INTERACTIVE CONTROL ENGINEERING
Principles and Applications

Volume 13 Control in Chemical Plants

CHAPTER 8

A Dividing-Wall Column Whose Spare Handle Moves Only the Energy

Pages 187–209

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How to cite this chapter. "A Dividing-Wall Column Whose Spare Handle Moves Only the Energy," in *Control in Chemical Plants*, John D. Hedengren, Ed., vol. 13 of *Interactive Control Engineering: Principles and Applications*. Advanced Process Solutions, LLC, 2026, ch. 8, pp. 187–209.

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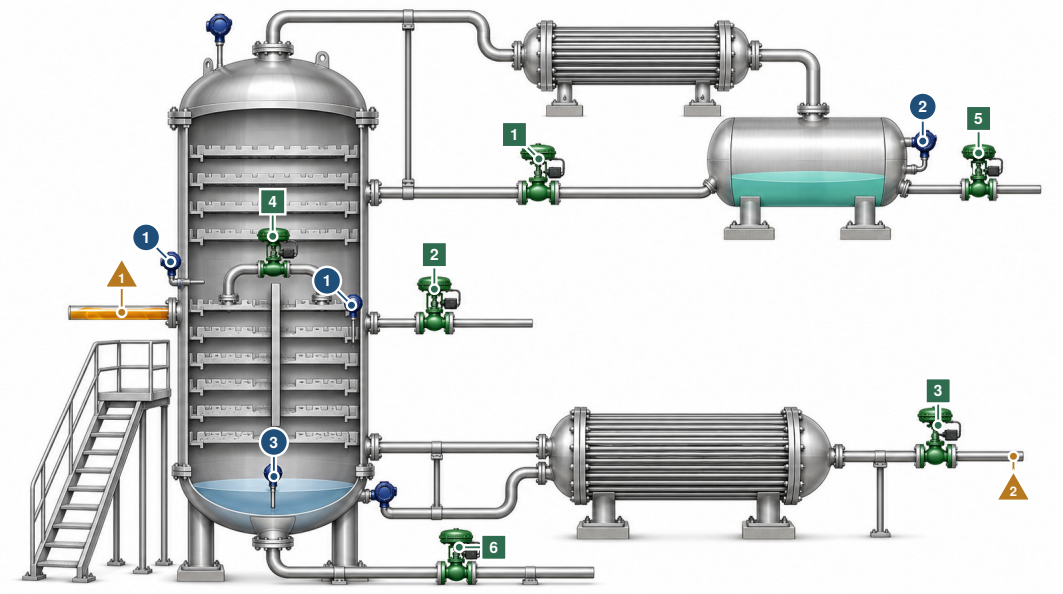
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CHAPTER 8

A Dividing-Wall Column Whose Spare Handle Moves Only the Energy



The controller moves 1 reflux valve 2 side draw valve 3 reboiler steam valve, which sets the boilup 4 liquid splitter above the wall 5 distillate valve, on the drum level 6 bottoms valve, on the base level

The controller reads 1 tray temperatures beside the wall 2 reflux drum level 3 base level

What disturbs it 1 a heavier or larger feed 2 a limit on the steam supply

Notice the wall up the middle of the tower and the splitter at its top: with the three products held pure, that one setting decides how much steam the reboiler at the lower right uses. Illustration, not to scale.

IN PLAIN TERMS One Tower Doing the Work of Two

The main idea. One tall tower with a wall up its middle splits a liquid mixture into three products. Three controllers keep the products pure, and a fourth setting decides how much of the liquid falling from the top goes to each side of the wall.

The challenge. With the products held pure, that setting changes only the steam used to boil the liquid at the bottom. The best value moves when the feed changes, and too low a value means no amount of steam makes the middle product.

Why it matters. A column with every product on target can still burn far more steam than it needs.

THREE WAYS TO READ THIS CHAPTER

Explore	13 min	the first page; the history boxes of Section 8.2; the fact box of Section 8.4; the try-it and fact boxes of Section 8.6; the key points
Study	45 min	the whole chapter with its pause points and the exercises
Practice	15 min	the first page; Section 8.6 with its result chart; Section 8.7; Section 8.8 and its open challenge

The control question Three purity loops use three of a dividing-wall column's four handles, and the fourth, the liquid split above the wall, moves only the reboiler duty along a valley whose minimum shifts with the feed. How is the column kept in that valley when the feed changes, and what does each control structure cost on the way?

Learning objectives

- Count the degrees of freedom of a dividing-wall column and explain why the spare handle moves only the energy.
- Compute the Underwood minimum vapor of each split, the thermally coupled saving, and the bound a fixed vapor split sets.
- Explain the steep side of the energy valley from the liquid-to-vapor ceilings on the two sides of the wall.
- Compare a fixed split, a split loop on the prefractionator, a feed-rate feedforward and an MPC through a feed change and a rate change.
- Judge when an inferred purity or a tray temperature can stand for the quantity a loop must hold.

Prerequisites Sections 1.4.5 (degrees of freedom and Underwood's method), 1.4.6 (inferred compositions and the bias update), 1.6.2 (velocity form) and 1.6.4 (scenarios and data). Section 1.6.3 is needed only for the predictive controller.

The app https://apmonitor.com/apps/dividing-wall-column/

See also Volume 6, Chapter 2 for pairing by the relative gain array and Volume 6, Chapter 7 for choosing a control structure. Volume 9, Chapter 8 for an optimum that moves with a disturbance and Volume 9, Chapter 4 for offset-free predictive control with a disturbance estimator. Volume 5, Chapter 3 for composition control through a slow analyzer.

8.1 Introduction

Three products from one feed normally need two distillation columns, two reboilers and two condensers. A dividing-wall column does the two splits in one shell. In the generic column simulated here, 300 kmol/h of equimolar benzene, toluene and o-xylene enters the feed side of a vertical wall, benzene leaves overhead at 99.2 mol %, toluene leaves by a side draw at 98.2 mol % and o-xylene leaves the base at 99.2 mol %, with one reboiler boiling 649 kmol/h (5.83 MW). That duty is a minimum, and it holds only while 31.4 % of the liquid leaving the section above the wall is sent down the feed side. With 40 % sent there instead, the same three purities need 17.7 % more steam, and with 28 % they need 21.4 % more. Below 28 % no boilup under the flooding rate makes the side product at all.

The simulator is built around one misconception, that holding every product on specification leaves nothing more for the operator to decide. Here three purities take three handles (reflux, side draw and boilup), and the fourth, the liquid split above the wall, is left free. Once the purities are held it cannot change any product flow or composition, so it moves only the internal flows and with them the energy. The same structure, more handles than specifications and a free one that sets the cost, appears in parallel trains that share a load, in heat-integrated units and wherever an optimum lies inside the constraints, and choosing what to hold constant there is the problem of self-optimizing control [1]. Chapter 6 couples two columns the other way, through one condenser-reboiler, so that one duty serves both. A control course meets the relative gain array [2] on a two-product column and rarely on a plant where a spare handle has a minimum to find and lose. Two more lessons come with the dividing wall. Its three purity loops interact strongly, and the column is ill-conditioned in the way high-purity distillation is [3]. Its minimum also moves with the feed, so a split fixed at commissioning wastes energy after the next feed change, which is the problem a measurement on the prefractionator was proposed to solve [4].

However, a student who reads the dividing-wall literature sees the energy valley as a figure from a steady-state solver and the control structures as trends from a commercial simulator [4, 5]. This chapter works with that column in a browser, with the liquid split as a handle and the valley computed

from the same equations the plant integrates. It measures what a fixed split, a split loop on the prefractionator, a feed-rate feedforward and a model predictive controller (MPC) do with one feed change and one rate change. The stage model, the shortcut methods of Fenske, Underwood and Gilliland [6–8], the four-point structure of Ling and Luyben [4] and the proportional-integral (PI) law are all established methods. The results are measured on one generic design. The valley computed by the app agrees with an independent steady-state solver to 0.01 kmol/h at twenty splits, its steep side is a ceiling on the prefractionator's liquid-to-vapor ratio, and an MPC on a fixed step-response model reaches the valley but lets the benzene fall below its specification on a feed change. The model has 138 states, is built on a distillation module that other apps share, closes its balances to 8.7×10^{-10} of the feed, and is given here with every equation, constant and default needed to build it again.

Section 8.2 traces the domain, from two columns in sequence to the wall in one shell. Section 8.3 sets out the shell as modeled: its stages, the wall, the drum and sump, the instruments and the parameters. Section 8.4 counts the degrees of freedom, computes the energy valley, checks it against an independent solver and the shortcut bounds, and explains why one side is steep. Section 8.5 describes the loops, the inferential measurements, the split loop, the feedforward and the MPC. Section 8.6 measures the nine cases of the app, from walking the valley by hand to the graded challenge, Section 8.7 names the real devices behind the loops, and Section 8.8 states the limitations. The exercises at the end of the chapter run several of the cases.

8.2 Two Columns in One Shell

Separating a ternary mixture by distillation takes two splits, and the classic answer is a sequence of two columns. In the direct sequence the first column takes the light component overhead and the second splits the other two, so the middle component is boiled in both. The thermally coupled alternative sends the feed to a prefractionator that splits it roughly, light and middle up, middle and heavy down, and returns both ends to a main column that draws the middle component from its side. That arrangement is the Petlyuk column, whose origin and first operating studies are told in the history boxes of this section. For infinite stages, constant relative volatility and constant molar flows, its minimum vapor rate equals that of the more difficult of the two binary splits done in a single column [9], the analytical form of Underwood's minimum reflux [7].

> ⧖ HISTORY **A Wall Through the Middle Trays, 1937 to 1965**
>
> In 1949 Wright proposed an alternative to columns in series for a three-component feed: an ordinary column shell in which a vertical wall through a set of trays divides the feed from the side draw, saving investment, with one shell and two heat exchangers, as well as operating cost. Brugma had proposed a similar design in 1937, with its own condenser and reboiler for the prefractionator. The arrangement carries the name of Petlyuk and coworkers, who studied it theoretically in 1965 to avoid the losses of mixing streams of different composition at the feed tray. Many authors predicted large savings, yet by 1995 few such columns had been built, and the only industrial one reported stood in Germany. A probable reason was that the column has many more degrees of freedom than an ordinary one, which complicates both its design and its control [10].

Putting both columns of the Petlyuk arrangement in one shell, with a vertical partition between the feed side and the draw side, gave the dividing-wall column. A 1987 account of columns with vertical partitions reported energy use 20 to 35 % lower than other distillation arrangements and production columns that were easily controlled [11]. Operation and control of the dividing wall were studied by the late 1990s [12], and reviews in 2010 and 2011 surveyed its design, its industrial record and its current activity [13, 14]. By 2009 about forty columns were reported in service [4].

Control arrived after design. Most published structures held the three purities with the reflux, the side draw and the boilup, while the vapor split was fixed when the wall was placed and the liquid split was left as a handle for some further objective [4]. Ling and Luyben proposed the four-point structure, which keeps the energy near its minimum implicitly by controlling the heaviest component

Table 8.1 Variables, Their Roles and Design Values (Case 4 at $t = 0$)

Symbol	Role	Design	Range
x_D	CV, benzene in the distillate (mol %)	99.20	SP 97–99.9
x_S	CV, toluene in the side draw (mol %)	98.20	SP 94–99.8
x_B	CV, o-xylene in the bottoms (mol %)	99.20	SP 97–99.9
x_P	CV (four-point), o-xylene on the prefractionator's top stage (mol %)	1.57	SP 0.2–8
ℓ_D, ℓ_B	CV, drum and base levels (%)	50, 50	SP 20–80
L	MV, reflux (kmol/h)	548.9	0–1500
S	MV, side draw (kmol/h)	100.2	0–300
V	MV, boilup (kmol/h)	649.3	0–V_{cap}
β	MV, liquid split to the prefractionator	0.314	0.15–0.70
D, B	MV, distillate, bottoms (kmol/h)	100.3, 99.5	0–400
F	DV, feed rate (kmol/h)	300	200–400
z_1, z_3	DV, benzene, o-xylene in feed (mol %)	33.3, 33.3	15–50
ΔT_{sub}	DV, feed subcooling (K)	0	0–40
V_{steam}	DV, boilup the steam allows (kmol/h)	1500	400–1500
M_i, x_{ij}	states, stage holdup (kmol), fractions	1 or 2, profile	40 stages
M_D, M_B	states, drum, sump holdup (kmol)	20, 30	cap 40, 60
Q	output, reboiler duty (MW)	5.83	—

in the prefractionator, and tested it on feed rate and feed composition changes [4]. Their study of the same benzene, toluene and o-xylene separation on temperatures found that one temperature on the prefractionator side and three in the main column handled feed rate changes, while product purities deviated for composition changes greater than about 10 % [5]. Multivariable model predictive control, by then the industrial standard for interacting units [15], became the other candidate.

> ⧖ HISTORY **The Energy Valley, 1995 and 1999**
>
> In 1995 a study of operating the three-product column found that the boilup could have two solutions at one liquid split, and that at a higher side-draw purity a hole opened where no split met the specifications. It warned of serious problems, at least at high purity [10]. A 1999 study noted that industrial use had been limited, with difficulties in operation reported as one reason. With three purities controlled, two degrees of freedom remained for optimization, and the optimal surface proved narrow, very steep in one direction and moved by disturbances, its optimum lying along the bottom of a valley. The authors proposed holding the column there by feedback on a variable that characterizes optimal operation, and called the heavy key at the top of the prefractionator very interesting, though probably in need of a composition analyzer [16]. The four-point loop of this chapter feeds back exactly that measurement.

8.3 The Shell as Modeled

No plant stands behind the simulated column, whose layout is shown in Figure 8.1. Forty theoretical stages are arranged as four sections, 8 above the wall, 12 on each side of it and 8 below. The feed enters stage 7 of the prefractionator, counted from the top of the wall, and the side draw leaves stage 7 of the main side. A total condenser feeds a reflux drum and a partial reboiler with its sump closes the shell. The liquid leaving the top section is divided above the wall by a splitter, and the vapor leaving the bottom section is divided at the foot of the wall by the wall's position. Sizes, volatilities and limits are teaching values picked so that the design point hangs together, and each export is labeled a synthetic educational model.

Table 8.1 lists the variables by role. Time runs in minutes while flows are in kmol/h, so the code multiplies each balance by $1/60$, a factor the equations below leave out. The model integrates 138 states, a holdup and two mole fractions on each of the 42 stages (drum, 40 stages, sump), six flow states and six ledgers that count the moles, the benzene and the o-xylene entering and leaving.

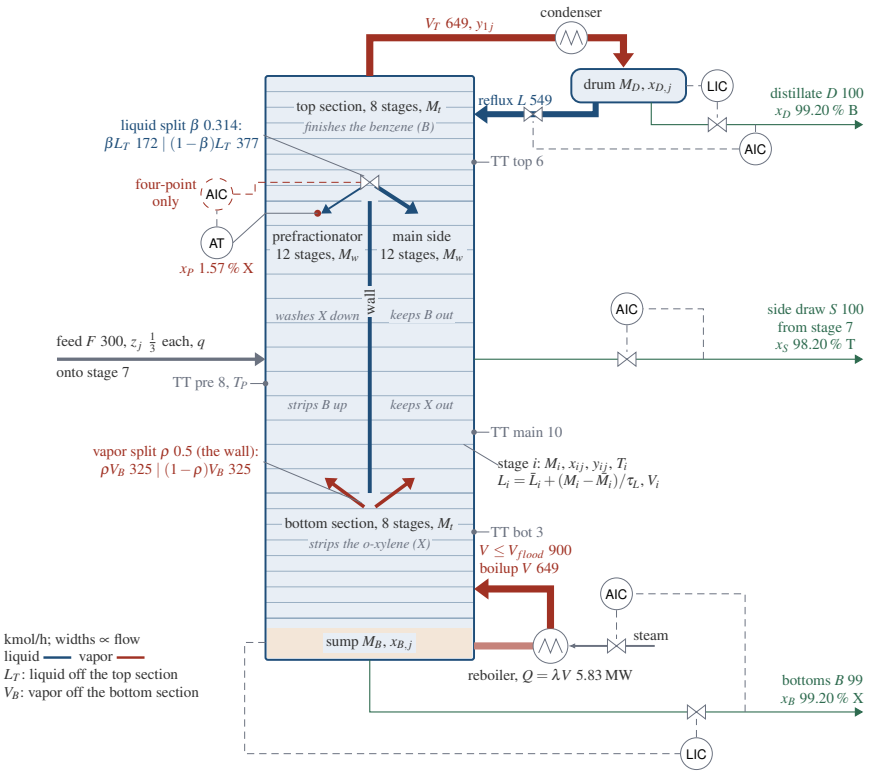


Figure 8.1 The dividing-wall column at its design point, following the application's Column view of case 4 at $t = 0$, where the split sits at the valley's minimum. Each section carries its job, the liquid split β above the wall and the vapor split ρ at its foot are drawn as the flows they send to the two sides (arrow widths proportional to flow), and the loops of the three-point structure are drawn with the fourth, four-point loop dashed in red, its controller bubble outlined dashed as well. Liquid runs down and vapor up, and every stream is labeled by name. TT marks the thermowells the inferential loops read. Flows in kmol/h. Process model only. Not to scale.

8.3.1 Stages, Equilibrium and Temperature

Each stage is an equilibrium stage with a liquid holdup, constant molar overflow and a linearized weir, as shown in Equation (8.1).

$$\begin{aligned} \frac{\mathrm{d}M_i}{\mathrm{d}t} &= L_{i-1} + V_{i+1} + F_i - L_i - V_i - S_i \\ \frac{\mathrm{d}(M_i x_{ij})}{\mathrm{d}t} &= L_{i-1}x_{i-1,j} + V_{i+1}y_{i+1,j} + F_i z_j \\ &\quad - (L_i + S_i)\,x_{ij} - V_i\,y_{ij} \\ L_i &= \bar{L}_i + \frac{M_i - \bar{M}_i}{\tau_L}, \qquad V_i = V_{i+1} + (1-q)\,F_i \end{aligned} \tag{8.1}$$

where i counts the stages of a section from its top, $j = 1,2,3$ are benzene, toluene and o-xylene, F_i is the feed on the feed stage and zero elsewhere, S_i is the side draw on the draw stage, q is the liquid fraction of the feed, and $\bar{L}_i$ and $\bar{M}_i$ are the weir's reference flow and holdup. The reference flows are those of a 500 kmol/h reflux, a split of 0.305, a 300 kmol/h feed and a 100 kmol/h draw, and $\tau_L = 0.1$ min. The reference holdup is $M_t = 2$ kmol on each stage above and below the wall and $M_w = 1$ kmol beside it. A draw takes at most the liquid there is on its stage. The vapor composition

follows constant relative volatility and the temperature a closed-form bubble point, as shown in Equation (8.2).

$$y_{ij} = \frac{\alpha_j x_{ij}}{\sum_k \alpha_k x_{ik}}, \qquad T_i = \frac{\Lambda}{\ln\left(\frac{P_0}{P}\sum_k x_{ik}\, e^{\Lambda/T_{b,k}}\right)} \tag{8.2}$$

where $\alpha = (2.4, 1, 0.44)$ relative to toluene, $\Lambda = 3890\,\mathrm{K}$ is one common latent heat over the gas constant, $P = P_0 = 1.013\,25\,\mathrm{bar}$, and the normal boiling points $T_{b,k}$ follow from α and toluene's 110.6 °C as 80.1 and 144.4 °C for benzene and o-xylene. One latent heat is the constant-molar-overflow assumption itself, and it makes α exactly constant. The latent heat $\lambda = R\Lambda = 32.3\,\mathrm{kJ/mol}$ turns the boilup into the duty $Q = \lambda V$, so 1 kmol/h of boilup is 0.008 984 MW. The stage stacks, the drum and the sump are a distillation module that the apps share, written for a reactor, column and recycle plant and moved into the framework when this column became its second user.

8.3.2 The Wall

The four sections are joined across the wall, as shown in Equation (8.3).

$$\begin{aligned} L_{P,0} &= \beta L_T, & L_{M,0} &= (1-\beta)\, L_T \\ V_{P,13} &= \rho V_B, & V_{M,13} &= (1-\rho)\, V_B \\ L_{bot,0} &= L_{P,12} + L_{M,12}, & V_{top,9} &= V_{P,1} + V_{M,1} \end{aligned} \tag{8.3}$$

where P and M are the prefractionator and the main side, index 0 marks the liquid entering a section's top stage and index $n+1$ the vapor entering its bottom stage, L_T is the liquid leaving the top section, V_B the vapor leaving the bottom section, the entering streams carry the composition of the stage they come from, and the two mixed streams carry the flow-weighted composition of their parts. The code computes the vapor bottom-up and the liquid top-down before any composition, and then evaluates the four stacks bottom-up. The vapor split $\rho = 0.5$ is equipment, not a handle.

8.3.3 Drum, Sump and Actuators

The drum is a total condenser's holdup and the sump a partial reboiler's equilibrium stage, as shown in Equation (8.4).

$$\begin{aligned} \frac{\mathrm{d}M_D}{\mathrm{d}t} &= V_T - L - D \\ M_D \frac{\mathrm{d}x_{D,j}}{\mathrm{d}t} &= V_T\,(y_{1j} - x_{D,j}) \\ \frac{\mathrm{d}M_B}{\mathrm{d}t} &= L_N - V - B \\ \frac{\mathrm{d}(M_B x_{B,j})}{\mathrm{d}t} &= L_N x_{N,j} - V y_{B,j} - B x_{B,j} \end{aligned} \tag{8.4}$$

where V_T is the vapor leaving the top stage at y_{1j}, L_N the liquid off the last stage at $x_{N,j}$, and $y_{B,j}$ is in equilibrium with the sump. The product purities are $x_D = 100\,x_{D,1}$, $x_S = 100\,x_{M7,2}$ on the draw stage, $x_B = 100\,x_{B,3}$, and x_P is the o-xylene on the prefractionator's top stage. Each manipulated flow follows its setpoint through a first-order lag, 0.2 min for the liquid flows, 1 min for the reboiler and 0.5 min for the splitter. As the drum or the base runs dry its pump delivers only the flow times $\min(1, M/(0.02\,M_{cap}))$. A subcooled feed enters with $q = 1 + c_{p,L}\Delta T_{sub}/\lambda$.

8.3.4 Instruments

A measurement packet carries everything the controllers see, and the application's test fails if it ever carries anything else. Level transmitters lag 0.1 min with 0.05 % of noise, flow meters lag 0.05 min with 0.3 kmol/h, and thermowells on four candidate stages per section lag 0.5 min with 0.05 K. Four analyzers on the shared analyzer module measure the three product purities and x_P. Each takes a sample every 10 min, after a 1 min transport delay, and publishes the result at the end of the following

Table 8.2 Parameters, Marked A When the Learner Can Change Them, H When the Panel Hides Them and S When Fixed in the Source

Symbol	Meaning	Value	Unit	
α_1, α_3	benzene, o-xylene volatility	2.4, 0.44	—	A
Λ	latent heat over R	3890	K	H
$T_{b,2}$	toluene normal boiling point	110.6	°C	H
ρ	vapor split to the prefractionator	0.5	—	A
M_t, M_w	stage holdup off, beside the wall	2, 1	kmol	A
τ_L	stage hydraulic lag	0.1	min	H
$M_{D,cap}, M_{B,cap}$	drum, base capacity	40, 60	kmol	A
V_{flood}	boilup at flooding	900	kmol/h	A
$c_{p,L}$	liquid heat capacity	0.16	kJ/(mol K)	H
—	specifications of x_D, x_S, x_B	99, 98, 99	mol %	A
$\tau_Q, \tau_V, \tau_\beta$	flow, reboiler, splitter lags	0.2, 1, 0.5	min	H
N_T, N_P, N_M, N_B	stages per section	8, 12, 12, 8	—	S
f, s	feed, draw stage (wall's top = 1)	7, 7	—	S
P	column pressure	1.01325	bar	S
$\bar{L}, \bar{\beta}, \bar{F}, \bar{S}$	weir references	500, 0.305, 300, 100	kmol/h	S
E	stage efficiency	1	—	S

cycle, with 0.01 mol % of noise (0.02 mol % on x_P). Every execution draws the same twelve normal deviates, so a seeded run replays bit for bit (Section 1.6.1).

8.3.5 Parameters, Initialization and Numerics

Table 8.2 gives every parameter. Each case opens lined out at its own split and setpoints, a state found by the Newton solver of Section 8.4 at the case's split and purity setpoints, with the holdups placed on the weirs and the drum and base at 50 %. The design point is an exact equilibrium, its largest derivative 4.5×10^{-15} per minute. Where no steady state exists at the case's split (case 8), the plant starts from the steady state at that split with the design's reflux and boilup and the side draw at the toluene in the feed. A fourth-order Runge-Kutta integrator advances the plant in 2 s steps, a third of the weir lag, the controllers act every 6 s, and one row is logged per 5 min. Halving the step moves case 4 at 4 h by 7.9×10^{-9} relative, and over a disturbed run the ledgers close the moles, the benzene and the o-xylene to 8.7×10^{-10} of the feed.

8.3.6 Assumptions

Constant molar overflow and constant relative volatility with one latent heat stand for the thermodynamics, so no energy balance is solved per stage and the volatilities do not drift with temperature. Benzene, toluene and o-xylene are close to ideal, and the error lies mostly there. The volatilities are teaching values. The Antoine fits of Willingham and coauthors, as the NIST Chemistry WebBook lists them [17], give 2.60 for benzene over toluene at 80 °C and 0.31, 0.34 and 0.37 for o-xylene over toluene at 70, 90 and 110 °C, so the 0.44 used is 19 to 42 % high and the toluene and o-xylene split is easier here than in a real column. The model's boiling points, 80.1, 110.6 and 144.4 °C, match the same fits' 80.1, 110.62 and 144.41 °C. The stages are theoretical with an efficiency of one, the shell has one pressure, and the vapor split is fixed, while a real wall's vapor split moves with the two sides' pressure drops. Flooding is a ceiling on the boilup, so the column has no flooded state. The flow loops, the condenser and the splitter are ideal lags, and the pressure and feed temperature loops are not shown.

8.4 The Spare Handle and Its Valley

8.4.1 Degrees of Freedom

The count follows Section 1.4.5. The drum and base levels take the distillate and the bottoms. Four handles remain, L, S, V and β, and three purities use three of them. With the purities fixed, the

component balances fix the three product flows, so the fourth handle can only redistribute the internal flows, as shown in Equation (8.5).

$$Q(\beta) = \lambda\, V(\beta)\big|_{x_D, x_S, x_B \text{ held}}, \qquad \beta^* = \arg\min_{\beta} Q(\beta) \tag{8.5}$$

The application computes $V(\beta)$ by Newton's method on every stage's two fractions and on L, S and V, with the three purities as equations, a numerical Jacobian, a step capped at 0.25 in any fraction and 30 % in any flow, and each stage projected into the simplex. The curve is walked from the minimum in steps of 0.005 until no solution exists or the boilup passes 1.6 times the flooding rate, and the minimum is refined by a parabola through its neighbors. It is computed at the purity setpoints in force, because those are what the loops hold, with the feed sampled at most every 10 min.

🕮 **Pause.** Try Exercise 8.1 before reading on.

At the design feed and the setpoints 99.2 mol %, 98.2 mol % and 99.2 mol %, the minimum is 649.3 kmol/h (5.83 MW) at $\beta^* = 0.314$, 72 % of flooding, with 548.9 kmol/h of reflux. The boilup is 788.5 kmol/h at 0.28 (21.4 % more) and 763.9 kmol/h at 0.40 (17.7 % more), and stays within 5 % of the minimum from 0.295 to 0.35. All three products can be made below flooding from 0.28 to 0.445. At the specifications the minimum would be 601.1 kmol/h at 0.305, so the 0.2 mol % margins cost 8.0 % of the duty. The heavier feed of cases 4, 5 and 9 (benzene 25, o-xylene 41.7 mol %) moves the minimum to 0.339 and 668.1 kmol/h (6.00 MW), as shown in Figure 8.3a. The plant lands on the curve when it lines out. In case 2 the split is moved every 3 h, and just before each move the duty is 7.31 against the curve's 7.31 (+0.03 %), 6.21 against 6.20 (+0.30 %) and 5.83 against 5.84 MW (−0.22 %), as shown in Figure 8.2.

8.4.2 An Independent Check and the Shortcut Bounds

A steady-state solver written for the technical review from the stage equations alone, by the bubble-point method at fixed flows with Newton's method on (D, S, V) for the purities, shares no code with the application. It reproduces the curve to 0.01 kmol/h at twenty splits from 0.275 to 0.50, puts the minimum at 0.3139 and 649.26 kmol/h against the application's 0.314 and 649.28 kmol/h, and returns the design purities at the application's design flows to six decimals, as Table 8.3 lists.

Underwood's method [7] at infinite stages, sharp splits and a saturated-liquid feed gives the roots of Equation (8.6) and the minimum vapor of each binary split. For $q = 1$ it is Equation (1.8) of Chapter 1.

$$\sum_j \frac{\alpha_j z_j}{\alpha_j - \theta} = 1 - q, \qquad V_{min,k} = F \sum_{j \le k} \frac{\alpha_j z_j}{\alpha_j - \theta_k} \tag{8.6}$$

With $\theta_1 = 1.4667$ and $\theta_2 = 0.5625$, the benzene and toluene split needs 257.1 kmol/h and the toluene and o-xylene split 359.2 kmol/h. The Petlyuk minimum is the larger of the two [9], here 359.2 kmol/h against 514.3 kmol/h for the direct sequence, a saving of 30.2 %. The wall fixes the vapor split, so the prefractionator can reach its preferred split (195.9 kmol/h of vapor) only when $\rho V \ge 195.9$, which puts the fixed-wall minimum at 391.8 kmol/h (3.52 MW) and a split of 0.231. The application's 649 kmol/h is 1.66 times that because its sections are short. Fenske's minimum [6] at the design compositions is 11.1 stages for the toluene and o-xylene split and 11.6 for the benzene and toluene split, against 14 stages for each (ratios of 1.26 and 1.21), and Gilliland's correlation [8] for the controlling split gives 894 kmol/h, an estimate rather than a bound. The prefractionator also needs a liquid-to-vapor ratio of 0.53 above the feed with its six stages, against the 0.344 of the preferred split, so the finite-stage minimum sits at a larger split, 0.314 against 0.231.

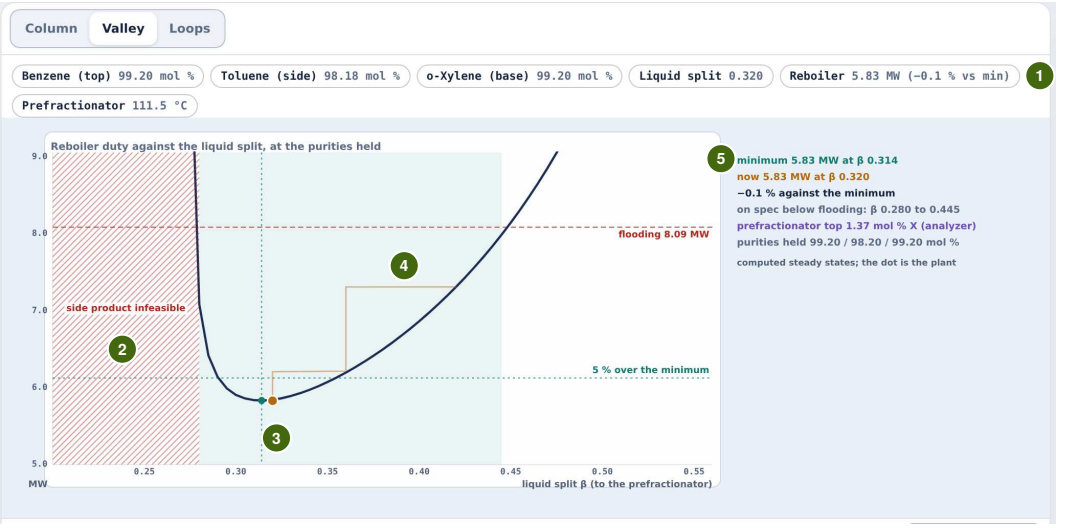


Figure 8.2 The energy valley of case 2 at $t = 9$ h on the Valley view, the three-point structure in Auto, light theme, cropped to the plot and its status chips. (1) The chips: benzene at 99.20 mol %, toluene at 98.18 mol % and still settling, o-xylene at 99.20 mol %, and the reboiler at 5.83 MW. (2) The zone below 0.28, hatched, where no boilup up to flooding (8.09 MW) makes the side product. The splits from 0.280 to 0.445 are on specification below flooding, and the dotted line lies 5 % over the minimum. (3) The computed curve holds 99.20 mol %, 98.20 mol % and 99.20 mol % at the design feed, with its minimum at 5.83 MW and a split of 0.314 (left dot). The plant's dot reads 5.83 MW at 0.320, 0.1 % under the minimum and 0.22 % under the curve at that split. (4) The plant's path down the gentle side through the case's moves from 0.42 to 0.36 at 3 h and 0.32 at 6 h. (5) The readout, with the analyzer's o-xylene on the prefractionator's top stage at 1.37 mol %.

Table 8.3 The Valley Against an Independent Solver and the Shortcut Bounds

Quantity	Application	Check
minimum split β^*	0.314	0.3139
minimum boilup (kmol/h)	649.28	649.26
boilup at 0.28, 0.40 (kmol/h)	788.5, 763.9	788.50, 763.89
largest difference on 20 splits (kmol/h)	—	0.01
RGA diagonal at the design	12.7, 0.44, 24.9	12.68, 0.44, 24.86
Underwood, Petlyuk V_{min} (kmol/h)	—	359.2
Underwood, $\rho = 0.5$ fixed (kmol/h, β)	—	391.8, 0.231
Fenske N_{min} against 14 stages	—	11.1, 11.6
vapor split for equal pressure drops	0.5	0.502

✦ DID YOU KNOW? Thirty Percent, If the Column Is Run Right

Studies of the three-product column report typical savings of about 30 percent in both energy and capital cost against two columns in series [16]. A four-product column with two side draws can save up to 40 percent of the energy, a saving that is lost when the column runs away from its optimum vapor split [18].

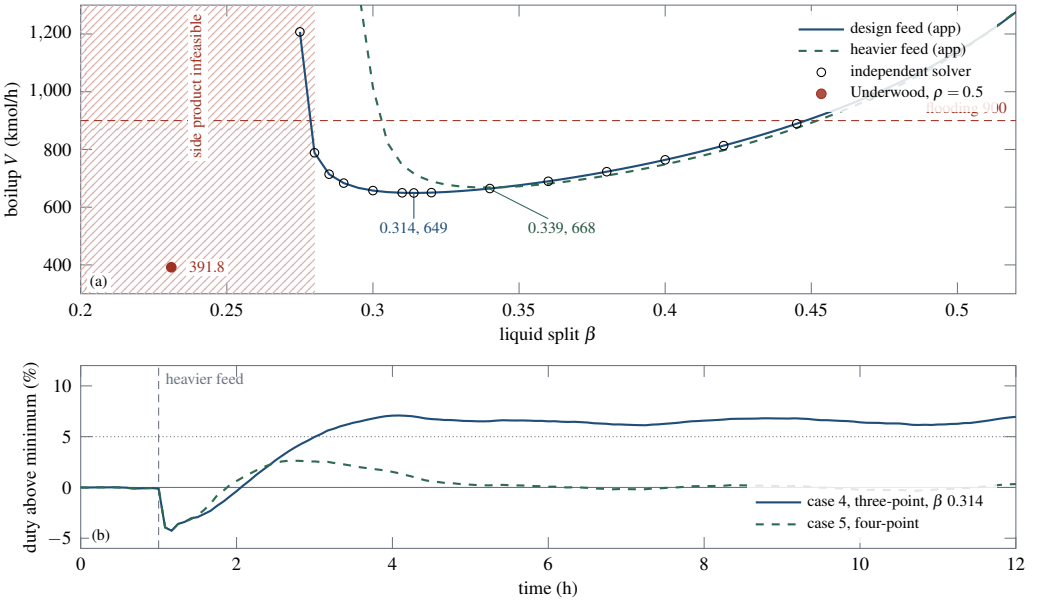


Figure 8.3 The valley and what the four-point loop does with it. (a) Boilup against the liquid split at the setpoints from the application at the design feed (solid) and at the heavier feed (dashed), the independent solver's points on the design curve (open circles), and the Underwood minimum with the vapor split fixed at 0.5 (filled dot). The hatched zone is the design feed's, and the flooding rate is the thin dashed line. (b) The duty against the valley's minimum in cases 4 (solid) and 5 (dashed) as shipped, every logged row, with the feed made heavier at 1 h.

8.4.3 Why One Side Is Steep

However hard the reboiler boils, each side of the wall has a ceiling on its liquid-to-vapor ratio set by the two splits, as shown in Equation (8.7).

$$\begin{aligned} \left(\frac{L}{V}\right)_{P,\text{above feed}} &= \frac{\beta L}{\rho V} < \frac{\beta}{\rho} \\ \left(\frac{L}{V}\right)_{M,\text{below draw}} &= \frac{(1-\beta)L - S}{(1-\rho)V} < \frac{1-\beta}{1-\rho} \end{aligned} \tag{8.7}$$

because $L < V$ whenever a distillate is drawn. The prefractionator needs a ratio of about 0.5 above the feed to wash the o-xylene down, 0.53 at the minimum against a ceiling of 0.63 and 0.49 at a split of 0.28 against 0.56. As the split falls the ceiling closes on the need, and the boilup climbs steeply, 788.5 kmol/h at 0.28, 1207 at 0.275, and about five times the flooding rate (4543 kmol/h) at 0.25. The main side below the draw needs 0.65 to 0.85, and its ceiling comes down to that only near a split of 0.675 (the boilup is 98 029 kmol/h at 0.674, and no steady state exists at 0.6765), so the high side rises gently over a far wider range. Below the minimum the o-xylene on the prefractionator's top stage rises, from 1.57 to 3.77 and 4.56 mol % at 0.28 and 0.275, and that o-xylene can leave only with the toluene. The asymmetry is in the stage balances, not in a correlation. The vapor split of 0.5 agrees with a wall on the centerline. With 12 trays on each side and equal pressure drops, taking a tray's drop as 40 % dry and the liquid head's crest share as 40 %, the two sides' weir-crest loads at the design are 550 and 567 (3 % apart) and equal drops need $\rho = 0.502$, between 0.488 and 0.515 across every split that runs below flooding.

🕮 **Pause.** Try Exercise 8.2 before reading on.

8.5 Loops as Implemented

8.5.1 Pairing and the Shared PI Law

The three-point structure pairs the reflux with the benzene in the distillate, the side draw with the toluene in the side draw and the boilup with the o-xylene in the bottoms, while the drum level moves the distillate and the base level the bottoms. At the design the relative gain array [2] of reflux, side draw and boilup against the three purities, each gain taken with the other two handles held and the levels closing the balance, has the diagonal 12.7, 0.44 and 24.9 and off-diagonal elements down to −24.4. Of the six pairings two have every element positive, the one in force and the swap of reflux and side draw, whose element of 0.006 for the side draw on the benzene rules it out. On the distillate and the bottoms the gain of the reflux alone is 476 and 124 times the gain of reflux and boilup moved together, the ill-conditioning of high-purity distillation [3]. All loops use the framework's velocity-form PID of Section 1.6.2, here without derivative action. In the loops' own symbols it reads as Equation (8.8).

$$\begin{aligned} e_k &= \sigma\,(r_k - y_k), \qquad s_k = s_{k-1} + K_c\,(e_k - e_{k-1}) \\ \hat{u}_k &= u_{b,k} + s_k + I_{k-1} \\ u_k &= \min(u_{max}, \max(u_{min}, \hat{u}_k)) \\ I_k &= I_{k-1} + \left[\frac{K_c}{\tau_I} e_k + \frac{u_k - \hat{u}_k}{\tau_I}\right]\Delta t_k \end{aligned} \tag{8.8}$$

where r_k is the setpoint, y_k the measurement, $u_{b,k}$ the feedforward term (zero when it is off, the starting flow being carried in the integral), and s_k, $\hat{u}_k$ and σ are the S_k, v_k and action a of Equations (1.14) to (1.17), with the tracking time equal to τ_I. The limit acts on the output only, and the integral alone carries the anti-windup. The action is $\sigma = +1$, reverse acting in Chapter 1's convention, for the reflux and boilup loops, and -1, direct acting, for the side draw (more draw, dirtier toluene), the levels and the split loop. Integral action is switched off once the integral time reaches 600 min. The levels move 10 kmol/h per percent with $\tau_I = 20$ min. On tray temperatures the purity loops move 50, 20 and 30 kmol/h per mol % with integral times of 10, 20 and 10 min and execute every 0.1 min. On the analyzers they run at 2, 1 and 2 with 60, 120 and 60 min and execute on each report with Δt_k the time since the last. Each measurement brings its own tuning, because on the analyzers the temperature gains run the side draw to zero 1.52 h into case 7. The boilup's upper limit is $V_{cap} = \min(V_{flood}, V_{steam})$, and the valve ranges of Table 8.1 limit the rest. Switching structure or mode is bumpless because every idle controller tracks its flow.

8.5.2 Tray Temperatures With an Analyzer Trim

By default each purity loop reads one tray temperature converted by a straight line fitted on the steady-state model at the design point, corrected by each analyzer report, as shown in Equation (8.9). The update is the laboratory bias update of Equation (1.11) with a first-order filter on the bias.

$$\begin{aligned} \hat{x} &= x_0 + m\,(T_k - T_{k,0}) + b_f, \qquad \tau_b \frac{\mathrm{d}b_f}{\mathrm{d}t} = b - b_f \\ b &\leftarrow b + \lambda_b \left(x_{an} - (x_0 + m(T_k - T_{k,0}))\big|_{t_{sample}} - b\right) \end{aligned} \tag{8.9}$$

where the slope m is −0.139, −0.750 and +0.118 mol %/K on top-section stage 6, main-side stage 10 and bottom-section stage 3, $\lambda_b = 0.5$ on the shared bias updater, which clamps the bias to ±3 mol %, $\tau_b = 5$ min, and the report is compared with the inferential's value when its sample was drawn. The bias starts lined out. Each loop can instead read its analyzer alone or the uncorrected temperature, which case 7 compares. Volume 12, Chapter 4 shows how a tray temperature that stands in for a product purity also answers to pressure, and Volume 5, Chapter 3 what an analyzer's delay does to a composition loop.

8.5.3 The Split Loop, the Feedforward and the MPC

The four-point structure adds the split on x_P, the o-xylene on the prefractionator's top stage read by its analyzer, at 0.015 per mol % with $\tau_I = 40$ min. More liquid on the feed side washes the o-xylene down [4], so the split must rise when x_P rises. The loop is direct acting ($\sigma = -1$) in Chapter 1's convention. Its setpoint, 1.57 mol %, is the value at the design valley's minimum. In the steady-state model, holding x_P there keeps the boilup within 0.31 % of each feed's minimum for six feed changes, while the best prefractionator tray temperature held the same way costs from 29.2 to 219 % when the benzene or the o-xylene changes, and a split fixed at 0.314 costs up to 13.97 %. In the language of self-optimizing control [1], x_P is a variable whose constant setpoint keeps the loss small. Volume 9, Chapter 8 meets an optimum that moves with the weather and follows it with a supervisory search instead. The temperature remains an Advanced option. The feed-rate feedforward adds $K(F_m - F_{ref})$ to the reflux, side draw and boilup loops' bias, with $K = 1.669$, 0.333 and 2.004 (the flows per unit of feed at the specifications and a split of 0.305) and F_{ref} the measured feed when it is switched on or the run starts.

The MPC runs every 5 min over a 5 h horizon of 60 steps on the apps' shared linear MPC module (Section 1.6.3) and moves L, S, V and β together. Its outputs are the logarithms of the three impurities and of x_P, and its model is the plant's step response at the design point fitted to first order plus dead time per pair, with the measured feed as a disturbance and an output bias held over the horizon. Reflux alone and reflux with boilup are identified apart because the column is ill-conditioned. The objective is given by Equation (8.10).

$$\begin{aligned} \min \; & \sum_{k,i} q_i \,(y_{ik} - r_i)^2 + \sum_i \left(400\, s_i^2 + 40\, s_i\right) \\ & + w_Q\, 10^{-3} \sum_k V_k + \sum_{j,k} \frac{w}{\delta_j^2}\, \Delta u_{jk}^2 \\ \text{s.t. } & y_{ik} \le r_i + s_i, \quad s_i \ge 0 \end{aligned} \tag{8.10}$$

where $q = (0.2, 0.2, 0.2, 2)$, the band applies to the three impurities only, $\delta = (10, 2, 10, 0.01)$ is a typical move of each handle, $w_Q = w = 1$, the moves are capped at 30, 6 and 30 kmol/h and 0.01 per execution, the split stays within 0.15 and 0.70, and a failed solve hands the handles back to the PI loops. On case 5 it solves 96 times with no fallback.

8.5.4 Annunciators and Model Separation

FLOODING marks the boilup request at V_{flood}, STEAM LIMIT at a lower steam supply, OFF SPEC a true purity below its specification, and SIDE PRODUCT INFEASIBLE a split below the lowest one at which the valley has a point under flooding. None of them trips the column. The flooding rate and the specifications are teaching values, and on a plant they would come from a tray or packing rating and from the buyer's contract. The application keeps three models apart. The plant is Section 8.3, the valley is its steady state at the setpoints, read only by the display, the infeasibility flag, the challenge's score and the helper that moves the split to the minimum, and the MPC's model is a fixed set of step responses.

8.6 Nine Cases, Measured

Table 8.4 names the nine cases. The figures in this section were taken headless at the default seed, advancing the engine one physics step at a time exactly as the page does (Section 1.6.1), each case opened the way the page opens it and each move of the learner applied at the time the text gives. Table 8.5 collects the scorecard tiles at the instants the cases are read. A case gives the same run whether it is opened first, picked after another case or restarted with Reset. At the fastest speed of 300 min per second a 12 h case plays in 2.4 s. The exported CSV file carries the structure and measurement in force, every setpoint, purity reading and handle, the split, the prefractionator's

Table 8.4 The Nine Cases

#	Settings and events	Teaching point
1	three-point, split 0.40, learner moves it to 0.34, 0.30, 0.28	the spare handle
2	split 0.42, to 0.36 at 3 h, 0.32 at 6 h, learner 0.29 at 9 h	the curve against the plant
3	purity loops in Manual, bottoms loop, then two loops	interaction, RGA
4	three-point at 0.314, heavier feed at 1 h	the valley moves
5	four-point, the same feed, then the MPC	a loop that holds it
6	four-point, steam 740 kmol/h, feed +20 % at 1 h	a reboiler limit
7	tray temperatures only, heavier feed at 1 h	inferential offset
8	split 0.25, side draw and boilup on stations	infeasible side product
9	challenge, 12 h, three-point at 0.40	the whole problem

Table 8.5 Scorecard Tiles, Purities and Split at the Instants Each Case Is Read

Case	Settings and instant	Duty (MW)	Against minimum (%)	Split, β^*	x_D / x_S / x_B (mol %)	Also
1	as shipped, 1 h	6.86	+17.5	0.400, 0.314	99.20 / 98.18 / 99.21	
1	split 0.34 at 1 h, 4 h	5.98	+2.6	0.340, 0.314	99.22 / 98.18 / 99.23	toluene low 98.11
1	split 0.30 at 4 h, 7 h	5.86	+0.5	0.300, 0.314	99.19 / 98.18 / 99.19	toluene low 97.95
1	split 0.28 at 7 h, 12 h	6.86	+17.5	0.280, 0.314	99.14 / 98.22 / 99.10	3.2 % under the curve
2	as shipped, 9 h	5.83	−0.1	0.320, 0.314	99.20 / 98.18 / 99.20	−0.22 % against the curve
4	as shipped, 5 h	6.39	+6.5	0.314, 0.339	99.21 / 98.18 / 99.22	x_P 3.22
4	as shipped, 8 h	6.40	+6.6	0.314, 0.339	99.19 / 98.20 / 99.18	
5	as shipped, 8 h	6.01	+0.1	0.345, 0.339	99.19 / 98.21 / 99.19	x_P 1.59
5	MPC, 8 h	6.05	+0.7	0.345, 0.339	99.15 / 98.24 / 99.20	benzene low 98.12
6	as shipped, 3 h	6.65	−5.0	0.312, 0.314	99.19 / 98.26 / 98.62	STEAM LIMIT from 95 min
6	setpoints 99.05 / 98.05 / 99.05 at 3 h, 7 h	6.57	−0.3	0.312, 0.307	99.04 / 98.02 / 99.06	boilup 731
7	as shipped, 3 h	5.82	−3.1	0.314, 0.339	99.36 / 98.01 / 99.02	loops read 99.20 / 98.17 / 99.21
8	as shipped, 2 h	5.86	+0.5	0.250, 0.314	99.21 / 97.31 / 98.09	x_P 6.38, INFEASIBLE

analyzer and temperature, the duty and the valley's minimum, the status flags, the disturbances, parameters and tunings. The true compositions and the balances sit in columns marked as truth, apart from the measurements a controller may use.

8.6.1 Walking the Valley

Case 1 starts at a split of 0.40 with the purities on their setpoints and the duty 6.86 MW, 17.5 % above the minimum. Moved to 0.34 at 1 h, the duty is 5.98 MW at 4 h, and moved to 0.30 it is 5.86 MW at 7 h. Moved to 0.28 it climbs, 5.95, 6.37, 6.62 and 6.72 MW at 8, 9, 10 and 11 h, toward the curve's 7.08 MW, and it is still 3.2 % under the curve at 12 h. On the curve the three moves are worth −0.89, −0.06 and +1.17 MW, so the smallest move changes the duty most. After each of the first two moves the duty is within 1 % of the curve for good after 2.31 and 2.35 h. Each move down dips the toluene first, to 98.11 mol % 83 minutes after the move to 0.34 and to 97.95 mol % half an hour after the move to 0.30, while the side loop catches up. In case 2 the learner's move to 0.29 at 9 h leaves the plant at 6.11 MW against the curve's 6.14 at 12 h, and within 1 % of the curve from 11.76 h.

> **TRY IT IN THE APP** **1 · The Fourth Handle: Move the Liquid Split**
>
> Load scenario 1 and press Run. At 1 h the three purities sit on their setpoints and the reboiler duty reads 6.86 MW, 17.5 % above the valley's minimum. Type 0.34 into the Liquid split box and run on. By 4 h the duty is 5.98 MW, while the purities have hardly moved.

8.6.2 Three Loops That Fight

Case 3 starts with the purity loops in Manual. With only the bottoms loop closed, its setpoint raised from 99.2 to 99.4 mol % reaches 99.35 mol % 9 min later on 0.4 kmol/h more boilup. The extra vapor leaves as distillate and takes toluene with it, so the benzene falls below 99.0 mol % 12 min after the move and stands at 98.86 mol % at 6 h. With the distillate loop closed as well, after Reset, the same move takes 75 min, 8.3 times as long, and by 8 h reflux and boilup have both risen about 45 kmol/h (the duty 6.24 MW). The relative gain of 24.9 for the boilup on the bottoms says the same thing, because with the other loops closed the boilup moves the bottoms about 25 times less than it does alone.

8.6.3 A Valley That Moves

Case 4 makes the feed heavier at 1 h. The distillate falls to 74.3 kmol/h and the bottoms rises to 125.2 kmol/h by 1.5 h as the levels pass the change through, and the toluene dips to 97.99 mol % and the o-xylene to 98.95 mol % before the loops recover them. The split stays at 0.314, now on the steep side of the new curve, and the duty is 6.39 MW at 5 h, 6.5 % above the new minimum, and 6.6 % above at 8 h, with x_P at 3.22 mol % from 1.57, as shown in Figure 8.3b. The helper that moves the split to the computed minimum, pressed at 5 h, takes it to 0.339, and by 10 h the duty is 5.97 MW. The helper uses the model and the true feed. Chapter 11 shows where an optimizer stops when its model is not exact. Case 5 repeats the feed change on the four-point structure. Without being told where the minimum went, the split loop takes the split to 0.345 by 8 h, a little on the gentle side of 0.339, the duty is 6.01 MW, 0.1 % above the minimum, and x_P is back at 1.59 mol %. The toluene dips to 97.98 mol % and the o-xylene to 98.86 mol % on the way.

The MPC on the same case also reaches the valley, with the split at 0.350 at 5 h, 0.345 and 0.7 % above the minimum at 8 h, but lets the benzene fall to 98.12 mol % and the toluene to 97.31 mol %, where the four-point PI loops hold the benzene above 99.08 mol %. It corrects an unmeasured feed change only through its output bias, and its first-order fits, with lags up to 290 min, describe responses that have two time scales.

> **TRY IT IN THE APP** **5 · Four-Point Structure: A Loop on the Prefractionator**
>
> Load scenario 5 and press Run. At 1 h the feed turns heavier. Watch the split on the Valley view: the loop, which has no model of the valley, takes it to 0.345 by 8 h, against the new minimum at 0.339, and the duty ends 0.1 % above it. Then choose MPC, press Reset and run again. It reaches the valley too, but the benzene falls to 98.12 mol %.

8.6.4 A Reboiler Limit and Inferential Measurement

Case 6 caps the steam at 740 kmol/h of boilup and raises the feed to 360 kmol/h at 1 h, where the valley's minimum at the setpoints is 779 kmol/h. STEAM LIMIT comes on at 95 min and the bottoms loop loses its handle, the o-xylene falling to 98.62 mol % by 3 h while the benzene and toluene hold. Lowering the setpoints to 99.05, 98.05 and 99.05 mol % lowers the minimum to 734 kmol/h, and by 7 h the boilup is 731 kmol/h with all three products on specification. Case 7 runs the loops on tray temperatures alone through the heavier feed. At 3 h the loops read 99.20, 98.17 and 99.21 mol % while the true purities are 99.36, 98.01 and 99.02 mol %, because the calibration made at the design feed misreads the heavier one. With the analyzer bias switched on at 3 h, the true purities are 99.17, 98.20 and 99.16 mol % by 5 h. On the analyzers alone, with their own tuning, the benzene falls to 86.0 mol % and the toluene to 81.2 mol % before the reports arrive.

Table 8.6 The Challenge Over 12 h, Default Seed

Settings	Low x_D (mol %)	Low x_S (mol %)	Low x_B (mol %)	Worst hour (%)	Verdict
three-point, 0.40 (shipped)	98.63	98.15	98.13	+12.4	fails
four-point and feedforward	99.11	98.07	99.07	+0.3	passes
four-point alone	98.61	98.15	98.07	+3.6	fails
feedforward alone	99.09	98.03	99.02	+12.4	fails
three-point, 0.339, feedforward	99.11	98.08	99.07	+0.0	passes
MPC	98.29	98.15	99.15	+16.7	fails

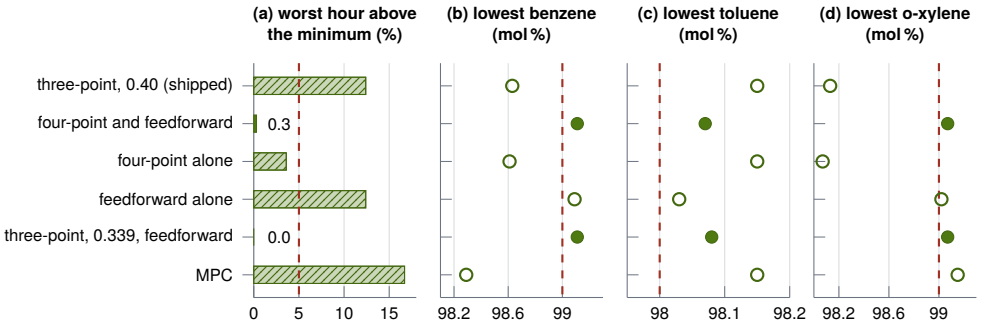


Figure 8.4 The challenge of Table 8.6 as a chart. (a) The worst judged hour against the valley's minimum, with the 5 % pass line dashed. (b) to (d) The lowest sample of each purity, with its specification dashed. Dark bars and filled dots are settings that pass, hatched bars and open dots settings that fail. Notice that the four-point structure alone holds the energy but lets the benzene and the o-xylene fall below their specifications, that the feedforward alone holds the purities but not the energy, and that only the settings with both a split on the minimum and the feedforward pass on every count.

🕮 **Pause.** Try Exercise 8.3 before reading on.

8.6.5 A Split That Cannot Be Fixed With Steam

Case 8 starts at a split of 0.25, where the curve has no point under flooding. With the side draw at 100 kmol/h and the boilup raised by hand, the side product holds 97.32 mol % toluene at the starting boilup, 97.31 at 750 kmol/h, 97.30 at 850 and 97.31 at 900 (flooding), while x_P reaches 7.2 mol %. The steady-state sweep at that split, with the benzene held, gives 97.32 to 97.34 mol % at every boilup from 650 to 900 kmol/h. Moved to 0.31, the side product reaches 98.83 mol % 2 h later. In Auto at that split, the side loop runs the draw to zero.

8.6.6 The Challenge

The challenge runs 12 h on the three-point structure at a split of 0.40. The feed turns heavier over 30 min from 2 h and rises 20 % over 30 min from 7 h. It passes when, from 2 h, every 10 min sample of the true purities is at or above 99 mol %, 98 mol % and 99 mol %, and when each of the six whole hours that start 2 h after a feed change has a mean duty within 5 % of the valley's minimum at the feed and setpoints in force. The changes arrive as ramps, the way a tank blend or a rate move arrives, although measured as steps the suggested settings also pass, with the toluene at 98.02 mol %. Table 8.6 lists the settings tried, and Figure 8.4 draws them as a chart. As shipped, the first judged hour is 12.4 % above the minimum, and the rate change drops the o-xylene to 98.13 mol %. The four-point structure fixes the energy and the feedforward fixes the rate change, and neither alone passes. Typing the new minimum, 0.339, on the three-point structure with the feedforward also passes, but only because the day's feed is known in advance.

The suggested settings pass at all 32 seeds from 0 to 31, with the lowest toluene between 98.040 and 98.107 mol % (mean 98.070, standard deviation 0.015). At the default seed and seeds 0 to 3 the lowest toluene sample falls between 7.33 and 7.5 h, in the half hour after the rate change starts. Halving the step leaves it at 98.073 mol %. The shipped settings fail at all 32. The toluene margin is thin, but it is set by the rate change and not by the noise.

DID YOU KNOW? Two Fixes That Fail Alone

From the simulator: on the twelve-hour challenge the four-point structure alone fails, with a worst hour 3.6 % above the minimum and the o-xylene down to 98.07 mol %, and the feedforward alone fails at 12.4 %. Together they pass at 0.3 %, while the MPC fails at 16.7 % (Table 8.6).

The MPC fails for its model's structure, not for a code defect. At the default seed and seeds 0 to 3, the benzene falls to between 98.27 and 98.33 mol % after the feed change and the worst hour is 15.8 to 17.0 % above the minimum. Its hourly excess falls from 16.7 through 14.5, 12.8, 10.6 and 8.0 to 4.5 %. The split is not the cause, since at 5 h it sits at 0.354 against the minimum's 0.339. The purities are, with the toluene at 98.61 mol % and the o-xylene at 99.33 mol % above their setpoints while the benzene, at 98.93 mol %, is still under its own. The slow directions of its step-response model take hours to bring all three back.

The side draw carries a visible fuzz, 0.58 to 0.78 kmol/h root mean square from one logged row to the next on lined-out stretches of cases 1, 2 and 4. It is the side loop answering thermowell noise. The loop's gain through the calibration is 15 kmol/h per kelvin, and 0.05 K of noise gives 0.75 kmol/h, against a measured standard deviation of the request of 0.82 kmol/h. The fuzz vanishes with every random draw set to zero and does not change when the step is halved.

8.7 Technology in Practice

What Measures It

Figure 8.5 draws the loops of Section 8.5 with their devices. Each purity loop reads a tray temperature, and an analyzer above it corrects the conversion. Monitoring and controlling distillation columns is a very common use of process chromatographs, which quantify the purity of the separated products [19], and the chapter's four analyzers, sampling every 10 min and reporting a cycle later, stand for such instruments. The tray temperatures come from thermocouples or resistance thermometers in thermowells, and nearby elements on a column can read differently where the flow patterns differ [19].

TECHNOLOGY Sensor: A Resistance Thermometer in a Tray Thermowell

A resistance temperature detector is a winding of pure metal wire, usually platinum, whose resistance rises with temperature. It is relatively insensitive but very linear [19]. Platinum elements cover about -200 to 800 °C and are chosen for their accuracy and precision [20]. On a column the element sits in a thermowell, so that it can be replaced without depressurizing, and the well adds a first-order lag. An air gap at the bottom of the well adds a second lag that can push a loop toward oscillation, and transmitters close together on a column can disagree where the flow patterns differ [19]. On a trend a badly seated element shows as a reading that trails its neighbors. The model's thermowells are a 0.5 min lag with 0.05 K of noise.

What Moves It

The reflux, the side draw, the distillate and the bottoms are liquid flows, and the boilup is set by the steam to the reboiler. In the model each manipulated flow follows its setpoint through a first-order lag, 0.2 min for the liquid flows and 1 min for the reboiler, which stands for a flow loop around a valve. The fourth handle is the liquid split above the wall, the one final element a conventional column does not have, and the model keeps the vapor split at its foot fixed at $\rho = 0.5$.

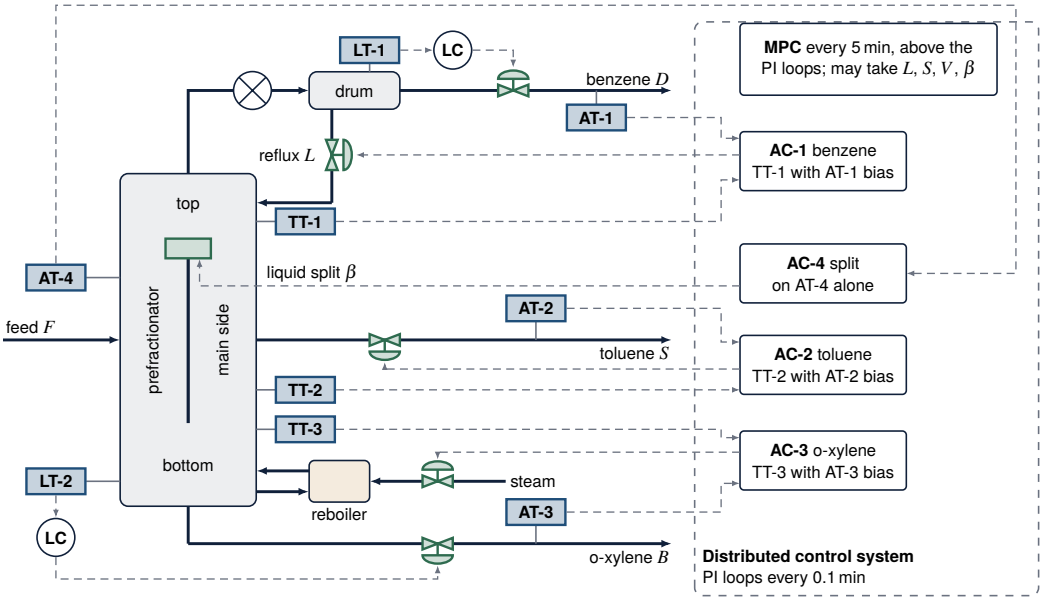


Figure 8.5 The loops of the dividing-wall column with their hardware. Lettered boxes are sensing devices: a tray temperature (TT) and a product analyzer (AT) behind each purity loop, the analyzer on the prefractionator's top stage (AT-4) and the two level transmitters, whose level controllers (LC) are drawn beside their vessels. Valve symbols and the splitter are final elements, and dashed arrows are signals. Notice that each purity loop reads its tray temperature through the analyzer's bias update, that the split loop alone reads an analyzer directly, and that the splitter above the wall is the one handle a conventional column lacks. The feed-rate feedforward and the flow loops are left out. Not to scale, and not a piping diagram.

TECHNOLOGY **Final Element: The Liquid Splitter Above the Wall**

The liquid split is made outside the shell. All the liquid leaving the trays above the wall can be drawn into an external accumulator and returned to the two sides under flow control [16], and controlling one of the two streams is enough, because tray overflow regulates itself [10]. A laboratory column split its reflux with a swinging funnel driven by solenoids, an on-off device that a PI controller set through pulse-width modulation [18]. A return valve with excess stem friction moves in jerks and ignores small reversals [19], so on a trend the split moves in steps. The vapor split is fixed by the wall, since vapor in an open column cannot be throttled like flow in a pipe [10]. The model's splitter follows its setpoint through a 0.5 min lag between 0.15 and 0.70.

Where the Controller Runs

A distributed control system runs nested and cascaded loops under a supervisory level, with cycle times from milliseconds to minutes [21]. The app executes its temperature loops every 0.1 min, its analyzer loops on each report and its predictive controller every 5 min, inside that range. The PI loops, the bias update and the feedforward sum belong to the regulatory layer, and the predictive controller to the layer above it, which takes the four handles when it runs. Industrial predictive controllers skip the bias update of an output whose analyzer has not reported, and they must cope with ill-conditioning such as that of adjacent tray temperatures in a column, where small errors call for large moves [15]. Section 8.5 measures the same property with the relative gain array.

IN PRACTICE **Temperature Control and Purity Give-Away**

Columns are widely controlled on a tray temperature instead of a product analyzer, because chromatographs and similar analyzers carry large delays and high costs. The practice assumes the product is on specification while the temperature is held, which is hard to keep when the feed composition or rate changes in a multicomponent column, and pressure moves the temperatures too [22]. Plants also tend to purify beyond need. Energy guidance asks for steam use to be compared with reflux and purity daily, and the reflux lowered in small steps until the purity is just met, which lowers the reboiler duty [23]. In this chapter the 0.2 mol % margins over the specifications cost 8.0 % of the duty.

What Is Modernizing It

Three developments bear on this column. A vapor split valve on a laboratory column has been shown to work as a handle under closed-loop temperature control, with feedback correcting the valve's inaccuracy [18]. It would add the fifth handle that the model keeps fixed. Soft sensors, which estimate a composition from several measurements, have distillation as their main target, and keeping their models up to date is the most critical issue that engineers report [22]. Such a sensor would replace the single-temperature lines of Equation (8.9), which case 7 shows misreading a heavier feed. And multivariable predictive control, with a solid foundation in refining and petrochemicals [15], has been suggested for this column in a nonlinear form built on a physical model [24], where the chapter's predictive controller uses one fixed linear model.

8.8 Limitations

Every size and setting is a generic teaching value. Constant molar overflow, constant relative volatility and one latent heat stand for the thermodynamics, and the o-xylene volatility of 0.44 is 19 to 42 % above the measured vapor-pressure data, so the toluene and o-xylene split here is easier than on a real column and the valley's position would move on a rigorous model. The stages are ideal, the pressure is uniform, and the vapor split is fixed at 0.5, while a real wall's vapor split moves with the liquid loads. Flooding is a ceiling on the boilup, and the column has no hydraulic limit of its own.

The four-point loop's setpoint is the value at the design minimum, which commissioning would have to find by stepping the split. The feedforward's gains are the flows per unit of feed at the specifications rather than at the setpoints, which moves the challenge's lowest toluene by 0.006 mol %. The MPC has a fixed model identified at one point and an output-bias disturbance model, and an industrial MPC would be identified on the plant and would often sit above temperature loops. When the reflux stops, the side draw is capped at the liquid on its stage while the side flow meter still reports the request, a state no shipped case reaches. The disturbances arrive as steps and ramps. A feed that turns heavier in one step would not happen on a real column, but it separates the valley's movement from the loops' response.

OPEN CHALLENGE **Holding the Valley With a Fixed Vapor Split**

The window of minimum energy is narrow and moves with the feed composition and the feed's vapor fraction [18]. With the vapor split fixed, as it normally is, the two ends of the prefractionator cannot both be controlled, and for some disturbances the column must use more than its minimum energy. Industry prefers decentralized PI loops with selectors where they work, but tuning them can be difficult, and a linear predictive controller would need models from several operating regions, so nonlinear predictive control on a physical model may be the better route [24]. Progress would be a vapor split that can be moved reliably on a full-scale column, with controllers that hold the minimum across feeds.

8.9 Conclusion

This chapter modeled a benzene, toluene and o-xylene dividing-wall column on four coupled stage stacks whose balances close to 8.7×10^{-10} of the feed, with the energy valley computed from the same equations and drawn under the running plant. With the three purities held, the liquid split

moves only the duty, from 5.83 MW at 0.314 to 17.7 % more at 0.40 and 21.4 % more at 0.28, and an independent solver puts the minimum at 0.3139 and 649.26 kmol/h. The Underwood minimum with the vapor split fixed at 0.5 is 391.8 kmol/h, and the column needs 1.66 times that because its 14 stages per split sit close to the Fenske minimum. The steep side is the prefractionator reaching its ceiling on liquid-to-vapor ratio. A heavier feed moves the minimum to 0.339 and leaves a fixed split 6.6 % above it, while the split loop on the prefractionator's o-xylene ends 0.1 % above. With the feedforward the four-point structure passes the challenge at 32 of 32 seeds, and the MPC fails it with the benzene at 98.29 mol %. The volatilities are teaching values and the hydraulics a ceiling. A fuller model would add rigorous thermodynamics, a vapor split that follows the pressure drops, temperature-based split control with a differential measurement, and an MPC whose model includes an input disturbance. The app shows that a column holding every specification can still be burning 17.7 % more steam than it needs.

KEY POINTS

- A dividing-wall column makes three products in one shell, and with the purities held its fourth handle, the liquid split, moves only the energy.
- At the design feed the duty is 5.83 MW at a split of 0.314, 17.7 % more at 0.40 and 21.4 % more at 0.28. The steep side is the prefractionator's ceiling on liquid-to-vapor ratio.
- A heavier feed moves the minimum to 0.339 and leaves a fixed split 6.6 % above it, while the split loop on the prefractionator ends 0.1 % above.
- With the feedforward the four-point structure passes the challenge at 32 of 32 seeds, and the MPC fails it.

Where else this applies. Volume 9, Chapter 8 meets an optimum that moves with a disturbance, and Chapter 11 shows where an optimizer stops when its model is not exact.

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8.10 Exercises

8.1 ○ Concept check · 2 min

In scenario 1 the three purity loops hold 99.2, 98.2 and 99.2 mol % while the liquid split is moved from 0.40 to 0.34. The distillate, side draw and bottoms stay near 100 kmol/h each, but the reboiler duty falls from 6.86 to 5.98 MW. Why can the split change the duty but not the product flows?

(a) The level loops hold the distillate and bottoms at fixed flows, so only the boilup is left free

(b) The vapor split at the wall follows the liquid split, so each side of the wall keeps its own flows

(c) With the feed and three purities fixed, the balances fix the products, so the split only moves internal flows

(d) The duty belongs to the bottoms loop alone, and the liquid split does not reach the boilup

8.2 ○ Concept check · 1 min

Below the valley's minimum the duty climbs steeply, and at a split of 0.25 no boilup up to flooding makes the side product. What makes that side steep?

(a) The main side runs short of liquid, so benzene reaches the side draw

(b) The boilup reaches flooding, so the bottoms loop loses its handle

(c) The side loop closes the draw, so the toluene backs up into the bottoms

(d) The prefractionator's ratio L/V cannot exceed β/ρ, so o-xylene climbs over the wall

8.3 Concept check · 2 min

In scenario 7 the purity loops read tray temperatures converted by straight lines fitted at the design feed. At 3 h, two hours after the feed turns heavier, the loops read 99.20, 98.17 and 99.21 mol % while the true purities are 99.36, 98.01 and 99.02 mol %. What causes the gap?

(a) A tray temperature depends on the whole composition, and the calibration fitted at the design feed misreads the heavier one

(b) The thermowells lag the trays, so the loops still read the compositions from before the feed change

(c) The analyzer bias update has reached its clamp and pushes each reading off by the same amount

(d) The loops run without integral action, so each settles with a proportional offset

8.4 Theory and calculation · 8 min

Use Equation (8.6) with $\alpha = (2.4,\ 1,\ 0.44)$, $z_j = 1/3$ each, $F = 300\,\mathrm{kmol/h}$ and a saturated-liquid feed ($q = 1$).

(a) Check that $\theta_1 = 1.4667$ and $\theta_2 = 0.5625$ are roots, and compute the minimum vapor of the benzene and toluene split (θ_1, benzene in the distillate) and of the toluene and o-xylene split (θ_2, benzene and toluene in the distillate). Give four significant figures. *Checkpoint:* 257.1 kmol/h and 359.2 kmol/h.

(b) In the direct sequence the second column receives 200 kmol/h of equimolar toluene and o-xylene. Find its root and minimum vapor, the direct sequence's total, and the saving of the thermally coupled column, whose minimum is the larger of the two values in part (a). *Checkpoint:* $\theta = 0.6111$, 257.1 kmol/h; 514.3 kmol/h; 30.2 %.

(c) The wall fixes $\rho = 0.5$, and the prefractionator reaches its preferred split only with 195.9 kmol/h of vapor. Compute the fixed-wall minimum boilup, its duty at 0.008 984 MW per kmol/h, and the ratio of the app's 649.3 kmol/h to it. *Checkpoint:* 391.8 kmol/h, 3.52 MW; 1.66.

8.5 Theory and calculation · 6 min

The latent heat is $\lambda = R\Lambda$ with $\Lambda = 3890\,\mathrm{K}$ and $R = 8.314 \times 10^{-3}\,\mathrm{kJ/(mol\,K)}$. On the design valley the boilup is 649.3 kmol/h at the minimum ($\beta^* = 0.314$), 763.9 kmol/h at 0.40 and 788.5 kmol/h at 0.28, and $\rho = 0.5$.

(a) Compute λ, the duty of 1 kmol/h of boilup in MW, the duty at the three splits, and how far the two outer points lie above the minimum. *Checkpoint:* 32.34 kJ/mol, 0.008 984 MW; 5.83, 6.86 and 7.08 MW; 17.7 % and 21.4 %.

(b) Compute the prefractionator's ceiling β/ρ at splits of 0.314, 0.28 and 0.25. It needs a ratio of 0.53 above the feed at the minimum and 0.49 at 0.28. Say what the ceiling at 0.25 means for scenario 8. *Checkpoint:* 0.628, 0.56, 0.50.

(c) The main side below the draw needs a ratio of 0.65 to 0.85. At what split does its ceiling $(1-\beta)/(1-\rho)$ fall to the lower value? *Checkpoint:* 0.675.

8.6 Theory and calculation · 6 min

The feed-rate feedforward adds $K(F_m - F_{ref})$ to the reflux, side draw and boilup. Its gains are the flows per unit of feed at the specifications and a split of 0.305, where the valley gives $L = 500.6\,\mathrm{kmol/h}$, $S = 100.0\,\mathrm{kmol/h}$ and $V = 601.1\,\mathrm{kmol/h}$ at $F = 300\,\mathrm{kmol/h}$. At the setpoints the minimum is $V = 649.3\,\mathrm{kmol/h}$ with $L = 548.9\,\mathrm{kmol/h}$.

(a) Compute the three gains. *Checkpoint:* 1.669, 0.333, 2.004.

(b) The feed rises from 300 to 360 kmol/h. Compute what the feedforward adds to each flow, and the duty its boilup adds. *Checkpoint:* 100.1, 20.0 and 120.2 kmol/h; 1.08 MW.

(c) With constant molar overflow the steady state at a fixed split and fixed purities scales with the feed. Compute the boilup and reflux the setpoints need at 360 kmol/h, and how much the purity loops must add to what the feedforward supplies. *Checkpoint:* 779.2 and 658.7 kmol/h, about 9.6 kmol/h each (9.7 from the rounded values).

8.7 App challenge · 8 min

Open scenario 1, *The fourth handle: move the liquid split*, at the default seed and the default speed of 60 min per second. Read the *Reboiler duty* and *Duty against the valley* tiles of the scorecard.

(a) Run as shipped (split 0.40) to 1 h and read both tiles. *Checkpoint:* 6.86 MW, +17.5 %.

(b) Reload the scenario, type 0.34 into the *Liquid split* box before Run and run to 4 h. Then reload, type 0.28 before Run and run to 4 h. Read both tiles each time, to within 0.02 MW and 0.2 points. *Checkpoint:* 5.98 MW, +2.5 %; 6.86 MW, +17.5 %.

(c) Run the 0.28 case on to 12 h and read the tiles again. The valley curve gives 7.08 MW at 0.28 and 6.86 MW at 0.40. Explain why 0.28 and 0.40 read the same at 4 h and what the run at 0.28 shows about the two sides of the valley. *Checkpoint:* 7.02 MW, +20.3 %.

8.8 App challenge · 8 min

Run scenario 4, *Three-point structure: a heavier feed*, and then scenario 5, *Four-point structure: a loop on the prefractionator*, each as shipped at the default seed to 8 h. The feed turns heavier at 1 h in both.

(a) For each run read the *Reboiler duty* and *Duty against the valley* tiles, and on the Liquid split card the split and the valley's minimum. *Checkpoint:* Scenario 4: 6.40 MW, +6.6 %, 0.314 and 0.339. Scenario 5: 6.01 MW, +0.1 %, 0.345 and 0.339.

(b) Export the CSV file of each run and read column `truth_xPX_pct`, the true o-xylene on the prefractionator's top stage, in the row at `Time (h)` 8, to within 0.02 mol %. *Checkpoint:* 3.22 mol % and 1.59 mol %.

(c) The split loop's setpoint, 1.57 mol %, is the value at the design feed's minimum. At the heavier feed's minimum, 0.339, the steady-state model puts x_P at 1.80 mol %. Explain where the loop settles and what that costs. *Checkpoint:* A little above 0.339, on the gentle side; about 0.1 % of duty.

8.9 App challenge · 8 min

Open scenario 9, the challenge *twelve hours in the valley*, at the default seed. Each run stops at 12 h, and the verdict gives the lowest sample of each true purity and the worst judged hour of duty against the valley's minimum.

(a) Run as shipped (three-point, split 0.40, feedforward off). Read the verdict and say which half of the target fails. *Checkpoint:* 98.63 / 98.15 / 98.13 mol %, +12.4 %; both halves fail.

(b) Reload, set *Control structure* to Four-point and *Feed-rate feedforward* to On before Run, and run again. *Checkpoint:* 99.11 / 98.07 / 99.07 mol %, +0.3 %; passes.

(c) Reload, keep the three-point structure, set the feedforward On and type the new minimum, 0.339, into the *Liquid split* box before Run. Say what the box shows, read the verdict, and explain why the setting of part (b) is still the one to keep. *Checkpoint:* 0.340; 99.11 / 98.08 / 99.07 mol %, +0.0 %; passes.

8.10 Application area · 3 min

The model's o-xylene volatility relative to toluene is 0.44, while vapor-pressure data give 0.31 to 0.37 between 70 and 110 °C.

(a) Does a real benzene, toluene and o-xylene column find the toluene and o-xylene split easier or harder than the model, and what does that ask of its stages or its boilup? *Checkpoint:* Harder; more stages or more boilup for the same purities.

(b) What would a plant team do before trusting the model's minimum or the four-point setpoint of 1.57 mol %? *Checkpoint:* Find both on the plant by stepping the split.

8.11 Application area · 4 min

At the design feed the setpoints sit 0.2 mol % above the specifications of 99, 98 and 99 mol %, and the valley's minimum is 649.3 kmol/h at the setpoints against 601.1 kmol/h at the specifications.

(a) Compute the cost of the margins as a share of the duty and in MW. *Checkpoint:* 8.0 %, 0.433 MW.

(b) In scenario 6 the steam supports 740 kmol/h of boilup and the feed rises to 360 kmol/h, where the minimum at the setpoints is 779 kmol/h. Lowering the setpoints to 99.05, 98.05 and 99.05 mol % lowers it to 734 kmol/h. What does the operator trade, and what must stay true for the trade to be safe? *Checkpoint:* Margin for throughput; the disturbances must stay inside the smaller margin.

8.12 Review the agent · 5 min

An AI assistant reviews the four-point structure and writes: *"The prefractionator analyzer reports only every 10 min and is costly to maintain. Set* Split loop measurement *to the prefractionator tray temperature at its shipped setpoint, 111.7 °C, the value near the design minimum. A tray temperature answers in a minute and follows the composition, so the split loop will find the valley after a feed change just as well."* Find the flaw, and say how you would check the claim in the app.