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.

$$\frac{dT_R}{dt} = \frac{1}{C_p H_R} \times [F_0 C_p(T_0 - T_R) + DC_p(T_D - T_R) - UA(T_R - T_C) - H_R \lambda k_R z] \qquad \text{(H-1)}$$

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 H.1 Parameters Used in the Energy Balance.

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

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

Table H.2 Controller Settings for the Reactor/Distillation Column Closed-Loop Responses (Figures 22.9a and 22.9b).

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

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.

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 ρ 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:

$$r_C = k' \left[\frac{\rho \, x_{R,A}}{MW_A}\right]\left[\frac{\rho \, x_{R,B}}{MW_B}\right] \tag{H-2}$$

where x denotes mass fraction; the mass density ρ, 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.

$$r_C = \rho \left(\frac{\rho k'}{MW_A MW_B}\right) x_{R,A} x_{R,B} \tag{H-3}$$

$$= \rho \, k \, x_{R,A} \, x_{R,B} \tag{H-4}$$

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

$$\alpha \overset{\Delta}{=} \frac{MW_A}{MW_C} \tag{H-5}$$

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:

$$r_A = -\alpha r_C \tag{H-6}$$

and

$$r_B = -(1-\alpha) r_C \tag{H-7}$$

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

The mass holdup in the reactor is controlled and constant. With constant ρ, the overall balance is

$$\rho \frac{dV_R}{dt} = w_1 + w_2 + w_8 - w_3 = 0 \tag{H-8}$$

yielding

$$w_3 = w_1 + w_2 + w_8 \tag{H-9}$$

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

$$\frac{d(\rho V_R x_{R,A})}{dt} = w_1 - w_3 x_{R,A} - \rho V_R \alpha k x_{R,A} x_{R,B} \tag{H-10}$$

$$\frac{d(\rho V_R x_{R,B})}{dt} = w_2 x_{2B} + w_8 x_{T,B} - w_3 x_{R,B} - \rho V_R (1-\alpha) k x_{R,A} x_{R,B} \tag{H-11}$$

$$\frac{d(\rho V_R x_{R,C})}{dt} = -w_3 x_{R,C} + \rho V_R k x_{R,A} x_{R,B} \quad \text{(H-12)}$$

$$\frac{d(\rho V_R x_{R,D})}{dt} = w_2 x_{2D} + w_8 x_{T,D} - w_3 x_{R,D} \quad \text{(H-13)}$$

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:

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

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,

$$w_5 = w_3 - w_4 = w_1 + w_2 + w_8 - w_4 \quad \text{(H-15)}$$

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

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

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

$$x_{4A} = \frac{x_{R,A}}{x_{R,A} + x_{R,C}} \quad \text{(H-17)}$$

$$x_{4C} = \frac{x_{R,C}}{x_{R,A} + x_{R,C}} = 1 - x_{4A} \quad \text{(H-18)}$$

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

$$w_5 = w_3(x_{R,B} + x_{R,D}) = (w_1 + w_2 + w_8)(x_{R,B} + x_{R,D}) \quad \text{(H-19)}$$

$$x_{7B} = x_{6B} = x_{5B} = \frac{x_{R,B}}{x_{R,B} + x_{R,D}} = 1 - x_{7D} \quad \text{(H-20)}$$

$$x_{7D} = x_{6D} = x_{5D} = \frac{x_{R,D}}{x_{R,B} + x_{R,D}} \quad \text{(H-21)}$$

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:

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

Recycle tank:

The overall mass balance is given by

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

and the component balances by

$$\rho \frac{d(V_T x_{T,B})}{dt} = w_7 x_{7B} - w_8 x_{T,B} \quad \text{(H-24)}$$

$$\rho \frac{d(V_T x_{T,D})}{dt} = w_7 x_{7D} - w_8 x_{T,D} \quad \text{(H-25)}$$

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

$$\rho \frac{dV_T}{dt} x_{T,D} + \rho V_T \frac{dx_{T,D}}{dt} = w_7 x_{7D} - w_8 x_{T,D} \quad \text{(H-26)}$$

$$(w_7 - w_8) x_{T,D} + \rho V_T \frac{dx_{T,D}}{dt} = w_7 x_{7D} - w_8 x_{T,D} \quad \text{(H-27)}$$

so that

$$\rho V_T \frac{dx_{T,D}}{dt} = w_7(x_{7D} - x_{T,D}) \quad \text{(H-28)}$$

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

$$x_{8D} = x_{T,D} \quad \text{(H-29)}$$

and the holdup of the recycle tank by

$$H_T = \rho V_T \quad \text{(H-30)}$$

Feed stream concentration relations:

Stream 1 is pure A. Therefore,

$$x_{1A} = 1 \quad \text{(H-31)}$$

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

$$x_{2B} = 1 - x_{2D} \quad \text{(H-32)}$$

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 V4, 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_{8D}, x_{4A}, and H_T.
14. Primary disturbance variable is x_{2D}.

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

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

Controlled Variables	Manipulated Variables
w_4	w_1
x_{4A}	w_2
x_{8D}	w_6
H_T	w_8

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:

$$\frac{dx_{R,A}}{dt} = \frac{1}{\rho V_R}[w_1 - (w_1 + w_2 + w_8)x_{R,A} - \rho V_R \alpha k x_{R,A} x_{R,B}] \tag{H-34}$$

$$\frac{dx_{R,B}}{dt} = \frac{1}{\rho V_R}[w_2(1 - x_{2D}) + w_8(1 - x_{T,D}) - (w_1 + w_2 + w_8)x_{R,B} - \rho V_R(1-\alpha)k x_{R,A} x_{R,B}] \tag{H-35}$$

$$\frac{dx_{R,D}}{dt} = \frac{1}{\rho V_R}[w_2 x_{2D} + w_8 x_{T,D} - (w_1 + w_2 + w_8)x_{R,D}] \tag{H-36}$$

$$\frac{dV_T}{dt} = \frac{1}{\rho}[(w_1 + w_2 + w_8)(x_{R,B} + x_{R,D}) - w_6 - w_8] \tag{H-37}$$

$$\frac{dx_{T,D}}{dt} = \left[\frac{(w_1 + w_2 + w_8)(x_{R,B} + x_{R,D}) - w_6}{\rho V_T}\right] \times \left[\frac{x_{R,D}}{x_{R,B} + x_{R,D}} - x_{T,D}\right] \tag{H-38}$$

$$w_4 = (w_1 + w_2 + w_8)(1 - x_{R,B} - x_{R,D}) \tag{H-39}$$

$$x_{4A} = \frac{x_{R,A}}{1 - x_{R,B} - x_{R,D}} \tag{H-40}$$

$$x_{8D} = x_{T,D} \tag{H-41}$$

$$H_T = \rho V_T \tag{H-42}$$

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

$$x_{R,A} = \frac{H_{R,A}}{H_R} \tag{H-43}$$

$$x_{R,B} = \frac{H_{R,B}}{H_R} \tag{H-44}$$

$$x_{R,C} = \frac{H_{R,C}}{H_R} \tag{H-45}$$

$$x_{R,D} = \frac{H_{R,D}}{H_R} \tag{H-46}$$

and, in the recycle tank, by

$$x_{T,B} = \frac{H_{T,B}}{H_T} \tag{H-47}$$

$$x_{T,D} = \frac{H_{T,D}}{H_T} \tag{H-48}$$

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

$$\frac{dH_{R,A}}{dt} = w_1 - (w_1 + w_2 + w_8)\frac{H_{R,A}}{H_R} - \frac{\alpha k}{H_R} H_{R,A} H_{R,B} \tag{H-49}$$

$$\frac{dH_{R,B}}{dt} = w_2(1 - x_{2D}) + w_8 \frac{H_{T,B}}{H_{T,B} + H_{T,D}} - (w_1 + w_2 + w_8)\frac{H_{R,B}}{H_R} - \frac{(1-\alpha)k}{H_R} H_{R,A} H_{R,B} \tag{H-50}$$

$$\frac{dH_{R,D}}{dt} = w_2 x_{2D} + w_8 \frac{H_{T,D}}{H_{T,B} + H_{T,D}} - (w_1 + w_2 + w_8)\frac{H_{R,D}}{H_R} \tag{H-51}$$

$$\frac{dH_{T,B}}{dt} = (w_1 + w_2 + w_8)\frac{H_{R,B}}{H_R} - w_6 \frac{H_{R,B}}{H_{R,B} + H_{R,D}} - w_8 \frac{H_{T,B}}{H_{T,B} + H_{T,D}} \tag{H-52}$$

$$\frac{dH_{T,D}}{dt} = (w_1 + w_2 + w_8)\frac{H_{R,D}}{H_R} - w_6 \frac{H_{R,D}}{H_{R,B} + H_{R,D}} - w_8 \frac{H_{T,D}}{H_{T,B} + H_{T,D}} \quad \text{(H-53)}$$

with the four outputs that remain to be controlled given by

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

$$x_{4A} = \frac{H_{R,A}}{H_R - H_{R,B} - H_{R,D}} \quad \text{(H-55)}$$

$$x_{8D} = \frac{H_{T,D}}{H_T} \quad \text{(H-56)}$$

$$H_T = H_{T,B} + H_{T,D} \quad \text{(H-57)}$$

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 H.3 Parameters of the Core Reactor/Flash Unit Model

Parameter	Value
H_R (kg)	3000
k (h^{-1})	330
α	0.5
ρ (kg/m^3)	1000

Table H.4 Initial Values of Inputs for the Core Reactor/Flash Unit Model

Parameter	Value
w_1 (kg/h)	1010
w_2 (kg/h)	1100
w_6 (kg/h)	110
w_8 (kg/h)	890
x_{2D}	0.01

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 H.5 Steady-State Values of the Core Reactor/Flash Unit Model

Variable	Steady-State Value
$H_{R,A}$ (kg)	20
$H_{R,B}$ (kg)	900
$H_{R,D}$ (kg)	100
$H_{T,B}$ (kg)	450
$H_{T,D}$ (kg)	50
w_4 (kg/h)	2000
x_{4A}	0.01
x_{8D}	0.10
H_T (kg)	500

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

Table H.6 Steady-State Flow Rates of Stream Variables.

	Stream Number, S							
Variable	1	2	3	4	5	6	7	8
w_{SA}	1010	0	20	20	0	0	0	0
w_{SB}	0	1089	900	0	900	99	801	801
w_{SC}	0	0	1980	1980	0	0	0	0
w_{SD}	0	11	100	0	100	11	89	89
w_S	1010	1100	3000	2000	1000	110	890	890

Table H.7 Controller Settings for Figure G-6.

Control Loop	CV − MV	Value of K_c	Dimensions of K_c
Composition Loop 7	$x_{4A} - w_8$	-1.6×10^6	kg/h
Level Loop 10	$H_T - w_6$	-5.0	h^{-1}
Flow Loop 11 Primary controller only	$w_4 - w_1$	2.5	dimensionless
Composition Loop 12 Modified to manipulate w_2 (V2) directly	$x_{8D} - w_2$	-6.3×10^3	kg/h

Table H.8 Controller Settings for Figure G-7.

Control Loop	CV − MV	Value of K_c	Dimensions of K_c
Composition Loop 7	$x_{4A} - w_8$	-1.6×10^6	kg/h
Level Loop 10	$H_T - w_6$	-5.0	h^{-1}
Flow Loop 11 Primary controller only	$w_4 - w_1$	2.5	dimensionless
Composition Loop 12 Manipulate $w_2 : w_1$ ratio	$x_{8D} - R$	-6.3	dimensionless

Notes:
1. All controller gains include measurement/transmitter and valve gains. The values were obtained by sequential trial-and-error tuning to obtain minimum-overshoot responses for step changes in set point.
2. All controllers are proportional-integral with τ_I = 1 h.
3. The initial value of R ($w_2 : w_1$ ratio) is 1.09.

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

Wu, K.-L., and C. C. Yu, Reactor/Separator with Recycle-1. Candidate Control Structure for Operability, *Computers Chem. Engng.*, **20**, 1291 (1996).