>
<tr>
<td></td>
<td>Level</td>
<td>Not used</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Composition</td>
<td>$x_B - V$</td>
<td>$-1.05 \times 10^4$ lb-mol/h</td>
<td>37.6</td>
</tr>
<tr>
<td></td>
<td>Level</td>
<td>$H_R - D$</td>
<td>$1.44 \times 10^3$ h$^{-1}$</td>
<td>45.7</td>
</tr>
<tr>
<td></td>
<td>Composition</td>
<td>$x_D - H_{R,sp}$</td>
<td>$12.2$ lb-mol</td>
<td></td>
</tr>
</tbody>
</table>

$K_c$ normally is dimensionless. For simulation purposes, the controller is assumed to contain the gains of both the measurement transmitter and the control valve.

$$r_C = \rho \left( \frac{\rho k'}{MW_A MW_B} \right) x_{R,A} x_{R,B}$$

$$= \rho \left( k x_{R,A} x_{R,B} \right)$$

where $k$ has units of time$^{-1}$. Then, define a dimensionless mass ratio,

$$\alpha = \frac{MW_A}{MW_C}$$

to represent the relationship between the masses of 1 kg-mol of component A that reacts to yield a kg-mol of C; thus $1 - \alpha$ represents the mass of B used in the same reaction:

$$r_A = -\alpha r_C$$

and

$$r_B = -(1 - \alpha) r_C$$

where the dimensions are mass (of component i)/time.

The mass holdup in the reactor is controlled and constant. With constant $\rho$, the overall balance is

$$\rho \frac{dV_R}{dt} = w_1 + w_2 + w_8 - w_3 = 0$$

yielding

$$w_3 = w_1 + w_2 + w_8$$

The balance for each component in the reactor can be written as follows (recall subscript $T$ denotes the recycle tank):

$$\frac{d(\rho V_{R,A})}{dt} = w_1 - w_3 x_{R,A} - \rho V_R \alpha k x_{R,A} x_{R,B}$$

$$\frac{d(\rho V_{R,B})}{dt} = \rho V_R (1 - \alpha) k x_{R,A} x_{R,B}$$
\[
\frac{d(\rho V_R x_{R,C})}{dt} = -w_3 x_{R,C} + \rho V_R k x_{R,A} x_{R,B} \quad (H-12)
\]
\[
\frac{d(\rho V_R x_{R,D})}{dt} = w_2 x_{2D} + w_8 x_{T,D} - w_3 x_{R,D} \quad (H-13)
\]

Because \( V_R \) is constant, only three of these balances are independent. We eliminate the C balance, Eq. H-12, which contains no inputs, using in its place:

\[
x_{R,C} = 1 - (x_{R,A} + x_{R,B} + x_{R,D}) \quad (H-14)
\]

**Flash Unit (modeled as a splitter):**

The flash unit liquid volume \( V_F \) is controlled, hence assumed to be constant. It also is negligible (\( V_F \approx 0 \)) for modeling purposes. Therefore,

\[
w_5 = w_3 - w_4 = w_1 + w_2 + w_8 - w_4 \quad (H-15)
\]

In a hypothetical splitter, only A and C leave in the liquid phase while B and D leave as vapor. Thus a mass balance on the A and C components in the flash unit yields

\[
w_4 = w_3 (x_{R,A} + x_{R,C}) = (w_1 + w_2 + w_8) (x_{R,A} + x_{R,C}) \quad (H-16)
\]

The exiting liquid-phase compositions (including critical quality measurement \( x_{4A} \)) are

\[
x_{4A} = \frac{x_{R,A}}{x_{R,A} + x_{R,C}} \quad (H-17)
\]
\[
x_{4C} = \frac{x_{R,C}}{x_{R,A} + x_{R,C}} = 1 - x_{4A} \quad (H-18)
\]

Similarly, the exiting vapor-phase flow rate and compositions are obtained from a mass balance on the vapor-phase components:

\[
w_5 = w_3 (x_{R,B} + x_{R,D}) = (w_1 + w_2 + w_8) (x_{R,B} + x_{R,D}) \quad (H-19)
\]
\[
x_{7B} = x_{6B} = x_{5B} = \frac{x_{R,B}}{x_{R,B} + x_{R,D}} = 1 - x_{7D} \quad (H-20)
\]
\[
x_{7D} = x_{6D} = x_{5D} = \frac{x_{R,D}}{x_{R,B} + x_{R,D}} \quad (H-21)
\]

Note that substituting H-16 and H-19 into the overall mass balance around the flash unit (H-15) satisfies it exactly, as it must.

**Purge stream node mass balance:**

\[
w_7 = (w_1 + w_2 + w_8) (x_{R,B} + x_{R,D}) - w_6 \quad (H-22)
\]

**Recycle tank:**

The overall mass balance is given by

\[
\rho \frac{dV_T}{dt} = w_7 - w_8 \quad (H-23)
\]

and the component balances by

\[
\frac{d(V_T x_{T,B})}{dt} = w_7 x_{T,B} - w_8 x_{T,B} \quad (H-24)
\]
\[
\frac{d(V_T x_{T,D})}{dt} = w_7 x_{T,D} - w_8 x_{T,D} \quad (H-25)
\]

Only two of these relations are independent. Because we are primarily interested in the D component in the recycle, we choose Eqs. H-23 and H-25. Using the methods of Chapter 2, the derivative in Eq. H-23 can be expanded as

\[
\rho \frac{dV_T}{dt} x_{T,D} + \rho V_T \frac{dx_{T,D}}{dt} = w_7 x_{T,D} - w_8 x_{T,D} \quad (H-26)
\]
\[
(w_7 - w_8) x_{T,D} + \rho V_T \frac{dx_{T,D}}{dt} = w_7 x_{T,D} - w_8 x_{T,D} \quad (H-27)
\]

so that

\[
\rho V_T \frac{dx_{T,D}}{dt} = w_7 (x_{T,D} - x_{T,D}) \quad (H-28)
\]

The D composition of Stream 8 is provided by the output relation

\[
x_{8D} = x_{T,D} \quad (H-29)
\]

and the holdup of the recycle tank by

\[
H_T = \rho V_T \quad (H-30)
\]

**Feed stream concentration relations:**

Stream 1 is pure A. Therefore,

\[
x_{1A} = 1 \quad (H-31)
\]

Because Stream 2 consists only of reactant B and contaminant D,

\[
x_{2B} = 1 - x_{2D} \quad (H-32)
\]

**H.2.2 Control Degrees of Freedom (CDOF) Analysis**

**Additional Assumptions for Control Structure Analysis:**

10. \( V_R \) is assumed to be controlled by V3, so \( V_R \) and \( w_3 \) are removed from further consideration in control structure analysis.
11. $V_F$ is assumed to be controlled by $V_4$, so $V_F$ and $w_4$ also can be eliminated from further consideration in control structure analysis.

12. Manipulated inputs are $w_1, w_2, w_6,$ and $w_8$.

13. Controlled outputs are $w_4, x_{SD}, x_{4A},$ and $H_T$.

14. Primary disturbance variable is $x_{SD}$.

$$N_{CF} = 4 \text{ (maximum number of independently controlled variables)} \quad (H-33)$$

This formulation of the model leads to the following set of CVs and MVs used in Appendix G:

<table>
<thead>
<tr>
<th>Controlled Variables</th>
<th>Manipulated Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>$w_4$</td>
<td>$w_1$</td>
</tr>
<tr>
<td>$x_{4A}$</td>
<td>$w_2$</td>
</tr>
<tr>
<td>$x_{SD}$</td>
<td>$w_6$</td>
</tr>
<tr>
<td>$H_T$</td>
<td>$w_8$</td>
</tr>
</tbody>
</table>

### H.2.3 The Simplified “Composition Model”

By eliminating extraneous variables, the model can be simplified to a set of equations containing only the desired four input and four output variables used in the control simulations of Appendix G, yielding the following:

$$\frac{dx_{RA}}{dt} = \frac{1}{\rho V_R} \left[ w_1 - (w_1 + w_2 + w_3)x_{RA} - \rho V_R k x_{RA} x_{RB} \right] \quad (H-34)$$

$$\frac{dx_{RB}}{dt} = \frac{1}{\rho V_R} \left[ w_2(1 - x_{2D}) + w_3(1 - x_{TD}) + (w_1 + w_2 + w_3)x_{RB} - \rho V_R (1 - \alpha) k x_{RA} x_{RB} \right] \quad (H-35)$$

$$\frac{dx_{RD}}{dt} = \frac{1}{\rho V_R} \left[ w_2 x_{2D} + w_3 x_{TD} - (w_1 + w_2 + w_3)x_{RD} \right] \quad (H-36)$$

$$\frac{dV_T}{dt} = \frac{1}{\rho} \left[ (w_1 + w_2 + w_3)(x_{RB} + x_{RD}) - w_6 - w_8 \right] \quad (H-37)$$

$$\frac{dx_{TD}}{dt} = \frac{(w_1 + w_2 + w_3)(x_{RB} + x_{RD}) - w_6}{\rho V_T} \times \left[ \frac{x_{RD}}{x_{RB} + x_{RD} - x_{TD}} \right] \quad (H-38)$$

$$w_4 = (w_1 + w_2 + w_3)(1 - x_{RB} - x_{RD}) \quad (H-39)$$

$$x_{4A} = \frac{x_{RA}}{1 - x_{RB} - x_{RD}} \quad (H-40)$$

$$x_{8D} = x_{TD} \quad (H-41)$$

$$H_T = \rho V_T \quad (H-42)$$

### H.2.4 The Simplified “Holdup Model” Used for Analysis and Simulation

In developing the component balances, there are alternative ways of defining the state variables—i.e., the dependent variables in the accumulation terms (Chapter 3). Another alternative is to use the species mass holdups in each vessel as the state variables and then to find the compositions from the mass holdups, as in Equations H-43 – H-48, below. The compositions in the reactor are given by

$$x_{RA} = \frac{H_{RA}}{H_R} \quad (H-43)$$

$$x_{RB} = \frac{H_{RB}}{H_R} \quad (H-44)$$

$$x_{RC} = \frac{H_{RC}}{H_R} \quad (H-45)$$

$$x_{RD} = \frac{H_{RD}}{H_R} \quad (H-46)$$

and, in the recycle tank, by

$$x_{TB} = \frac{H_{TB}}{H_T} \quad (H-47)$$

$$x_{TD} = \frac{H_{TD}}{H_T} \quad (H-48)$$

Making this change of variables in the previous model equations prior to expanding H-24 and H-25, we obtain

$$\frac{dH_{RA}}{dt} = w_1 - (w_1 + w_2 + w_3) \frac{H_{RA}}{H_R} - \alpha k \frac{H_{RA}}{H_R} \frac{H_{RB}}{H_R} \quad (H-49)$$

$$\frac{dH_{RB}}{dt} = w_2(1 - x_{2D}) + w_3 \frac{H_{TB}}{H_T} + \frac{H_{RD}}{H_R} \quad (H-50)$$

$$\frac{dH_{RD}}{dt} = w_2 x_{2D} + \frac{H_{RD}}{H_R} \quad (H-51)$$

$$\frac{dH_{TB}}{dt} = (w_1 + w_2 + w_3) \frac{H_{RB}}{H_R} - w_6 \frac{H_{TB}}{H_T} + \frac{H_{TD}}{H_T} \quad (H-52)$$
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with the four outputs that remain to be controlled given by

\[ w_4 = (w_1 + w_2 + w_8) \left( \frac{H_R - H_{R,B} - H_{R,D}}{H_R} \right) \]  (H-54)

\[ x_{4A} = \frac{H_{R,A}}{H_R - H_{R,B} - H_{R,D}} \]  (H-55)

\[ x_{8D} = \frac{H_{T,D}}{H_T} \]  (H-56)

\[ H_T = H_{T,B} + H_{T,D} \]  (H-57)

Note that the holdup model, while complicated slightly by the quotient terms, has an advantage in that Eq. H-53 is symmetric with H-52 and thus is easier to manipulate symbolically than with Eqs. H-37 and, particularly, H-38. The model also has one less parameter.

**H.2.5 Plant Parameters and Steady-State Operating Values**

Table H.3 gives the parameters used in this case study. In addition, values of the input variables (both manipulated and disturbance variables) are specified in Table H.4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( w_1 ) (kg/h)</td>
<td>1010</td>
</tr>
<tr>
<td>( w_2 ) (kg/h)</td>
<td>1100</td>
</tr>
<tr>
<td>( w_6 ) (kg/h)</td>
<td>110</td>
</tr>
<tr>
<td>( w_8 ) (kg/h)</td>
<td>890</td>
</tr>
<tr>
<td>( x_{2D} )</td>
<td>0.01</td>
</tr>
</tbody>
</table>

These parameters and constant model inputs result in the steady-state in Table H.5. Note that the first five variables listed are the state variables in the mass holdup formulation of the model; the last four are the output variables:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Steady-State Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_{R,A} ) (kg)</td>
<td>20</td>
</tr>
<tr>
<td>( H_{R,B} ) (kg)</td>
<td>900</td>
</tr>
<tr>
<td>( H_{R,D} ) (kg)</td>
<td>110</td>
</tr>
<tr>
<td>( H_{T,B} ) (kg)</td>
<td>450</td>
</tr>
<tr>
<td>( H_{T,D} ) (kg)</td>
<td>50</td>
</tr>
<tr>
<td>( w_4 ) (kg/h)</td>
<td>2000</td>
</tr>
<tr>
<td>( x_{4A} )</td>
<td>0.01</td>
</tr>
<tr>
<td>( x_{8D} )</td>
<td>0.10</td>
</tr>
<tr>
<td>( H_T ) (kg)</td>
<td>500</td>
</tr>
</tbody>
</table>

The resulting steady-state flow rates are then found as shown in Table H.6.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Stream Number, ( S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( w_{SA} )</td>
<td>1010  0  20  20  0  0  0  0  0</td>
</tr>
<tr>
<td>( w_{SB} )</td>
<td>0  1089  900  0  900  99  801  801</td>
</tr>
<tr>
<td>( w_{SC} )</td>
<td>0  0  1980  1980  0  0  0  0  0</td>
</tr>
<tr>
<td>( w_{SD} )</td>
<td>0  11  100  0  100  11  89  89  89</td>
</tr>
<tr>
<td>( w_S )</td>
<td>1010  1100  3000  2000  1000  110  890  890</td>
</tr>
</tbody>
</table>
H.2.6 RGA Analysis

The model equations can now be linearized about the nominal steady state. The gain matrix (Eq. G-1) is then obtained, and the RGA (Eq. G-2) is calculated. Note that in linearizing these relations, the steady state is defined by the values of the steady-state holdups. Therefore, the gain matrix and the RGA may differ slightly from those obtained using the previous model in terms of the recycle tank total holdup and the process concentrations.

H.2.7 Closed-Loop Control

Two sets of closed-loop simulations were made using the holdup version of the core reactor/flash unit model; the results are plotted in Figures G.6 and G.7. For each case, the four control loops listed in Table G.4 were implemented as shown in Tables H.7 and H.8, respectively.

REFERENCE