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CHAPTER 7

Switchable Control Structures and the Snowball Effect in a Reactor–Column Recycle Plant

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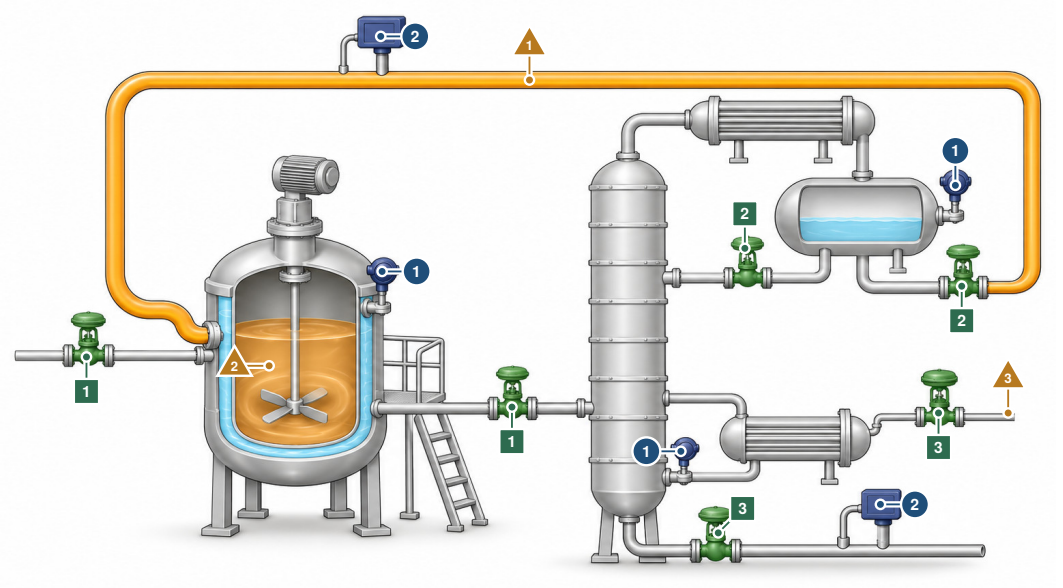
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CHAPTER 7

Switchable Control Structures and the Snowball Effect in a Reactor–Column Recycle Plant



The controller moves 1 fresh feed valve and reactor outlet valve 2 reflux valve and recycle valve under the drum 3 product valve and reboiler steam valve

The controller reads 1 levels of the reactor, the reflux drum and the column sump 2 purity analyzers on the recycle and on the product

What disturbs it 1 a production step, which the recycle multiplies 2 loss of catalyst activity 3 a limit on the reboiler steam

The fresh feed enters at the far left while the much wider recycle returns over the top, and at a fixed reactor holdup a production step swells that recycle and with it the vapor the column must boil. Illustration, not to scale.

IN PLAIN TERMS A Loop That Turns a Nudge Into a Shove

The main idea. A reactor turns a liquid into a product but leaves part of it unchanged. A tall column boils that leftover off and pipes it back to the reactor, so the same liquid goes round and round.

The challenge. Ask for a little more product and the returning stream grows far more: ten percent more feed swells it by more than half. The column must boil all of it, and it can only boil so fast.

Why it matters. Which flow the operators set, and where, decides whether the reactor, the returning stream or the column takes the strain.

THREE WAYS TO READ THIS CHAPTER

Explore	12 min	the first page, the fact on the windup in Section 7.1, the history at the end of Section 7.2, the try-its and the fact on a catalyst loss in Section 7.6, and the key points at the end of Section 7.9
Study	40 min	the whole chapter with its three pause points and the twelve exercises at its end
Practice	15 min	the first page, the results (Section 7.6), Technology in Practice (Section 7.7), Limitations (Section 7.8) and the open challenge

The control question A reactor that leaves part of its feed unconverted sends that reactant round a column and back, and a small production change can become a large load on the column. Which flow of the recycle loop should be held fixed, where should production be set, and what does each choice do to the recycle, the reactor and the column's vapor limit?

Learning objectives

- Derive the steady recycle of the reactor-column plant from two balances, and its elasticity and pole.
- Distinguish the five quantities called a snowball gain by their definitions and units.
- Explain why every structure that holds the holdup and both purities lands on one curve, so the structure chooses only the production handle.
- Compute the reactor holdup that moves production on CS2 and the recycle purity a fixed recycle would need on CS3.
- Show on the app why a purity loop cannot recover a column at its vapor limit, and pass the graded day by choosing structure and holdup.

Prerequisites Sections 1.4.1, 1.4.3 and 1.4.4 (the ideal-separator example, the throughput manipulator and the snowball), 1.6.2 (velocity-form PI) and 1.6.4 (scenarios and data).

The app https://apmonitor.com/apps/recycle-snowball/

See also Volume 13, Chapter 2 for a recycle with a converter inside it and inventory pairing, and Volume 13, Chapter 7 for a recycle that changes a loop's gain rather than its speed. Volume 13, Chapter 8 for a column whose spare handle moves only the energy, and Volume 13, Chapter 11 for setpoints moved by a steady-state optimizer.

7.1 Introduction

A reaction that stops short of completion leaves reactant that has to be separated from the product and sent back, and the flowsheet that results has a loop in it. In the generic plant simulated here, 200 kmol/h of fresh reactant A meets 500 kmol/h of recycled distillate in a stirred reactor holding 400 kmol, which converts 196 of the 675 kmol/h of A it receives, 29.0 % per pass. A column of twenty trays boils 1115 kmol/h, 67.6 % of its flooding rate, to return the unconverted A at 95 mol % and to send the product B out at 98 mol %. With the reactor holdup and both purities held, 10 % more fresh feed takes the recycle from 500 to 812 kmol/h in 12 h, on its way to a steady 817 kmol/h, and leaves the column 3.1 % of vapor margin.

Three beliefs about such a plant fail on the running simulator. The first is that a recycle stream grows in proportion to production. The steady recycle here grows 63.4 % for a 10 % step, because the reactor can convert more A in the same holdup only by running richer in A, and the column returns that richer effluent's A. The second is that fixing a flow inside the loop removes the problem. With the reactor effluent fixed and production moved by the holdup, the recycle falls 4.2 % while production rises 10.4 % by 6 h, but the holdup has to rise 14 % for each 10 % of production, and the same structure moved by its effluent lands back on the curve of the first. The third is that the snowball has one size. Five different quantities carry the name snowball gain on this one design point, in two units, and they read 4.61, 11.5, 11.55, 63.4 and 9.4 to 11.1, as Table 7.3 sets out.

The shape of the problem is general. A recycle is a feedback path inside the plant, so it moves the plant's poles and with them its speed and possibly its stability [1], and some recycle is a common feature of most plants [2]. Wherever a unit inside a recycle loop is pushed toward its capacity, the loop amplifies the push. An esterification plant whose extraction step limited it showed the same windup, with flooding of its extractor and columns when the throughput was set too high [3]. The ammonia synthesis loop of Volume 13, Chapter 2 circulates several times its makeup flow for the same reason, a low conversion per pass, and the gas recycle of Chapter 8 carries an inert that only a purge removes. A second decision is attached to every such loop. The point where production is set, the throughput manipulator, fixes how every inventory upstream and downstream of it has to be held [3–6], as Section 1.4.3 sets out, and whether that point lies inside or outside the recycle decides which flows move when production does.

✦ DID YOU KNOW? Half a Day Before the Windup Shows

On that esterification plant the recycle windup, which its authors liken to the snowball effect, took 12 to 24 hours to engage fully. A rate that was stable one day could wind up the next, so operators set production below the optimum [3].

The reactor, column and recycle plant of the plantwide control literature is usually met as steady-state curves and as simulation studies reported in papers [7, 8]. A reader of those seldom switches the plant's control structure during a run, measures the plant against the curve, or watches the column's vapor rate reach its limit. This chapter places that plant in a browser with the control structure as a switch, and measures on it what each structure does with one production change, a catalyst loss and a vapor limit. The balances, the analytical steady state, which is the one Larsson, Govatsmark, Skogestad and Yu derived [8], and the proportional-integral (PI) loops are established methods. The measurements on one generic design show three things. At a fixed holdup every structure that holds both purities settles on one curve, to 0.005 %, so a structure decides only which handle moves production. The holdup handle removes the snowball from the recycle and moves it into the reactor. Switching the recycle purity loop off raises the recycle's 12 h rise from 62.3 to 93.5 %. Behind the measurements are a sixty-nine-state model whose mole and A balances close to 1×10^{-11} of the throughput, a column module with a closed-form bubble point that other columns of the series reuse, and an analytical overlay computed apart from the dynamic model. Each of the nine cases carries a rule that credits its completion (Section 1.6.4).

Section 1.4.4 derived the snowball on a plant with an ideal separator. This chapter adds the column, its vapor limit and the line between them. Section 7.2 traces plantwide control of recycle plants from 1964. Section 7.3 builds the reactor, the line and the column, Section 7.4 derives the steady state and compares the three handles, and Section 7.5 describes the loops as coded. Section 7.6 measures the nine cases, Section 7.7 describes the real meters, valves and controllers, Section 7.8 states what the model leaves out, and Section 7.9 sums up.

7.2 Recycle, Inventory and the Throughput Handle Since 1964

The control of a whole plant, rather than of its units one by one, was first discussed at length by Page Buckley in a chapter on overall process control in his 1964 book [4]. A later review finds there the material balance control that runs in the direction of flow or against it, production rate control, surge tanks as low-pass filters, and the observation that inventory and flow cannot be set independently at one point of a plant, because the material balance ties them [2]. The same review credits Buckley with the point that where the production rate is set determines the structure of the inventory loops, and it judges that industrial practice had not moved far from his chapter in the thirty-five years that followed. In the same year Gilliland, Gould and Boyle used a plant with a reaction, a separation and a recycle to show how the positive feedback of the recycle changes the dynamics and the steady state [9], as Larsson and coauthors summarize that study [8].

The name came three decades later. In a 1993 series on recycle systems, Luyben took up the high sensitivity of the recycle flow to the fresh feed and named it the snowball effect [8, 10], then gave the reactor and separator case a paper of its own [7]. His remedy was to let the reactor holdup vary and, as a generic rule, to put one flow somewhere in the recycle loop on flow control [8]. The rule became part of the nine-step plantwide procedure of Luyben, Tyreus and Luyben, which was applied to a vinyl acetate process, the Eastman plantwide control process and a hydrodealkylation plant [2, 11]. Price and Georgakis built a tiered procedure on Buckley's ideas and, after 318 simulations of a reactor, separator and recycle, advised that an internal flow be preferred as the throughput manipulator and that the inventory loops be consistent with it [2, 5].

The rule was soon tested on the same plant. Wu and Yu proposed balanced structures that hold the reactor composition and found that Luyben's structure moves the snowball from the recycle into the reactor holdup, while a fixed flow at a constant holdup could take only small throughput

changes [8, 12]. Larsson and Skogestad's review then argued that the snowball occurs because the reactor is too small for the feed, which makes it a steady-state design problem [2]. Skogestad framed the choice of what to control as self-optimizing control, a search for controlled variables that keep the economic loss acceptable at constant setpoints [13]. Applied to this plant, the argument places a liquid reactor at its largest holdup, an active constraint, where the conventional structure gives less recycle than Luyben's structure at every feed rate [8]. Skogestad's procedure for complete plants then sets the production rate at the bottleneck, which for this plant is the reactor holdup at steady state and the column's vapor capacity dynamically [14]. Aske and Skogestad stated the requirement on the inventory loops as local consistency [6].

Industry had moved the handle before these procedures were published, as the history segment at the end of this section tells, and one justification offered for Luyben's rule is that a fixed flow in the loop avoids the recycle's slow dynamics [1, 3]. The column that sits in the loop is modeled here the way the distillation tutorial literature models it, with constant relative volatility, constant molar flows and linearized liquid dynamics on the trays [15], while a real column's flooding limit comes from tray evaluation procedures built on Fair's flooding and entrainment data of 1961, which were refitted as algebraic correlations as recently as 2025 [16].

> ⧖ HISTORY **Late 1970s: Production Set Away From the Feed**
>
> In the late 1970s and early 1980s one chemical company moved the throughput manipulator of numerous plants away from the process feeds. On an esterification plant whose units had been designed with the throughput set at the feed, the handle went first to the distillate of the first column and later to the feed of the extraction step, once that step had become the bottleneck. Early adoption was hard for three reasons: a mindset that the process feeds must stay constant, the operators' grasp of an inventory-to-feed strategy, and pneumatic hardware that made the control decision difficult to reverse. Setting the handle somewhere other than the feed is now common there, driven by variability propagation and ease of operation [3].

7.3 The Reactor, the Column and the Line as Modeled

The plant has three units, as shown in Figure 7.1. Pure A enters a stirred tank, where it reacts to B. The tank's effluent feeds tray 9 of a twenty-tray column, whose condensed overhead collects in a reflux drum. The drum's liquid is split between the reflux and the distillate, and the distillate returns to the reactor through a pipe as the recycle. A partial reboiler with its sump boils the column's bottom liquid and releases the bottoms as the product. Every size, rate constant and limit is a generic teaching value chosen for a consistent design point, not a measurement on any plant, and exports carry the label synthetic educational model.

Table 7.1 lists the variables by role. The clock is in minutes and the flows in kmol/h, so every balance below carries the factor $1/60$ in the code, which the equations omit. Sixty-nine states are integrated, four in the reactor (holdup, composition, temperature and coolant temperature), ten in the recycle line, two on each of the column's twenty-two stages (drum, trays and sump), six flow states and five ledgers that count the moles and the A entering, leaving and reacting.

7.3.1 Reactor Holdup and Composition

The irreversible reaction $A \rightarrow B$ conserves moles, so the reactor holdup changes only with the flows, and its A changes with the flows and the reaction, as shown in Equation (7.1).

$$\begin{aligned} \frac{\mathrm{d}M_R}{\mathrm{d}t} &= F_0 + D - F, \qquad M_R = \rho\, V_{vessel}\, \frac{L_R}{100} \\ \frac{\mathrm{d}(M_R z)}{\mathrm{d}t} &= F_0 z_0 + D x_{rec} - F z - k M_R z \end{aligned} \tag{7.1}$$

where z is the mole fraction of A in the reactor, z_0 in the fresh feed and x_{rec} in the recycle as it reaches the reactor, $\rho = 4\,\mathrm{kmol/m^3}$ is the molar density and V_{vessel} the vessel volume. The design

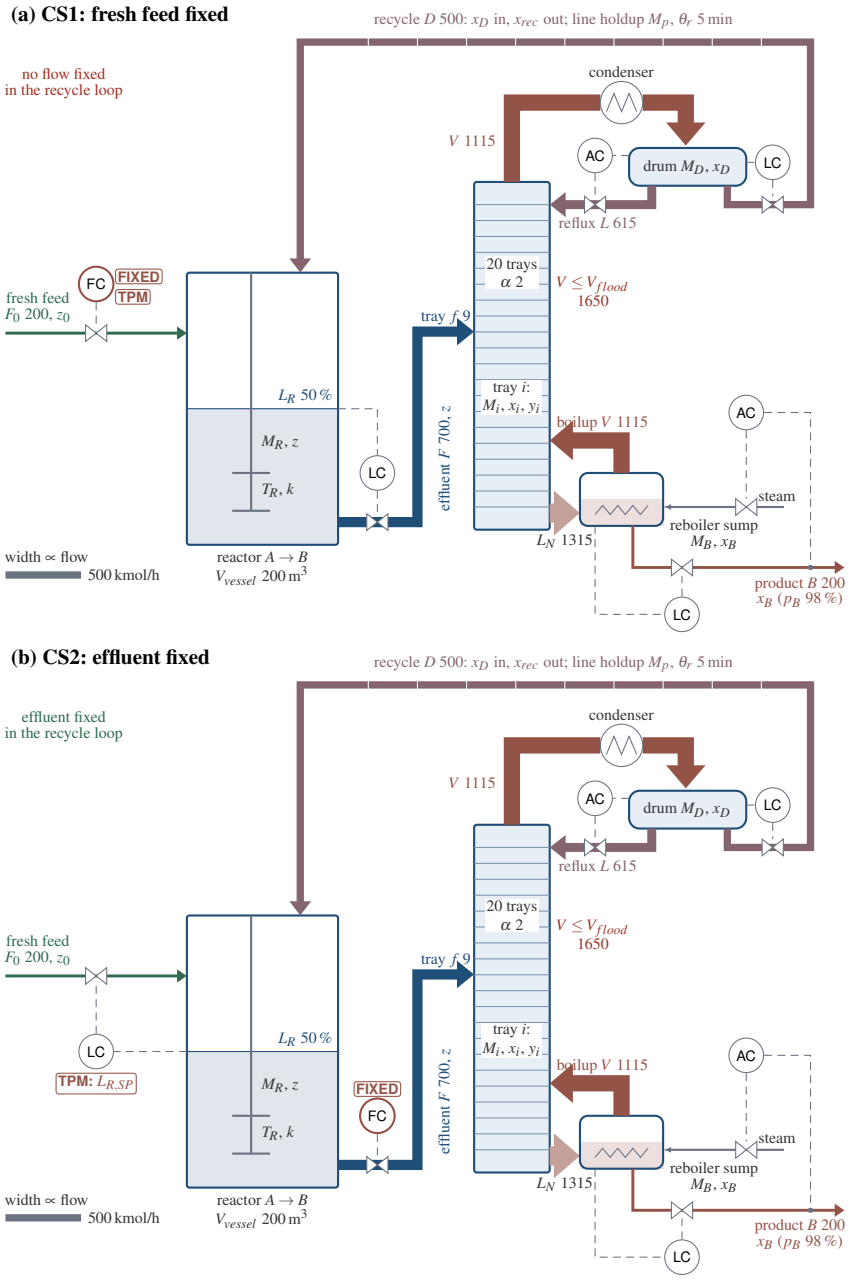


Figure 7.1 The plant at its design point, drawn like the application's Plant view. Every stream's line width is proportional to its flow on one scale (500 kmol/h in the key), flows are in kmol/h, and each valve carries the controller that moves it. (a) In CS1, the conventional structure, the fresh feed F_0 is on flow control and is the throughput manipulator (TPM), and the reactor level controller moves the effluent F. (b) In CS2 the effluent is fixed, the reactor level controller moves the fresh feed, and production is set by the reactor level setpoint. In both, the drum level moves the recycle D, the recycle purity x_D moves the reflux L, the product purity p_B moves the reboiler's steam and so the boilup V, and the sump level moves the product B. CS3 is described in Table 7.4. Not to scale.

Table 7.1 Plant Variables, Their Roles and Design Values

Symbol	Role	Design	Range
L_R	CV, reactor level (%)	50	SP 10–90
x_D	CV, recycle purity (mol % A)	95.00	SP 85–99.5
p_B	CV, product purity (mol % B)	98.00	SP 90–99.9
L_D, L_B	CV, drum and sump levels (%)	50, 50	SP 20–80
F_0	MV, fresh feed (kmol/h)	200	0–400
F	MV, reactor effluent (kmol/h)	700.19	0–2400
D	MV, recycle (distillate, kmol/h)	500.19	0–2000
L	MV, reflux (kmol/h)	614.76	0–3000
V	MV, boilup (kmol/h)	1114.95	0–V_{cap}
B	MV, product (bottoms, kmol/h)	200	0–500
a	DV, catalyst activity (%)	100	50–120
z_0	DV, A in the fresh feed (mol %)	100	80–100
V_{steam}	DV, boilup the steam allows (kmol/h)	2000	800–2000
M_R, z	states, reactor holdup (kmol), A (mol %)	400, 68.44	—
T_R, T_c	states, reactor, coolant (°C)	70, 59.6[a]	—
x_j	states, A in the line's cells (mol %)	95.00	$j = 1 \ldots 10$
M_i, x_i	states, stage holdup (kmol), A	4, profile	$i = 1 \ldots 20$
M_D, M_B	states, drum, sump (kmol)	50, 60	cap 100, 120

[a]The coolant matters only with the jacket option.

holds 100 m^3 of liquid in a 200 m^3 vessel, so one percent of level is 8 kmol and the holdup can rise as a handle. The residence time at design is $M_R/F = 34.3$ min and the reaction's own time constant $1/k$ is 83.8 min.

7.3.2 Kinetics and the Optional Jacket

The rate constant follows the Arrhenius law about the design temperature, scaled by the catalyst activity, as shown in Equation (7.2).

$$
\begin{aligned}
k &= k_0\, a \exp\Big[-\frac{E_a}{R}\Big(\frac{1}{T_R}-\frac{1}{T_0}\Big)\Big] \\
\tau_T \frac{\mathrm{d}T_R}{\mathrm{d}t} &= T_{R,SP} - T_R \qquad \text{(isothermal default)} \\
M_R c_p \frac{\mathrm{d}T_R}{\mathrm{d}t} &= (-\Delta H_r)\, k M_R z + c_p (F_0 + D)(T_f - T_R) \\
&\quad - UA\,(T_R - T_c), \qquad \tau_J \frac{\mathrm{d}T_c}{\mathrm{d}t} = T_{c,SP} - T_c
\end{aligned}
\tag{7.2}
$$

where R is the gas constant, temperatures in the exponent are absolute, a is the catalyst activity, $k_0 = 0.716\,\mathrm{h}^{-1}$ at $T_0 = 70\,^\circ$C and $E_a = 60$ kJ/mol, so near the design one kelvin raises k by 6.3 %. In the energy balance the flows are taken per second and c_p is per mole. By default an ideal temperature loop holds the reactor with $\tau_T = 5$ min. The jacket option replaces it with the energy balance, in which the reaction releases 2.18 MW at design, the feeds enter at $T_f = 50\,^\circ$C and a temperature controller sets $T_{c,SP}$, which the coolant temperature T_c follows with $\tau_J = 3$ min. The coolant sits at 59.6 °C at the design steady state.

7.3.3 A Line That Carries Composition Late and Flow at Once

The recycle line is ten well-mixed cells of fixed holdup, as shown in Equation (7.3).

$$
\begin{aligned}
\frac{M_p}{N_p}\frac{\mathrm{d}x_j}{\mathrm{d}t} &= D\,(x_{j-1} - x_j), \qquad j = 1 \ldots N_p \\
x_0 &= x_D, \qquad x_{rec} = x_{N_p}
\end{aligned}
\tag{7.3}
$$

where $N_p = 10$ and $M_p = \theta_r D_{ref}/60$, so the line holds 41.7 kmol, the content of a $\theta_r = 5$ min transit at $D_{ref} = 500$ kmol/h. Because the holdup is fixed, the line runs full of liquid and delivers the recycle

at the rate it leaves the drum at every instant. Only the composition arrives late. The minimum θ_r is 1 min, which keeps the explicit 2 s step on these cells stable up to the 2000 kmol/h valve limit (a step size times eigenvalue of 1.33 against the 2.79 that the fourth-order Runge-Kutta method tolerates on the real axis).

7.3.4 Twenty Trays, a Drum and a Reboiler Sump

The column follows the binary model of the distillation tutorial literature [15], with constant molar overflow, constant relative volatility and a linearized weir on each tray, as shown in Equation (7.4).

$$\begin{aligned} \frac{\mathrm{d}M_i}{\mathrm{d}t} &= L_{i-1} + F\,\delta_{if} - L_i, \qquad L_i = \bar{L}_i + \frac{M_i - \bar{M}}{\tau_L} \\ \frac{\mathrm{d}(M_i x_i)}{\mathrm{d}t} &= L_{i-1}x_{i-1} + V y_{i+1} + F z\,\delta_{if} - L_i x_i - V y_i \\ y_i &= \frac{\alpha x_i}{1 + (\alpha - 1)x_i} \\ T_i &= \Lambda \Big/ \ln\Big(\frac{P_0}{P}\sum_j x_{ij}\,\mathrm{e}^{\Lambda/T_{b,j}}\Big) \end{aligned} \tag{7.4}$$

where trays are numbered $i = 1 \ldots 20$ from the top, the feed enters as saturated liquid on $f = 9$, δ_{if} is one on the feed tray, the vapor V is the same on every tray, $L_0 = L$ and $x_0 = x_D$, and $y_{21} = y_B$ is the vapor leaving the sump, x_{ij} is the fraction of component j on tray i, $T_{b,j}$ its normal boiling point, and $P = P_0 = 1.01325$ bar. The weir's reference flows $\bar{L}_i$ are those of a 615 kmol/h reflux and a 700 kmol/h feed, $\bar{M} = 4$ kmol and $\tau_L = 6$ s, and $\alpha = 2$. Temperatures come from one common latent heat, $\Lambda = 3600$ K in units of the gas constant, which makes α exactly constant and the bubble point closed form, with normal boiling points of 80.0 and 105.75 °C for A and B. A total condenser feeds the drum, and the partial reboiler is an equilibrium stage with its sump, as shown in Equation (7.5).

$$\begin{aligned} \frac{\mathrm{d}M_D}{\mathrm{d}t} &= V - L - D, \qquad M_D\frac{\mathrm{d}x_D}{\mathrm{d}t} = V\,(y_1 - x_D) \\ \frac{\mathrm{d}M_B}{\mathrm{d}t} &= L_{20} - V - B \\ \frac{\mathrm{d}(M_B x_B)}{\mathrm{d}t} &= L_{20}x_{20} - V y_B - B x_B \end{aligned} \tag{7.5}$$

where x_B is the A in the sump and the product, $p_B = 100(1 - x_B)$ is the product purity in mol % B, and y_B is in equilibrium with x_B. At design the drum boils at 80.9 °C and the sump at 105.0 °C.

7.3.5 Flows, Pumps and Instruments

Each manipulated flow follows its setpoint q_{SP} through a first-order loop, $\tau_Q\,\mathrm{d}q/\mathrm{d}t = q_{SP} - q$ with $\tau_Q = 0.2$ min, and the boilup through the reboiler with $\tau_V = 1$ min. A pump loses suction as its vessel empties, so the delivered flow is the flow times $\mathrm{clip}(M/(0.02M_{cap}), 0, 1)$ of the vessel it draws from. Level transmitters lag 0.1 min with noise of 0.05 % of span (0.1 % on the drum and sump), flow meters lag 0.05 min with 0.3 kmol/h of noise, and the reactor thermowell lags 0.5 min. The two purity analyzers are continuous by default, a 1 min sample line with 0.02 mol % of noise, and the Advanced options replace them with a chromatograph that draws a sample every 2, 5 or 10 min through the same 1 min sample line and reports it one cycle later. A measurement packet carries only these readings to the controllers, and a packet holding anything beyond them fails the application's own test suite. The logged flow columns are the delivered flows rather than the meter readings.

7.3.6 Parameters, Starting State and Integration

Table 7.2 gives every parameter. A case begins at the steady state of its own settings. The analytical steady state of Section 7.4 supplies the reactor and the flows, a damped Newton solution of the

Table 7.2 Parameters (A Adjustable in the Parameters Panel, H Hidden From It, S Written Into the Source)

Symbol	Meaning	Value	Unit		Symbol	Meaning	Value	Unit	
V_{vessel}	reactor vessel volume	200	m^3	A	α	relative volatility, A to B	2	—	A
ρ	liquid molar density	4	$kmol/m^3$	H	$T_{b,B}$	normal boiling point of B	105.75	°C	H
k_0	rate constant at T_0	0.716	h^{-1}	A	Λ	latent heat over R	3600	K	H
T_0	design reactor temperature	70	°C	H	N	theoretical trays	20	—	S
E_a	activation energy	60	kJ/mol	A	f	feed tray, from the top	9	—	H
ΔH_r	heat of reaction (jacket)	−40	kJ/mol	A	$\bar{M}$	tray holdup at the reference	4	kmol	A
c_p	liquid heat capacity	0.16	kJ/(mol K)	H	τ_L	tray hydraulic lag	0.1	min	A
UA	jacket conductance	150	kW/K	A	$\bar{L}, \bar{F}$	weir reference reflux, feed	615, 700	kmol/h	S
T_f	feed temperature (jacket)	50	°C	H	$M_{D,cap}$	drum capacity	100	kmol	A
τ_J	coolant response	3	min	H	$M_{B,cap}$	sump capacity	120	kmol	A
τ_T	isothermal temperature loop	5	min	S	V_{flood}	boilup at flooding	1650	kmol/h	A
$L_{R,max}$	reactor high-level alarm	90	%	A	θ_r	line transit at D_{ref}	5	min	A
τ_Q	flow loop response	0.2	min	H	D_{ref}, N_p	line reference recycle, cells	500, 10	kmol/h, —	S
τ_V	reboiler response	1.0	min	H	P	column pressure	1.01325	bar	S

column at those flows supplies every stage's composition, and a bisection on the reflux makes the distillate meet its purity. The largest derivative at $t = 0$ is 4.9×10^{-9} in the state's units per minute. Settings with no steady state start from the design. Integration uses a fixed 2 s step of the classical fourth-order Runge-Kutta scheme, control executes every 6 s, and the historian writes one row per 5 min, on the engine of Section 1.6.1. Halving the step moves the recycle, the boilup, both purities and the reactor's A in case 1 at 6 h by 3.5×10^{-11} relative. Over a disturbed test run with structure switches, an activity loss, a feed composition change, a chromatograph and the steam limit, the moles and the A held plus the ledgers close to 1.0×10^{-11} of the throughput.

7.3.7 Assumptions

One irreversible first-order reaction at constant molar density stands for the chemistry, and a reversible or second-order reaction would move the steady curve without changing its shape. The column is binary with constant relative volatility and constant molar overflow, which is the same assumption as one latent heat, and the pressure, the condenser and the reboiler's heat transfer are ideal. Flooding is a fixed ceiling on the boilup rather than a hydraulic model, so the model has no flooded state. At the ceiling the trays keep their full separation and their weir holdups, and what the plant loses is the vapor the product loop asks for. A real column loses efficiency gradually as it approaches flooding, and its limit moves with the liquid load. The recycle line's ten cells add some mixing to the delay, where a real line is closer to plug flow. The flow loops are fast first-order lags whose own tuning is outside the lesson, and the reactor temperature is held ideally unless the jacket is chosen.

7.4 One Steady State and Three Handles

7.4.1 The Curve From Two Balances

With the holdup M_R and both purities held, the steady state follows from the balances alone. Overall, $F_0 = B$, because the reaction conserves moles. The A in the fresh feed either reacts or leaves in the product, and the column's feed leaves as recycle or product, as shown in Equation (7.6).

$$z^* = \frac{F_0(z_0 - x_B)}{kM_R}, \qquad D^* = F_0 \frac{z^* - x_B}{x_D - z^*}$$
$$F_0^{pole} = \frac{kM_R x_D}{z_0 - x_B} \tag{7.6}$$

These are equations 1 to 3 of Larsson, Govatsmark, Skogestad and Yu [8], which give z^*, the column feed $F = F_0 + D^*$ with z^* eliminated, and the holdup below which no steady state exists, here rearranged as the fresh feed at which z^* would reach x_D. With an ideal separator, $x_D = 1$ and $x_B = 0$ with $z_0 = 1$, the recycle reduces to Equation (1.3) and the pole to $F_0 = kM_R$. Their own design,

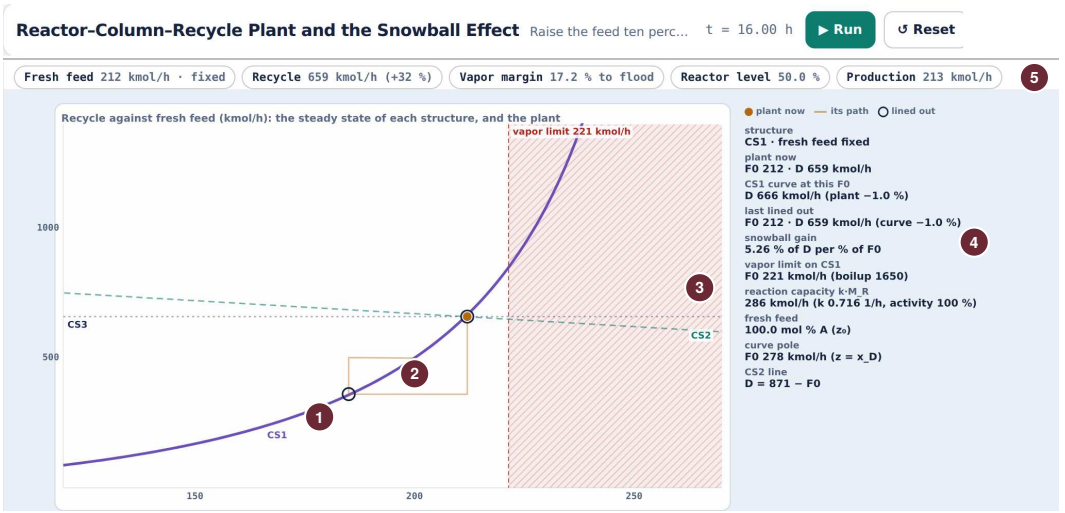


Figure 7.2 The snowball curve of case 2 at $t = 16$ h on the Snowball view, CS1, a composite of the application's header above its Snowball view, with the control panel and the trends cut. The CS1 curve (1), CS2's line $D = 871 - F_0$ and CS3's flat line are drawn with the region beyond the vapor limit at 221 kmol/h hatched (3). The plant's path (2) runs from the design down to 185 kmol/h and up to 212 kmol/h (Table 7.5), with a ring where the fresh feed and the recycle held within 1 % for an hour. The run places the rings at 360.8 kmol/h at 185, 0.84 % above the curve, and 659.3 at 212, 1.00 % under it and still climbing. The panel (4) reads the curve's 666, the gain 5.26 % per percent, the reaction capacity kM_R of 286 kmol/h and the pole at 278 kmol/h. The badges (5) read a recycle 32 % above its start, a vapor margin of 17.2 % to flooding and 213 kmol/h of production.

Table 7.3 Five Quantities Called a Snowball Gain on One Plant

Definition	Value	Where it appears
local elasticity $\mathrm{d}\ln D^*/\mathrm{d}\ln F_0$ on the CS1 curve, % per %	4.61 at design, 4.03 and 5.26 at 185 and 212, 2.63 with the vessel doubled	scorecard tile, Snowball view, cases 2 and 6
local slope $\mathrm{d}D^*/\mathrm{d}F_0$, kmol/h per kmol/h	11.5 at design	Model dialog
secant after ±2 % production steps lined out 32 h, kmol/h per kmol/h	CS1 11.55, CS2 by the holdup −1.00 (−0.40 % per %)	Instructions, application tests
finite step, steady $\Delta D/D$ for +10 % of F_0	+63.4 % (6.3 % per %)	case 1, Model dialog
secants between points not yet lined out, kmol/h per kmol/h	9.4 down, 11.1 up (curve: 9.5, 11.4)	case 2

460 kmol/h of feed at 0.9 mole fraction A, $x_B = 0.0105$, $k = 0.341\,\mathrm{h}^{-1}$ and 2800 kmol, gives their $z^* = 0.43$ (0.4285). At the app's design, $kM_R = 286.4\,\mathrm{kmol/h}$, $z^* = 68.44\,mol\,\%$, $D^* = 500.19\,\mathrm{kmol/h}$, so $D/F_0 = 2.50$, and the pole is at 277.6 kmol/h. The dynamic model is not built from Equation (7.6). Stepped from the design and run 32 h, its recycle lands within 0.005 % of D^* at seven fresh feeds from 185 to 220 kmol/h, as shown in Figure 7.3a. The application draws the curve on its Snowball view with the plant's path over it, as shown in Figure 7.2.

🕮 **Pause.** Try Exercise 7.1 before reading on.

7.4.2 Five Quantities Called a Snowball Gain

Differentiating Equation (7.6) at a fixed holdup, where $\mathrm{d}\ln z^*/\mathrm{d}\ln F_0 = 1$, gives the elasticities of Equation (7.7).

$$\begin{aligned}\frac{\mathrm{d}\ln D^*}{\mathrm{d}\ln F_0} &= 1 + \frac{z}{z - x_B} + \frac{z}{x_D - z} \\ \frac{\mathrm{d}\ln D^*}{\mathrm{d}\ln k} &= -\left(\frac{z}{z - x_B} + \frac{z}{x_D - z}\right)\end{aligned} \tag{7.7}$$

At design the first is 4.61 and the second −3.61. With the ideal separator of Section 1.4.1 the first is the elasticity of Equation (1.3). The application and its texts quote five different numbers under the name snowball gain, and Table 7.3 names each by its definition. The local elasticity is a percent per percent, and the local slope $\mathrm{d}D^*/\mathrm{d}F_0 = 11.5$ is the same tangent in kmol/h per kmol/h, larger by D/F_0. A finite step reads more than either, because the curve steepens on the way, and 10 % of fresh feed is 63.4 % of recycle at steady state. The secant over ±2 % steps lined out, 11.55, sits just above the tangent because the curve is convex. The recycle purity enters through the same denominator, and each mol % of x_D lost at design costs 18.8 kmol/h of recycle at steady state.

🕮 **Pause.** Try Exercise 7.2 before reading on.

7.4.3 The Other Two Structures

A structure that holds the holdup and both purities lands on Equation (7.6) whatever flow it fixes, so the structures differ in which handle moves production. Fixing the effluent (CS2) or the recycle and the effluent (CS3) gives the relations of Equation (7.8).

$$\begin{aligned}&\text{CS2:} \quad D = F - F_0, \qquad F_0 = F\,\frac{x_D - z}{x_D - x_B} \\ &\text{CS3:} \quad F_0 = F - D, \qquad x_D = \frac{F z - F_0 x_B}{D}\end{aligned} \tag{7.8}$$

On CS2 the recycle is the fixed effluent less the product, so production moved by the holdup moves the recycle the other way, −1 kmol/h per kmol/h, or −0.40 percent per percent at design. Lined out, five holdups from 46.6 to 57.2 % of level put the plant on that line to 0.018 kmol/h. The effluent at a fixed holdup is a different handle. Three effluents of 670, 730 and 760 kmol/h settle the plant at fresh feeds of 197.5, 202.3 and 204.5 kmol/h with recycles within 0.016 kmol/h of the steady state the balances predict, and those steady states lie on the CS1 curve, as Figure 7.3a shows. This measurement is why CS2's production handle in the app is the reactor level setpoint rather than the effluent. On CS3 production is the difference of two flow setpoints, and the recycle purity floats to whatever closes the column's balance, which on a lined-out run at 704 kmol/h of effluent it does to 3×10^{-4} mol %.

7.4.4 Where the Column Stops the Snowball

The boilup the column needs grows with the recycle. From the column's own steady state at both purities, the CS1 steady states at 216, 220, 221.4, 223, 226 and 230 kmol/h of fresh feed need 1485, 1604, 1649, 1703, 1812 and 1974 kmol/h of boilup, so the largest fresh feed the column can boil under its 1650 kmol/h flooding rate is 221.4 kmol/h, 10.7 % above the design. The boilup controller never asks for more than $V_{cap} = \min(V_{flood}, V_{steam})$, which is where the model holds the boilup when the snowball reaches the wall. The design sits at 67.6 % of flooding on purpose. At a design of 80 % the wall would come at 6.3 % more fresh feed, and the 10 % step of case 1 could not show the snowball's size before reaching it. Beyond the wall the product loop has no vapor left, A breaks into the product, and that A no longer returns, which is the end Larsson and coauthors describe for a real snowball [8].

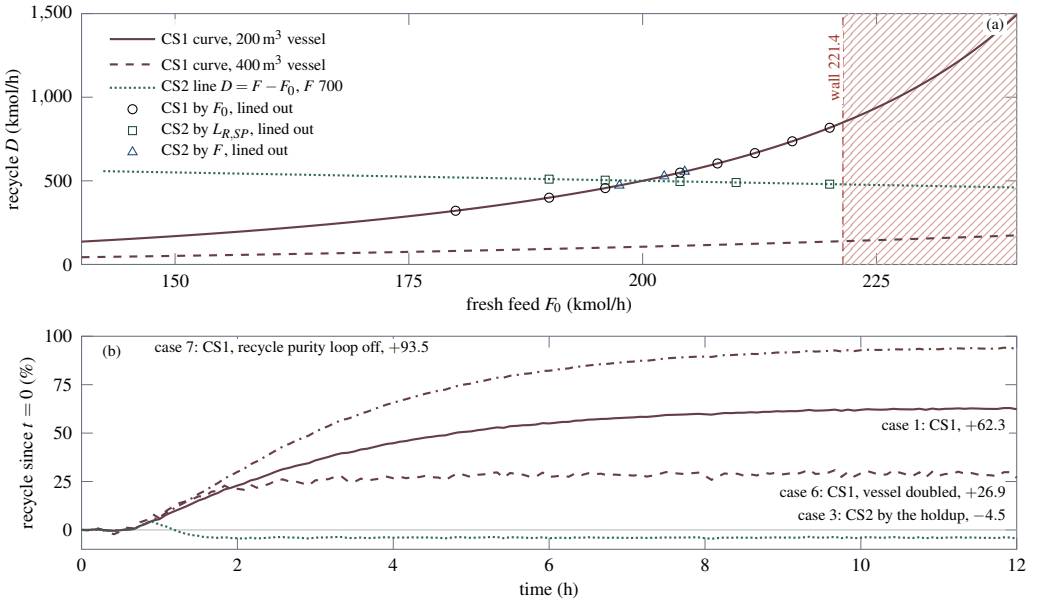


Figure 7.3 The steady state and the path to it. (a) Recycle against fresh feed from Equation (7.6) at the design holdup (solid) and with the vessel doubled (dashed), CS2's line (dotted), the vapor wall at 221.4 kmol/h (thin dashed, hatched beyond), and the plant lined out 32 h after steps from the design under three handles (circles, squares and triangles). (b) The recycle since $t = 0$ for the same production increase in cases 1 (solid), 3 (dotted), 6 (dashed) and 7 (dash-dotted) as shipped, with the values at 12 h.

Table 7.4 What Each Structure Fixes and Pairs

Loop	CS1	CS2	CS3
flow control	F_0	F	F and D
reactor level →	F	F_0	F_0
drum level →	D	D	L
recycle purity x_D →	L	L	floats
product purity p_B →	V	V	V
sump level →	B	B	B
production handle (TPM)	$F_{0,SP}$	$L_{R,SP}$	F_{SP}

7.5 The Loops as Coded

7.5.1 Pairings by Structure

The three structures are listed in Table 7.4. CS1 is the conventional structure, with nothing fixed inside the recycle loop. CS2 fixes the effluent and moves production by the reactor holdup, which is the structure the literature calls Luyben's [8]. CS3 fixes the recycle itself, which leaves no flow to hold the drum except the reflux, and so lets the recycle purity float. Each structure has its own production setpoint, marked TPM on the Plant view, rather than one setpoint routed to a different valve. The structure can change during a run. One PI controller exists per manipulated flow, the reactor level having one on F and one on F_0 and the drum level one on D and one on L, and every controller that is not driving its flow tracks it at every execution, so a switch is bumpless. A test makes each of the six possible switches at 60 min and finds no flow moving more than 1 % of its design value over the next control period. Manual mode holds the five level and purity controllers at their stations, while the structure's flow setpoints stay in force.

7.5.2 The Shared PI Law

Every loop uses the velocity-form PID of Section 1.6.2, Equations (1.11) to (1.14), without derivative action, with the clamp on the emitted output only and back-calculation whose tracking time equals τ_I. Its bias u_b is the flow when the controller starts, and the control period is $\Delta t = 0.1$ min. The action is $a = -1$ for a level held by an outflow (the reflux included) and $a = +1$ for the reactor level held by the fresh feed and for both purities. Integral action is dropped when the integral time is set to 600 min or longer. The reactor level moves 50 kmol/h per percent with $\tau_I = 30$ min, the drum and sump levels 30 kmol/h per percent with 30 min, both purity loops 40 kmol/h per mol % with 15 min, and the jacket's temperature loop 2 K of coolant per kelvin with 20 min. The level controllers see their transmitter through a 0.5 min first-order filter, which cuts the production jitter the level noise causes. The boilup's upper limit is V_{cap}, and the valve ranges of Table 7.2 limit the rest.

7.5.3 Why the Default Analyzer Is Continuous

A sampled analyzer is the realistic instrument for a purity, and the Advanced options offer one. With a 5 min cycle at the default purity tuning, case 1's product swings between 65.6 and 100 mol % B after 4 h, and the boilup sits at the flooding rate for 279 min from 2.08 h, so the snowball cases would spend hours off specification for a reason unrelated to the structure. Both purity loops at 20 kmol/h per mol % and 30 min hold the product between 96.3 and 97.8 mol % on the same chromatograph without reaching the flooding rate. The continuous analyzers are therefore the default, and the chromatograph stays an Advanced option. Volume 5, Chapter 3 measures what an analyzer's lag costs a single composition loop on a binary column.

7.5.4 The Line Delay and the Reactor Level

On CS1 the reactor level loop acts through the recycle, because more effluent is more column feed and the product purity loop boils most of it back up. With the level loop out of the way, nine tenths of a 20 kmol/h effluent step return as recycle within 11.9 min, at once in flow because the line runs full. The line's composition delay therefore barely touches the level loop. Case 1's largest reactor level error is 0.850, 0.853 and 0.870 % with a 1, 5 and 30 min line. At three faster tunings, up to 200 kmol/h per percent with 5 min, the largest error moves by less than 0.003 points between a 1 and a 30 min line, and at all four tunings the level's standard deviation from 8 to 12 h stays between 0.007 and 0.022 points.

7.5.5 Status Flags and the Three Models

FLOODING marks the boilup controller at the flooding rate and STEAM LIMIT at a lower steam supply. OFF SPEC marks the true product more than 0.5 mol % under its setpoint, and LEVEL HIGH the reactor above its 90 % alarm. These are annunciators, not trips, and the flooding rate, the alarm and the 98 mol % specification are teaching values, while real ones come from a tray rating [16], the vessel's design and the product's sales specification. The application keeps three models apart. The plant is Section 7.3. The analytical model of Section 7.4 is an overlay computed from the true activity and temperature, drawn on the Snowball view and logged, and no controller reads it. The controllers carry no model at all.

7.6 Nine Cases on the Running Plant

The nine cases are listed in Table 7.5. The numbers below come from the engine of Section 1.6.1 run without a browser at the default seed, each case loaded as the application loads it and each move made at the instant the text names. Cases 4, 6, 7 and 8 compare two runs, the second started by Reset after the change, because a structure, vessel or setpoint chosen before a run acts from $t = 0$ as a starting condition. The scorecard the application shows for each case at its reading instant is collected in Table 7.6, and Figure 7.4 draws its recycle and vapor margin columns. Every case loads identically on first selection, from the list after another case, and after Reset.

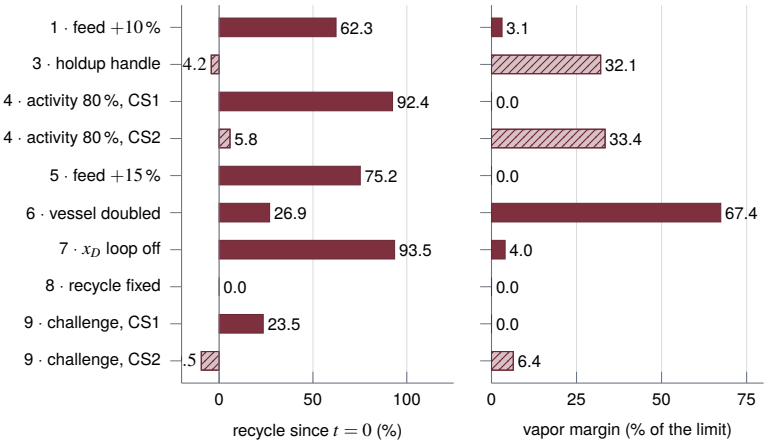


Figure 7.4 The scorecard of Table 7.6 for ten of its rows, at each row's reading instant: dark bars run on CS1, hatched bars on CS2 and the white bar on CS3. The margins of case 9 are to the steam limit, the others to flooding. Notice that the dark bars of cases 1, 4, 5, 7 and 9 end at or near a vapor margin of zero, while on the hatched bars the recycle barely moves.

Table 7.5 The Nine Cases

#	Structure and events	Teaching point
1	CS1, fresh feed 200 to 220 kmol/h at 30 min, 12 h	the snowball
2	CS1, fresh feed to 185 at 0.5 h, to 212 at 7.5 h, 16 h	the curve against the plant
3	CS2, level 50 to 57.2 % at 30 min	the holdup as the handle
4	CS1, activity to 80 % at 30 min, then CS2	who absorbs a kinetic loss
5	CS1, fresh feed +15 % at 30 min	the vapor wall, infeasible
6	CS1, 400 m^3 vessel, +10 %	holdup against recycle
7	CS1, recycle purity loop off, +10 %	the column's loops are plantwide
8	CS3, effluent 700 to 720 kmol/h over 0.5–2.5 h	what a fixed recycle costs
9	Challenge: steam 1200, target 240 at 15 min, activity 90 at 3 h, 8 h	the structure and the holdup

7.6.1 The Snowball and the Curve

Case 1 raises the fresh feed by 10 % at 30 min on CS1. The reactor's A climbs from 68.4 to 75.2 mol % by 12 h, the recycle from 500 to 812 kmol/h, still short of the curve's 817, and the boilup from 1115 to 1599 kmol/h, which takes the vapor margin from 32.4 to 3.1 % of the flooding rate, as shown in Figure 7.3b. The product loop falls behind the climb at first. The product is under 97.5 mol % B from 0.95 h, reaches 97.17 mol % at 1.8 h, and OFF SPEC clears at 4.7 h. At the new steady state the margin would be 2.8 %.

> **TRY IT IN THE APP** **1 · Fresh Feed +10 % on the Conventional Structure**
>
> Load the scenario, press Run and watch the Recycle since $t = 0$ tile after the fresh feed steps up by a tenth at 30 min. By 12 h the recycle has risen 62.3 %, still climbing, while the Vapor margin badge has fallen from 32.4 to 3.1 % of the flooding rate.

Case 2 takes the fresh feed down to 185 and then up to 212 kmol/h (Table 7.5) on the Snowball view, as shown in Figure 7.2. At 7.4 h the recycle is at 360 kmol/h, 0.6 % above the curve's 358 and still closing, and at 16 h it is at 659, 1.0 % under the curve's 666 and still climbing. The recycle stays within 2 % of the curve from 5.0 h after the first step and from 7.4 h after the second, because each new point is approached at the pace of the reactor and the level loop. Between the points the plant reached, 15 fewer kmol/h of fresh feed took 140 kmol/h off the recycle and 27 more added 299,

Table 7.6 The Application's Scorecard at Each Case's Reading Instant, With the Lowest True Product Purity of the Run

Case	Settings and instant	Recycle since $t = 0$ (%)	Production (kmol/h)	Vapor margin (% of the limit)	Lowest p_B (mol % B)	Also
1	as shipped, 12 h	+62.3	220	3.1 to flood	97.17	OFF SPEC 0.95–4.7 h
2	as shipped, 16 h	+31.8	213	17.2 to flood	96.98	OFF SPEC 7.8–11.5 h
3	as shipped, 6 h	−4.2	221	32.1 to flood	97.86	production dips to 178.7 at 0.92 h
3	effluent to 760 kmol/h at 6 h, 12 h	+6.4	225	26.5 to flood	96.79	60 more effluent, 4.7 more product
4	as shipped (CS1), 12 h	+92.4	200	0.0 to flood	91.67	FLOODING from 3.80 h
4	CS2 and Reset, 6 h	+5.8	170	33.4 to flood	97.88	production −14.9 %
5	as shipped, 12 h	+75.2	230	0.0 to flood	95.01	FLOODING from 3.96 h, 11.4 kmol/h of A in B
5	fresh feed to 220 at 6 h, 12 h	+64.8	220	1.9 to flood	95.28	crosses 97.5 mol % at 7.62 h; one hour above it off flooding by 9.0 h
6	as shipped, 12 h	+26.9	219	67.4 to flood	97.58	starts at 106 kmol/h of recycle
7	as shipped (loop off), 12 h	+93.5	220	4.0 to flood	97.28	x_D 91.83 mol %
8	as shipped, 8 h	0.0	219	0.0 to flood	92.68	x_D 99.32 mol %, FLOODING from 4.47 h
8	level 56.5 % and Reset, 8 h	0.0	219	30.7 to flood	97.58	x_D at most 95.79 mol %
9	as shipped (CS1), 8 h	+23.5	239	0.0 to steam	79.57	steam limit from 0.75 h, fails
9	suggested, CS2 at 75 %, 8 h	−9.5	245	6.4 to steam	97.87	passes

secants of 9.4 and 11.1 against the curve's own 9.5 and 11.4. In percent the curve's slope is 4.03 at 185 and 5.26 at 212 kmol/h.

7.6.2 The Holdup as the Handle

Case 3 runs on CS2 and raises the reactor level setpoint from 50 to 57.2 %, the holdup that the balances give for 10 % more product. Production first dips to 178.7 kmol/h at 0.92 h, 25 min after the step, because the fresh A that fills the reactor reaches the column first, and it is back above 200 by 1.22 h. By 6 h production is 220.8 kmol/h, the reactor's A has fallen from 68.4 to 65.8 mol % and the recycle from 500 to 479 kmol/h, with the boilup almost unchanged at 1120 kmol/h. The handle has a price. The holdup rose 14 % for 10 % of production, the snowball in the reactor holdup that Wu and Yu found on Luyben's structure [8, 12]. Raising the effluent to 760 kmol/h at 6 h instead brings the CS1 curve back. The recycle is at 536 kmol/h within half an hour, and at 12 h production is 225.4 kmol/h with 532 kmol/h of recycle, 60 more kmol/h of effluent for about 5 of product.

7.6.3 Activity Lost on Two Structures

Case 4 cuts the catalyst activity to 80 %. On CS1 the fresh feed stays at 200 kmol/h, so the recycle has to make up the lost conversion. The product slips under 97.5 mol % at 1.2 h, the boilup reaches the flooding rate at 3.8 h, and by 12 h the product is at 91.76 mol % with 962 kmol/h of recycle, while the steady state would need 1767 kmol/h. On CS2, after Reset, the same loss costs production instead, 170.3 kmol/h at 6 h (−14.9 %), with the recycle at 529 kmol/h and the boilup at 1099. Switched to CS2 during the flooded run without Reset, the structure fixes the effluent where the snowball left it, about 1130 kmol/h, and the column stays at its flooding rate to 12 h.

> **+ DID YOU KNOW? The Free Flow Takes the Catalyst Loss**
>
> From the simulator (Table 7.6). With a fifth of the catalyst activity gone, the fixed fresh feed of CS1 leaves the loss to the recycle, which has risen 92.4 % by 12 h, with the column flooding from 3.80 h. On CS2, after Reset, the recycle has risen only 5.8 % at 6 h, and production has fallen 14.9 % instead.

7.6.4 The Vapor Wall

Case 5 asks for 15 % more fresh feed, beyond the 10.7 % the wall allows. The boilup reaches the flooding rate at 3.96 h with the recycle at 856 kmol/h, and from then the column sends no more A overhead. A goes into the product instead, 11.4 kmol/h of it at 12 h, where the product is at 95.04 mol %. That A no longer returns, so the recycle stalls near 877 kmol/h, far short of the 1082 kmol/h the curve gives at 230. Doubling the product purity gain leaves the product at the same 95.04 mol %, because the loop asks for vapor that is not there. With the fresh feed cut to 220 kmol/h at 6 h, the product first crosses 97.5 mol % at 7.62 h while still flooding, and by 9.0 h has held above that value off the flooding rate for an hour.

Pause. Try Exercise 7.3 before reading on.

7.6.5 Vessel Size and the Recycle Purity Loop

Case 6 doubles the vessel to 400 m^3 at the same level. The reactor starts at 34.2 mol % A with 106 kmol/h of recycle and 453 kmol/h of boilup, far from the curve's pole, and the same step raises the recycle 26.9 % by 12 h (28.9 % at steady state), against 62.3 % in case 1. The local elasticity at 200 kmol/h falls from 4.61 to 2.63. This is the design side of the snowball that the literature points to [2, 8]. Case 7 repeats case 1 with the recycle purity loop off and the reflux held. More A arriving at a fixed reflux lets B into the distillate, whose purity falls to 91.83 mol %, and since the reactor still needs the same z, more kmol of a leaner recycle must come back. The recycle rises 93.5 % against 62.3 % with the loop on, where the reflux rose 171 kmol/h to hold 95 mol %.

> **TRY IT IN THE APP** **7 · The Column's Purity Loops Are Part of the Recycle**
>
> Load the scenario, in which the recycle purity loop is off, run to 12 h and read the Recycle since $t = 0$ tile: the same step as case 1 now raises the recycle 93.5 %, because the recycle purity sags to 91.83 mol %. Switch the loop On, press Reset and run again to compare with the 62.3 % of case 1.

7.6.6 A Fixed Recycle

Case 8 runs on CS3 and ramps the effluent from 700 to 720 kmol/h over two hours. Production follows, 221.0 kmol/h at 6 h, and the recycle stays at 500 kmol/h. By Equation (7.8), at the design holdup 10 % more production would need a recycle of 107.5 mol % A, purer than pure A. The recycle purity climbs to 97.89 mol % at 3 h, the boilup reaches the flooding rate at 4.47 h, and at 8 h the product is at 92.68 mol % with the recycle at 99.32 mol %. With the level setpoint at 56.5 %, the holdup that keeps x_D at 95, the recycle purity peaks at 95.79 mol % and the boilup at 1154 kmol/h. A fixed recycle protects the column only while something else raises the conversion with production.

7.6.7 A Graded Day

The challenge limits the reboiler's steam to 1200 kmol/h of boilup, 7.6 % above the design's, raises the production target to 240 kmol/h at 15 min and takes a tenth of the catalyst activity away at 3 h. Over 8 h it judges production as twelve half-hour means of at least 235.2 kmol/h from 2 h, the true product at or above 97.5 mol % and the true recycle at or above 94.0 mol % at every step, the boilup never at its limit, and the reactor never above its alarm. Table 7.7 lists the settings tried. On CS1 the steady state at 240 kmol/h would need 2496 kmol/h of boilup, and as shipped the boilup reaches the steam limit at 0.75 h and the product falls to 79.57 mol %. On CS2 at a 75 % level the day passes, with 245.9 kmol/h in the worst half hour and the recycle falling from 500 to 453 kmol/h while production rises, and at seven other noise seeds the worst half hour stays between 245.7 and 245.9 kmol/h. The lowest passing CS2 level is 70.5 %, against the 72.3 % that makes 240 kmol/h at 90 % activity at steady state.

The size of the loss was chosen by measurement. With a fifth of the activity lost, CS2 needs 81.3 % of level at steady state, and the day passes only between 79 and 87.5 %, because at 88 % the overshoot breaks the 90 % alarm. With a tenth lost, the passing band is 70.5 to 87.5 %. Both teach the

Table 7.7 The Challenge Over 8 h, Default Seed

Settings	Worst (kmol/h)	Min p_B (mol %)	Min x_D (mol %)	At limit (min)	Max L_R (%)	Verdict
CS1, level 50 (shipped)	238.6	79.57	94.69	434.9	51.3	fails
CS2, level 75 (suggested)	245.9	97.87	94.55	0	77.4	passes
CS2, level 50	185.2	97.95	95.00	0	50.2	fails
CS2, level 70	234.9	97.87	94.58	0	72.3	fails
CS2, level 70.5	236.0	97.87	94.58	0	72.8	passes
CS2, level 85	266.5	97.87	94.53	0	87.4	passes
CS1, level 75	236.2	96.80	76.18	0	77.9	fails
CS1, level 75, slow loop[a]	198.7	97.73	92.37	0	78.3	fails
CS3, F 745, level 70	242.7	85.49	93.89	324.2	71.9	fails

[a] 10 kmol/h per percent and 120 min on the reactor level.

same lesson, that the structure and the holdup decide the day rather than the tuning, and the wider band leaves a first estimate room to pass.

7.7 Technology in Practice

What Measures It

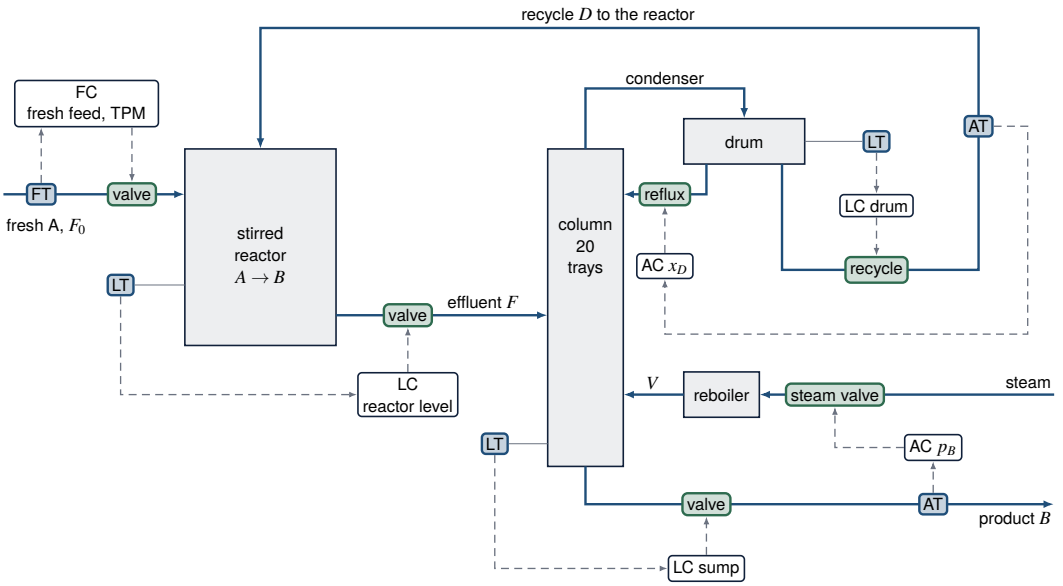
Every production handle of this plant is a flow setpoint: the fresh feed in CS1, the effluent in CS2 and CS3, and the recycle as well in CS3. Each sits on a flow loop, often metered by a pressure-based element whose signal is characterized by a square root [17]. The chapter's flow meters lag 0.05 min with 0.3 kmol/h of noise and read as well at the bottom of their range as at the top, which an orifice meter does not. The two purities come from analyzers. A process chromatograph separates species by time, so cycle times of minutes are not uncommon even on line, and some measurement dead time is inevitable [17]. The chapter's analyzers are continuous by default, with the chromatograph an Advanced option.

> **TECHNOLOGY Sensor: The Orifice Meter Under Each Flow Loop**
>
> The most common pressure-based flow element is the orifice plate, a metal plate with a hole, sandwiched between two pipe flanges. The pressure drop it develops grows with the square of the flow, so the transmitter's signal is characterized by a square root before an indicator or controller uses it as flow. Accuracy falls toward the bottom of the range: the practical turndown of pressure-based meters is often no more than 3 to 1. A dulled orifice edge or uneven liquid columns in the impulse tubes then cause large errors at low flow, even with a perfectly calibrated transmitter [17].

What Moves It

In the model each manipulated flow follows its setpoint through a first-order loop of 0.2 min, which stands for a control valve under its own flow controller, and the boilup follows through the reboiler in 1 min. The boilup controller never asks for more than V_{cap} and uses back-calculation, so the vapor wall of case 5 arrives as a saturated output without windup, as in a real controller that receives back-calculation feedback from its final element [17].

> **TECHNOLOGY Final Element: The Reboiler Steam Valve at Its Limit**
>
> Boilup is moved by the steam valve of the reboiler. When the steam supply cannot deliver what the loop asks for, a controller with integral action winds up, driving its output to saturation in a futile attempt to open the valve further, and when steam returns the saturated output overshoots. On a trend the output sits at its maximum while the measurement stays off setpoint. Back-calculation from the final element stops the controller from driving the valve farther than it is able to respond. A steam flow loop under the temperature or composition loop takes up steam-side upsets first, and it must respond faster than the loop above it [17].



Blocks FC, LC and AC: velocity-form PI in the distributed control system; the app executes all of them every 6 s. CS2 and CS3 re-pair the same blocks (Table 7.4).

Figure 7.5 The loops of CS1 on plant hardware. The fresh feed is the throughput manipulator, held by FC through a flow transmitter on an orifice, and the reactor level is held by the effluent valve. The drum level moves the recycle, the recycle analyzer moves the reflux, the product analyzer moves the reboiler steam valve and the sump level moves the product valve, each through a flow loop on its valve that is not drawn. Notice that no setpoint of the recycle is fixed in CS1: it is whatever the drum level controller sends back.

Where the Controller Runs

In a plant these loops run in a distributed control system, whose supervisory level oversees localized controllers. Loops are often nested or cascaded, and supervisory and lower-level loops run with cycle times from milliseconds to minutes [18]. Supervisory control in the process industry uses advanced regulatory control, a setpoint-based model predictive controller on top of the PID layer, or both, and usually no optimization layer exists [19]. The app integrates with a 2 s step and executes its controllers every 6 s, as Figure 7.5 shows for CS1. A structure is not a block of its own: one PI controller exists per manipulated flow, and those not driving their flow track it. Output tracking is also how a real controller picks up from its last manual value without a bump [17].

> ⚠ **IN PRACTICE** **Throughput First, Then the Bottleneck**
>
> After a new plant starts up, the operating staff usually turn first to raising throughput, because the extra profit there is usually much larger than from running more efficiently at a given rate. Yet the design phase usually makes no effort to give the plant a control system that runs at maximum throughput. At that point some unit is the bottleneck, and its maximum flow becomes an active constraint, which gives the rule of locating the throughput manipulator at the bottleneck unit. The design team should also say where the bottleneck is expected to appear when throughput rises [3].

What Is Modernizing It

Two directions stand out. The first designs self-optimizing behavior into simple, mostly single-loop regulatory strategies from the start. Against a centralized real-time optimizer, such strategies give simplicity, robustness and reliability, and they have found particular appeal in industry [3]. The

second moves the throughput manipulator automatically, where a handle moved to a new bottleneck would otherwise need several inventory loops rearranged. In a bidirectional structure each inventory has two controllers, one with a high setpoint on its inflow and one with a low setpoint on its outflow, and min-selectors choose between them. With unreachable flow setpoints it finds the bottleneck by itself and maximizes throughput [19]. The chapter's structures are switched by hand, and the bottleneck structure that would set production at the column's vapor rate is not offered (Section 7.8).

7.8 Limitations

Every size and setting here is a generic teaching value, chosen to give a consistent design point at 67.6 % of flooding, not a fit to any plant. The column is binary with constant relative volatility and constant molar overflow, its pressure is fixed, and flooding is a fixed ceiling on the boilup, so the model cannot show the gradual loss of efficiency near flooding, entrainment or the liquid limit of a downcomer. One irreversible first-order reaction stands for the chemistry, and side reactions, an equilibrium limit and an energy balance by default are absent. The recycle line mixes as well as delays.

The structures are three fixed pairings, so the bottleneck structure that sets production at the column's vapor rate [14], the balanced structures of Wu and Yu [12] and the reflux ratio as a self-optimizing variable [8] are not offered, and no supervisory layer moves the holdup or the temperature with production. A real-time optimizer that moves the setpoints of a reactor's loops is the subject of Volume 13, Chapter 11. The PI loops are tuned for continuous analyzers, the flow loops are ideal, and the status flags do not trip anything. The disturbances arrive as steps and ramps. A flow setpoint that the structure in force does not use follows the flow it names while the plant runs in Auto. In Manual the panel does not refresh it, so it keeps the value it held when Manual was selected.

> ⚠ **OPEN CHALLENGE** **A Structure Designed, Not Inherited**
>
> Heuristics, rules from case studies and optimization algorithms have all contributed to plantwide design over some forty years, yet much of that research has not gained enough acceptance in industry to have a profound influence. Process design and control design are still commonly segregated, and plants are run unit by unit with simple loops that operators understand. On an older plant even setting the throughput somewhere other than the feed can take years of work to win acceptance. What is missing is a formal yet simple procedure that ties the inventory structure to the plant's economics [3].

7.9 Conclusion

This chapter modeled the reactor, column and recycle plant of the plantwide control literature from balances that close to 1×10^{-11} of the throughput, with the control structure as a switch and the analytical steady state of Larsson and coauthors drawn beside the running plant. With the fresh feed fixed, 10 % more feed raises the recycle 62.3 % in 12 h toward 63.4 %. The five quantities called a snowball gain on this one design point, 4.61, 11.5, 11.55, 63.4 and 9.4 to 11.1, are consistent once each is named by its definition. Lined out, every structure that holds the holdup and both purities lands on one curve, so a structure chooses the production handle. The holdup moves the recycle -1 kmol/h per kmol/h at the price of 14 % more holdup for 10 % more product, the effluent at a fixed holdup brings the curve back, and a fixed recycle pushes the column's purity past pure A. The column's vapor limit ends the snowball by putting A into the product, and a recycle purity loop left open raises the recycle's rise to 93.5 %. The model's flooding is a ceiling and its chemistry one reaction. A fuller model would add the bottleneck structure with production set at the boilup, a reflux-ratio loop, a supervisory layer that moves the holdup with production, and a hydraulic flooding model. Where production is set in a recycle plant decides where the snowball goes.

KEY POINTS

- With the reactor holdup held and the fresh feed fixed, ten percent more feed raises the recycle 62.3 % in 12 h.
- Lined out, every structure that holds the holdup and both purities lands on one curve, so a structure chooses the production handle.
- The holdup handle moves the recycle -1 kmol/h per kmol/h at the price of 14 % more holdup for 10 % more product.
- The column's vapor limit ends the snowball by putting A into the product, and a stronger purity loop cannot recover it.

Where else this applies. A column that runs out of steam returns in Volume 10, Chapter 10, where a steam header trip pushes out of contract the one product with no controller on it.

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7.10 Exercises

7.1 Concept check · 2 min

In case 1 the fresh feed rises 10 % on CS1 while the reactor holdup and both purities are held, and the steady recycle rises 63.4 %. Which explanation is right?

(a) The reactor converts more A in the same holdup only by running richer in A, and the column returns that richer effluent's A

(b) The column separates less well under the larger load, so B circulates in the recycle and dilutes it

(c) The reactor level controller overshoots and lifts the effluent above what the production change needs

(d) The recycle line delays the returning A, so the recycle must grow to carry the A held in the line

7.2 Concept check · 1 min

At the design point the Snowball gain tile reads 4.61 % per percent, while the Model dialog gives a slope of 11.5 for the same curve at the same point. Why do the two differ?

(a) The tile is the secant of a 10 % step and the dialog is the tangent at the design point

(b) Both are the tangent of the CS1 curve, the tile in percent per percent and the dialog in kmol/h per kmol/h

(c) The tile is computed on CS2's line and the dialog on the CS1 curve, so they describe different structures

(d) The tile uses the analyzed purities and the dialog the setpoints, and the two differ by the analyzer noise

7.3 Concept check · 2 min

In case 5 the boilup reaches the 1650 kmol/h flooding rate and the product purity falls to 95.04 mol %. Doubling the Product purity gain leaves the product at the same 95.04 mol %. Why?

(a) The analyzer's sample line hides the improvement until after the 12 h reading

(b) Back-calculation freezes the integral at the limit, so only the small proportional term responds

(c) The boilup is already at its ceiling, so the loop asks for vapor that is not there and A leaves in the product

(d) The larger gain makes the loop oscillate about the ceiling, and the mean purity stays where it was

7.4 Theory and calculation · 6 min

The design reactor holds $M_R = 400\,\text{kmol}$ with $k = k_0 = 0.716\,\text{h}^{-1}$ at 70 °C and full activity. The fresh feed is pure A ($z_0 = 1$), the recycle purity is $x_D = 0.95$ and the product carries $x_B = 0.02$ of A. Use Equation (7.6).

(a) Find the reaction capacity kM_R, the reactor composition z^* and the steady recycle D^* at $F_0 = 200\,\text{kmol/h}$. *Checkpoint:* 286.4 kmol/h, 68.44 mol % and 500.2 kmol/h.

(b) Find the fresh feed at the curve's pole. *Checkpoint:* 277.6 kmol/h.

(c) Find the steady recycle at $F_0 = 220\,\text{kmol/h}$ and its rise over the design value. *Checkpoint:* 817.5 kmol/h, +63.4 %.

7.5 Theory and calculation · 6 min

Continue at the design point of the previous exercise, $z = 0.6844$, $x_D = 0.95$, $x_B = 0.02$, $F_0 = 200\,\text{kmol/h}$ and $D = 500.2\,\text{kmol/h}$.

(a) Evaluate both elasticities of Equation (7.7). *Checkpoint:* 4.61 and -3.61.

(b) Convert the first into the slope $\mathrm{d}D^*/\mathrm{d}F_0$ in kmol/h per kmol/h. *Checkpoint:* 11.5.

(c) Differentiate D^* of Equation (7.6) with respect to x_D at fixed F_0 and M_R, and find the recycle each mol % of recycle purity lost costs at steady state. *Checkpoint:* 18.8 kmol/h per mol %.

7.6 Theory and calculation · 6 min

Production is to rise from 200 to 220 kmol/h with both purities held ($x_D = 0.95$, $x_B = 0.02$, $z_0 = 1$). The design reactor converts $kM_R = 286.4\,\text{kmol/h}$ at a 50 % level.

(a) On CS2 the effluent stays at 700.19 kmol/h. Find the steady reactor composition and the reactor level setpoint that gives 220 kmol/h. *Checkpoint:* 65.78 mol % and 57.2 %.

(b) Find, for the CS2 move, the rise of the holdup in percent and the steady recycle. *Checkpoint:* $+14.4$ % and 480.2 kmol/h.

(c) On CS3 the recycle stays at 500 kmol/h and the effluent goes to 720 kmol/h at the design holdup. Find the recycle purity that would close the column's balance, and the level that keeps it at 95 mol %. *Checkpoint:* 107.5 mol % and 56.5 %.

7.7 App challenge · 8 min

Load scenario 1, Fresh feed +10 % on the conventional structure, and change no setting. Run to 12 h (720 min) at the default seed; the default 60 min/s plays it in 12 s.

(a) Read the Recycle since $t = 0$ and Vapor margin tiles at 12 h, and in the exported file the columns `recycle_kmolh` and `recycle_curve_kmolh` at 720 min. *Checkpoint:* $+62.3$ % and 3.1 % to flood; 811.9 kmol/h against 817.5 kmol/h, within 0.5 kmol/h.

(b) Compare the Snowball gain tile at $t = 0$ and at 12 h, and say why it changed. *Checkpoint:* 4.61 and 5.84 % per percent.

(c) Load scenario 7, The column's purity loops are part of the recycle, in which the recycle purity loop is off, run it to 12 h and read the Recycle since $t = 0$ tile and `truth_xD_pct` at 720 min. *Checkpoint:* $+93.5$ % and 91.83 mol %, within 0.02 mol %.

7.8 App challenge · 8 min

Load scenario 3, CS2: the same production increase by the reactor holdup, and use the default seed. The reactor level setpoint steps from 50 to 57.2 % at 30 min.

(a) Run to 6 h. Read the Production and Recycle since $t = 0$ tiles, and find in the exported file the lowest `production_kmolh` and its time. *Checkpoint:* 221 kmol/h and -4.2 %; lowest 178.7 kmol/h at 55 min, within 0.2 kmol/h.

(b) At 6 h raise the Reactor effluent setpoint to 760 kmol/h and run on to 12 h. Read the same two tiles. *Checkpoint:* 225 kmol/h and $+6.4$ %.

(c) Use the slope of the snowball curve to explain why 60 kmol/h more effluent buys only about 5 kmol/h more product. *Checkpoint:* $\Delta F_0 \approx \Delta F/(1 + \mathrm{d}D^*/\mathrm{d}F_0) \approx 60/12$.

7.9 App challenge · 9 min

Load scenario 9, the challenge, and use the default seed. Each run lasts 8 h; at 300 min/s it plays in under 2 s.

(a) Run as shipped (CS1). Read the three So far tiles at 8 h and say which criteria fail. *Checkpoint:* 238.6 kmol/h worst half hour; product 79.57 mol % B; boilup at its limit 434.9 min. Purity and limits fail.

(b) Choose CS2, set the Reactor level setpoint to 70 %, press Reset and run the 8 h. Repeat at 70.5 %. Read the production tile each time. *Checkpoint:* 234.9 kmol/h, which fails, and 236.0 kmol/h, which passes.

(c) Using the CS2 balances of the theory exercise above, find the level that makes 235.2 kmol/h, the production the verdict requires, at steady state with 90 % activity, and compare it with (b). *Checkpoint:* 70.1 %, so 70.5 % is the first setting on the slider's 0.5 % grid.

7.10 Application area · 3 min

The column was designed at 67.6 % of its 1650 kmol/h flooding rate. The CS1 steady states at 216, 220 and 221.4 kmol/h of fresh feed need 1485, 1604 and 1649 kmol/h of boilup.

(a) Find the vapor margin left at steady state after case 1's 10 % increase. *Checkpoint:* 2.8 % of the flooding rate.

(b) A project engineer proposes to size a new column of this plant at 80 % of flooding, as for a plant without recycle. What does the snowball do to that choice? *Checkpoint:* The wall moves to 6.3 % more fresh feed.

7.11 Application area · 4 min

Case 6 doubles the reactor vessel to 400 m^3 at the same level. The design recycle falls from 500 to 106 kmol/h, the boilup from 1115 to 453 kmol/h, and the snowball gain at 200 kmol/h from 4.61 to 2.63.

(a) The app's case 6 briefing prices a vessel at its volume to the 0.6 power. By what factor does doubling the vessel raise its cost? *Checkpoint:* About 1.52.

(b) Name the equipment whose size the larger reactor saves, and say what the lower snowball gain gives the operator. *Checkpoint:* Column, reboiler, condenser and recycle pumps; a smaller recycle swing per percent of production or activity.

7.12 Review the agent · 5 min

An AI assistant is asked how to keep the product on specification in case 5, where the fresh feed rises 15 % on CS1. It replies: "The product purity loop is too slow for the larger load. Double the Product purity gain to 80 kmol/h per mol % and shorten its integral time to 7 min; the product will return to 98 mol % within an hour of the FLOODING alarm." Find the flaw, and say how you would check the claim and what you would do instead.