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CHAPTER 4

A Propylene Splitter Simulator for Inferential Control and Quality Cascade Audit

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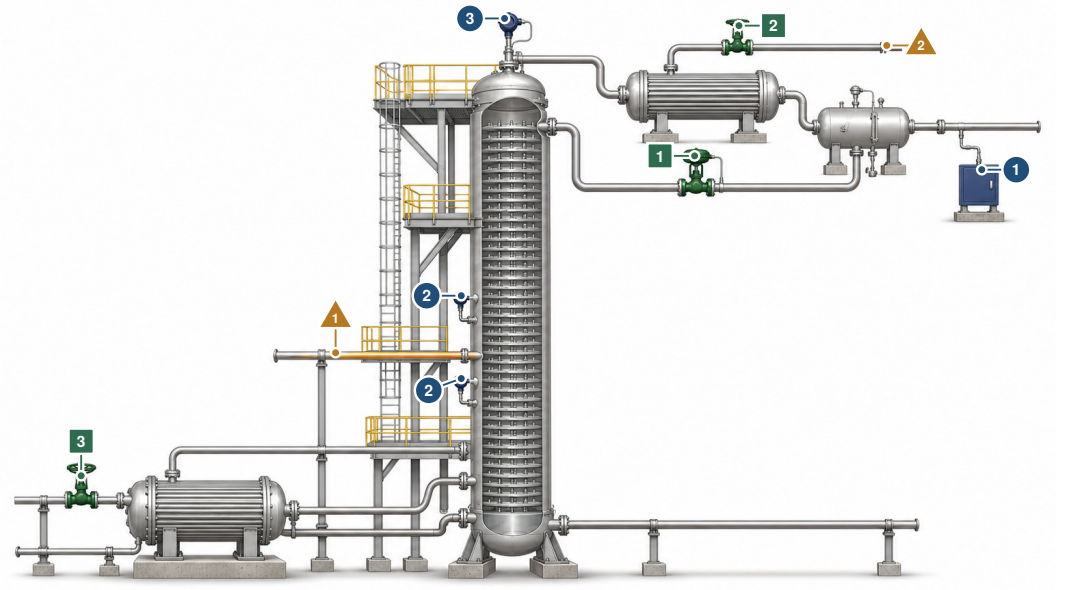
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CHAPTER 4

A Propylene Splitter Simulator for Inferential Control and Quality Cascade Audit



The controller moves 1 reflux valve, set as a ratio to the distillate flow
2 cooling water valve, which holds the overhead pressure
3 steam valve to the reboiler, set by the operator rather than a loop

The controller reads 1 product chromatograph, one result every twenty minutes
2 control and reference tray thermometers 3 overhead pressure transmitter

What disturbs it 1 changes in the feed's propylene content and rate
2 cooling water, cold at night and warm in the afternoon ▲ a chromatograph that freezes on its last result

Notice that the thermometers sit partway down the tower, close to the feed, while the only reading of the product's purity comes from the chromatograph at the far end of its line, every twenty minutes. Illustration, not to scale.

IN PLAIN TERMS A Thermometer Standing In for a Test

The main idea. A tall tower of trays splits propylene, which becomes plastic, from propane, which boils at almost the same point. The tower is so slow that a thermometer part way up stands in for the test of the product, which comes every twenty minutes.

The challenge. The thermometer also feels the pressure, and a tray far from the top sees changes the product never feels. If the test freezes on its last answer, a controller that trusts it does more harm than good.

Why it matters. This tower is often the biggest user of heat on its site, and plastic makers take only very pure propylene.

THREE WAYS TO READ THIS CHAPTER

Explore	12 min	This page, the Did you know? box in Section 4.1, the History boxes in Section 4.2, the Try it boxes in Sections 4.4 and 4.6, the second Did you know? box in Section 4.6.7, and Key points in Section 4.10. No equations.
Study	50 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
Practice	15 min	This page, Section 4.6 with Figure 4.2, Section 4.7, Section 4.8 with its Open challenge box, and the second Open challenge box in Section 4.9.

The control question A propylene splitter is about half settled four hours after a reflux step, so its step test does not finish within a shift and a tray temperature must stand in for a product analyzed every twenty minutes. Which tray, which pressure correction and which layer above it hold polymer grade, and what is the analyzer above the tray loop actually for?

Learning objectives

- Explain why an open-loop step test cannot identify this column within a shift, and read the settling time from the impurity drift.
- Compute the pressure term of a tray bubble point, and what compensation removes and leaves behind.
- Choose a control tray for fidelity to the product rather than for sensitivity, and justify the choice with the measured feed step.
- Compare the inferential, cascade and analyzer-only structures with a healthy and a frozen analyzer, and state what the validity hold buys.
- Evaluate a predictive controller that removes giveaway against the minutes it spends below the specification, and set a back-off.

Prerequisites Sections 1.4.6 (inferred quality), 1.4.8 (back-off from a limit), 1.6.2 (velocity-form PID), 1.6.3 (predictive control option) and 1.6.4 (scenarios and Reset).

The app https://apmonitor.com/apps/c3-splitter/

See also Volume 5, Chapter 3 for a small column whose composition loop does feel a slow analyzer, and Volume 5, Chapter 10 for an inferred quality corrected by a delayed laboratory. Volume 3, Chapter 2 for the structure of a cascade before its tuning. Volume 9, Chapter 4 for offset-free predictive control with a bias estimator, and Volume 9, Chapter 9 for a controller that spends a band.

4.1 Introduction

The first experiment in a process control course is an open-loop step test. A manipulated variable is moved, the controlled variable settles, and a gain, a time constant and a dead time are read off the record. On a propylene splitter that experiment cannot be performed. The column modeled here is 53 percent complete four hours after a three percent step in reflux ratio and 98 percent complete after twenty-four, so a student who watches for a shift sees a ramp and fits an integrator to a plant that is not one. The rate of change of distillate impurity falls below 20 ppm/h only after 715 min. Every practical consequence follows from that single fact. The product analyzer is not the bottleneck it is usually assumed to be, the tray temperature that replaces it measures something other than what the specification is written on, and the architecture that a textbook would recommend is not the one that performs best.

The shape is not unique to propylene. Any separation carried out close to both a minimum stage count and a minimum reflux ratio has a small stage-to-stage driving force, a large liquid inventory relative to the product rate, and a composition response measured in hours rather than minutes [1]. Ethylene splitters, xylene columns and deisobutanizers share it, and so does any unit whose quality measurement is intermittent while its inferential is continuous and biased. What generalizes is not the distillation but the structure: a slow plant, a fast measurement that is a proxy, a slow measurement that is the truth, and a supervisory loop that must decide which to believe. Section 1.4.6 sets out the practices that recur across this volume, and Volume 5, Chapter 10 meets the same structure in a dryer whose moisture a delayed laboratory corrects. Inferential estimation from secondary measurements

has been studied for distillation since the 1980s [2] and remains active as soft sensing and disturbance rejection are combined [3]. The control literature on this particular column is narrower [4, 5] and concentrates on what advanced control adds rather than on what the underlying measurement means.

> ✦ DID YOU KNOW? **Two Separations, a Share of the World's Energy**
>
> Purifying propylene and ethylene accounts for about 0.3 % of the world's energy use, a 2020 review reports, and it is counted among seven chemical separations that could change the world [6]. The reboiler of this chapter's column takes 25.4 MW continuously.

A student handed a first-order transfer function and a set of tuning rules never encounters the difficulty that dominates this service, which is that neither available measurement is both fast and faithful. The misconception the simulator is built to correct is that an analyzer with a twenty-minute cycle is slow. Against a composition response that needs about twelve hours to settle it is fast, and measurement on this column is limited by fidelity and validity rather than by speed. This chapter works with an interactive propylene splitter in which the stage count, the holdup, the volatility and the bubble-point pressure coefficient are hidden, so that the inferential must be built, the control tray chosen, and the analyzer layer audited rather than assumed. Its scenarios reach conclusions on tray selection and cascade architecture that contradict the usual rules of thumb, and each conclusion is measured rather than asserted.

The chapter is organized as follows. Section 4.2 recalls the Fenske and Underwood limits that make the column tall and the history of its control. Section 4.3 states the 159-state column with its instrument chain, in the detail needed to rebuild it, and Section 4.4 shows what a step test can and cannot identify on it. Section 4.5 describes the five quality control settings, the pressure-compensation options, the analyzer validity hold and a model predictive controller. Section 4.6 reports the measured results, from the tray loop and pressure compensation through tray selection, the architecture audit, floating pressure and the graded challenge to the comparison with predictive control. Section 4.7 names the hardware and the practice behind the model. Sections 4.8, 4.9 and 4.10 state the limitations, the three lessons that carry beyond distillation and a summary, and the exercises follow in Section 4.11.

4.2 Background

Propylene and propane differ by one double bond. At 18 bar their bubble points differ by 6.2 °C and the relative volatility is 1.12. Polymer-grade propylene at 99.5 mol% or better is a polypropylene feedstock and refinery-grade propylene at 70 percent is not, so the separation is worth doing and expensive to do.

> ⧖ HISTORY **From Short-Cut Methods to Column Dynamics, 1920s to 1965**
>
> A survey of distillation dynamics and control, first given in 1992, looks back over some seventy years of study. From the 1920s into the 1950s the work mainly treated the steady state, with graphical and short-cut models. When the digital computer arrived in the 1950s, research turned to rigorous models that simulate the dynamic as well as the steady behavior, and to control. Up to about 1965 the leading contributions came from industrial researchers in the United Kingdom and the Netherlands, who did pioneering work on dynamic models and simulation, on controlling both product compositions at once, on choosing the control configuration and on the interactions between loops. The same survey noted that most columns respond sluggishly, almost like a pure integrator [7].

Two results from the 1930s and 1940s fix how expensive. Fenske's total-reflux analysis, developed while fractionating Pennsylvania gasoline [8], gives the minimum theoretical stage count, which for this duty is 72. No reflux ratio is large enough to shorten the column below it. Underwood's treatment of minimum reflux at infinite stages [9] gives 11.4 for the same duty, so no stage count is large enough to make the column cheap. Real splitters therefore carry 150 to 250 trays, frequently

in two shells because a single column that tall will not stand, and run reflux ratios of 14 to 20. The reboiler on the column modeled here is 25.4 MW continuously, which on many olefin plants is the largest single heat consumer on the site.

Control of the service developed in three stages. Before continuous analysis was available the column was run on a tray temperature and a reflux flow, with laboratory samples once a shift to confirm that the temperature still corresponded to the product. Tray temperature is a bubble point and therefore a function of composition and pressure together, so the arrangement was tolerable only while pressure was held constant and the feed did not change. Process gas chromatographs made a direct composition measurement available from the 1960s and made the modern cascade possible, with the analyzer adjusting the setpoint of the temperature loop rather than the valve. The estimation literature formalized what a secondary measurement can and cannot recover [2], and the configuration question of which flows to pair with which compositions was settled in the same period by studies of dual composition control and its interaction [1, 10]. Model predictive control of the splitter followed once the economics of an energy consumer this size justified it [4, 5].

> ⧖ HISTORY **A Temperature Loop Under an Analyzer, 1973 to 1991**
>
> Product composition measurements were often expensive, unreliable and late, so the most popular way to control a column's product became a tray temperature. To be sensitive, that tray sits some distance from the column's ends, where it may not follow the product well, and works of 1973 and 1990 answer with a fast temperature loop cascaded with an analyzer. A 1978 estimator that inferred composition from temperatures and flows proved very sensitive to model errors on high-purity columns. In 1991 a regression on about five temperatures spread along the column worked in simulation and in implementation, could also correct for pressure, and almost removed the measurement delay. By 1989 an industrial predictive controller on benzene and toluene towers was adjusting a tray temperature setpoint [7].

Energy became the second driver. Shinskey's treatment of distillation in an energy conservation context introduced floating pressure, the practice of letting the column run at the lowest pressure the condenser can hold, because relative volatility rises as pressure falls and the separation becomes cheaper [11]. The practice is standard now and the savings are still being quantified for this specific column [12, 13]. Whether a saving created in reflux ratio is collected in megawatts is a separate question, treated in Section 4.6. The alternatives to distillation are under active development, with membranes and metal-organic frameworks offering polymer-grade propylene at a fraction of the energy [14], but the installed base of superfractionators is large and will be operated for decades.

4.3 Process Model

Column C-401 is a 200-tray superfractionator with a total condenser, a reflux drum, a partial reboiler and a sump, operating at 18 bar on a feed of 700 kmol/h containing 72 mol% propylene. Reflux returns at 7000 kmol/h for a distillate of 494 kmol/h, a reflux ratio of 14.17. Figure 4.1 shows the arrangement, the instrument tags and every symbol used in the equations that follow.

Table 4.1 classifies what the loops interact with. The plant is expressed in the units of olefin operation, flows in kmol/h, holdups in kmol, pressure in bar, temperature in degrees Celsius and time in minutes. Every material balance therefore carries a factor of $1/60$. One hundred and fifty-nine states are integrated: 152 compositions covering the total condenser, 150 theoretical stages and the partial reboiler, the two holdups, the overhead pressure, and four actuator and hydraulic lags.

4.3.1 Stage Material Balances

Each theoretical stage carries a balance on the light key given by Equation (4.1), with vapor-liquid equilibrium Equation (4.2).

$$M\,\frac{\mathrm{d}x_n}{\mathrm{d}t} = L_{n-1}x_{n-1} + V y_{n+1} - L_n x_n - V y_n \tag{4.1}$$

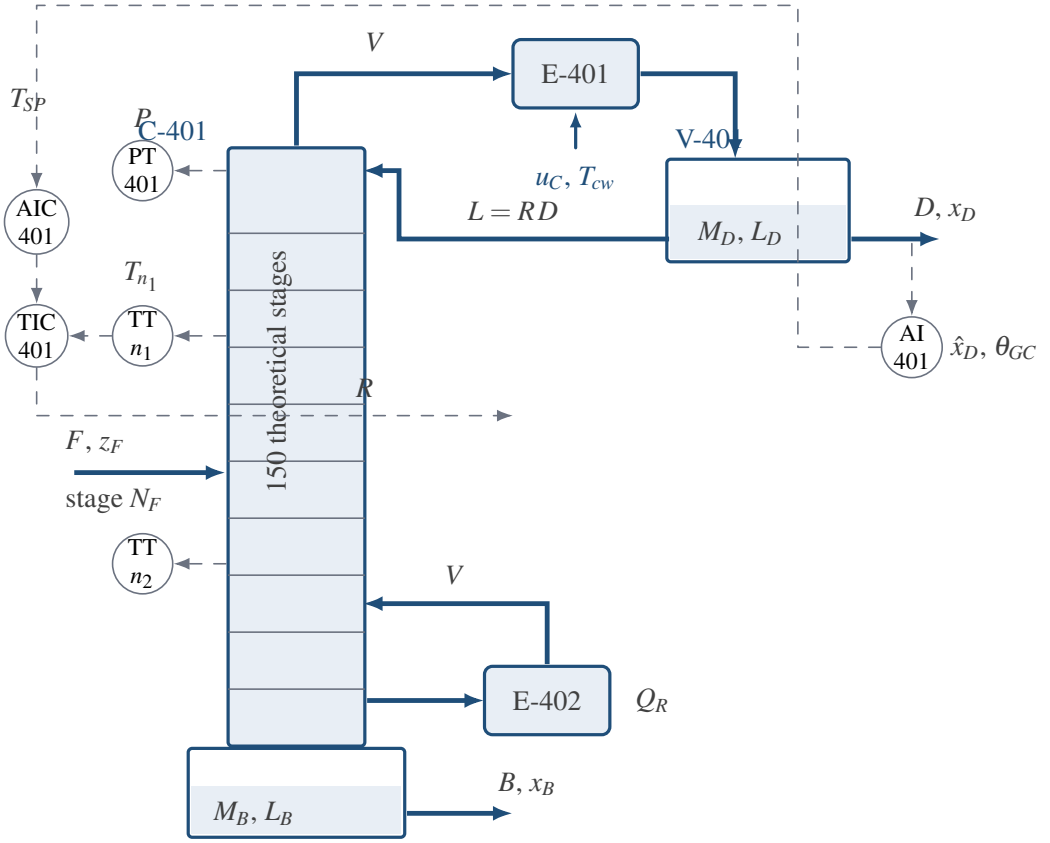


Figure 4.1 Superfractionator C-401 with its condenser E-401, reflux drum V-401, reboiler E-402 and sump. Feed F of composition z_F enters at stage N_F. Boilup V leaves the top, is condensed against cooling water at T_{cw} through valve u_C, and collects in V-401 at holdup M_D and level L_D. Reflux L is set as the ratio R times the distillate D, which leaves at propylene mole fraction x_D. The sump holds M_B at level L_B and the bottoms B leaves at x_B. TT-n_1 and TT-n_2 are the control and reference tray thermometers, PT-401 measures the overhead pressure P, and AI-401 is the product chromatograph of cycle time θ_{GC}. TIC-401 manipulates the reflux ratio and AIC-401 sets its setpoint T_{SP}.

$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1) x_n} \tag{4.2}$$

where M is the liquid holdup per stage in kmol, x_n and y_n are propylene mole fractions in the liquid and vapor leaving stage n, L_n and V are the internal liquid and vapor flows in kmol/h, and α is the relative volatility. Constant molar overflow is assumed, so V is the same on every stage and L_n changes only at the feed.

The holdup is 14.6 kmol per stage, which is about 2200 kmol of liquid against a reflux of 7000 kmol/h. Liquid turns over in eighteen minutes and composition responds in hours, because near a pinch the stage-to-stage driving force is small and re-inventorying the profile is far slower than moving liquid through it.

The stage count is deliberately not reduced. Collapsing 150 stages into 40 with an effective relative volatility of $\alpha^{3.75} = 1.53$ preserves the total separation power and looks like a defensible reduction. It is not. The reduced column makes 99.99 mol% propylene at a reflux ratio of 10, below the true Underwood minimum of 11.4, where the 150-stage model reaches only 95.98 mol%, because the coarse stepping walks over the tangency between the equilibrium curve and the operating line. The

Table 4.1 Classification of Variables. Nominal Values Are Those of the Design Operating Point at Which the Scenarios Start Unless They Set Otherwise.

Symbol	Role	Nominal	Range
x_D (AI-401)	CV, intermittent	99.53 mol%	99.0–99.9 SP
T_{n_1} (TT)	CV, continuous	46.71 °C	44.0–50.5 °C SP
P (PT-401)	CV, continuous	18.0 bar	15.0–21.0 bar
R	MV	14.17	8–24
u_C	MV	65 %	0–100 %
V	MV, operator set	7494 kmol/h	4000–11 000 kmol/h
F	DV, measured	700 kmol/h	450–900 kmol/h
z_F	DV, unmeasured	0.72	0.60–0.88
T_{cw}	DV, measured	28 °C	12–36 °C
analyzer freeze	DV, unmeasured	off	on/off
$x_0 \ldots x_{151}$	states	profile	0–1
M_D, M_B	states	700, 450 kmol	0–1400, 0–900
P, lags	states	18 bar	—

pinch is the reason superfractionators exist, and the application carries an automated test that fails if it is ever lost.

4.3.2 Relative Volatility and the Tray Thermometer

Relative volatility falls with pressure, Equation (4.3), which is the entire economic content of floating pressure.

$$\alpha(P) = \alpha_0 - \frac{\mathrm{d}\alpha}{\mathrm{d}P}\,(P - P_0) \tag{4.3}$$

with $\alpha_0 = 1.12$ at $P_0 = 18\,\mathrm{bar}$ and $\mathrm{d}\alpha/\mathrm{d}P = 0.0075/\mathrm{bar}$.

A tray temperature is a bubble point, so it depends on composition and pressure together, Equation (4.4).

$$T_n = x_n\, T^{sat}_{C_3^=}(P) + (1 - x_n)\, T^{sat}_{C_3}(P) \tag{4.4}$$

$$\begin{aligned} T^{sat}_{C_3^=}(P) &= T^{sat}_{C_3^=,0} + \frac{\mathrm{d}T}{\mathrm{d}P}\,(P - P_0) - \beta\,(P - P_0)^2 \\ T^{sat}_{C_3}(P) &= T^{sat}_{C_3,0} + \left(\frac{\mathrm{d}T}{\mathrm{d}P} + \delta\right)(P - P_0) - \beta\,(P - P_0)^2 \end{aligned} \tag{4.5}$$

where the bubble points at P_0 are $T^{sat}_{C_3^=,0} = 45.6\,^\circ\mathrm{C}$ for propylene and $T^{sat}_{C_3,0} = 51.8\,^\circ\mathrm{C}$ for propane, the pressure slope is $\mathrm{d}T/\mathrm{d}P = 3.10\,^\circ\mathrm{C/bar}$, the propane curve is steeper by $\delta = 0.15\,^\circ\mathrm{C/bar}$, and the curvature is $\beta = 0.05\,^\circ\mathrm{C/bar^2}$. The composition term and the pressure term of Equations (4.4) and (4.5) are what the application is about. The composition term spans 5.80 °C from the top of the column to the bottom, about 0.038 °C per stage. The pressure term is about 3.1 °C per bar (3.12 °C/bar at stage 70, where the liquid is 82 percent propylene). A tenth of a bar therefore reads like almost seven percent of the reflux ratio, and a 0.4 bar excursion is more temperature than the entire composition profile between the control tray and the top of the column.

4.3.3 Why the Manipulated Variable Is a Ratio

With constant molar overflow and the drum level on the distillate valve, $D = V - L$. Reflux is 7000 kmol/h and distillate is 494 kmol/h, so one percent on the reflux flow is fourteen percent on the product rate, and the bottoms composition moves from 6 to 29 mol% propylene for it. Ratioing reflux to distillate instead gives Equation (4.6).

$$D = \frac{V}{1 + R}, \qquad L = R\,D \tag{4.6}$$

Table 4.2 Model Parameters. Adjustable Parameters Can Be Changed in the Model Dialog, and Hidden Parameters Are Fixed.

Symbol	Meaning	Value	Class
α_0	volatility at 18 bar	1.12	adjustable
$\mathrm{d}\alpha/\mathrm{d}P$	volatility fall with P	0.0075/bar	adjustable
$\mathrm{d}T/\mathrm{d}P$	bubble point vs. pressure	3.10 °C/bar	adjustable
M	holdup per stage	14.6 kmol	adjustable
N	theoretical stages	150	fixed
N_F	feed stage	84	hidden
τ_h	reflux to sump transit	8.0 min	adjustable
τ_V	reboiler thermal lag	2.5 min	adjustable
C_V	overhead capacitance	12.0 kmol/bar	adjustable
k_C	condenser duty coefficient	6.55	adjustable
θ_{GC}	analyzer cycle	20 min	adjustable
τ_T	thermowell lag	0.6 min	adjustable
x_D^{spec}	polymer grade	99.5 mol%	adjustable
x_B^{max}	propylene in bottoms	8.0 mol%	adjustable

One percent on R is then one percent on the product. The LV configuration is not wrong in general and the configuration question has a long literature [1, 10]. It is wrong at a reflux ratio of fourteen, where the manipulated flow is fourteen times the flow that closes the material balance.

4.3.4 Condenser, Pressure and Holdups

Overhead pressure is a small capacitance driven by the imbalance between boilup and condensation, Equation (4.7).

$$C_V \frac{\mathrm{d}P}{\mathrm{d}t} = V - k_C\, u_C\, f\left(T_{C_3^=}^{sat}(P) - T_{cw}\right) \tag{4.7}$$

where $C_V = 12.0\,\mathrm{kmol/bar}$, $k_C = 6.55\,\mathrm{kmol/h}$ per percent of valve per kelvin of approach, u_C is the cooling water valve in percent, and f is a condenser condition factor that is 1.0 when clean. At design the valve sits at 65 % with 17.6 K of approach. The resulting pressure time constant is about half a minute (0.55 min), which makes pressure the fast loop on a column whose composition is the slow one. The drum and sump integrate their own flow imbalances. A reflux change reaches every rectifying stage at once, because constant molar overflow carries no tray hydraulics, and a single eight-minute lag τ_h carries it to the stripping section and the sump.

4.3.5 Assumptions

The model is calibrated to produce the right sensitivities rather than to size equipment, and six assumptions bound what it can teach.

The separation is binary. A real feed carries propadiene, methylacetylene, ethane and C4 traces, and polymer-grade specifications include several of them, so the reader would not learn here that a product can fail on a contaminant this separation does not address.

Constant molar overflow is assumed with no energy balance, so subcooled reflux and changes in feed enthalpy do not alter the internal traffic the way they do on a real column.

Relative volatility is a single number linear in pressure. Real propylene/propane volatility varies along the column with temperature and composition, and the variation matters most where the driving force is smallest.

Tray efficiency is fixed and folded into the stage count. Efficiency on a real splitter falls at turndown and near flooding, which is a common way for a column to lose separation while every instrument reads normally.

There is no hydraulic capacity limit. Flooding, weeping, entrainment and tray pressure drop are absent, so the application cannot show the constraint that usually stops a splitter being pushed, which is that the column floods before the reboiler runs out.

Liquid transport is one eight-minute lag rather than 150 weir calculations, so a reflux change arrives at the sump smoothed rather than as a wave, while the rectifying section sees it without delay.

4.4 Dynamic Analysis

4.4.1 What Can Be Identified

The distillate composition response to a three percent step in reflux ratio (14.17 to 14.60, which moves the distillate from 99.528 to 99.638 mol%) is 29 percent complete at two hours, 53 percent at four and 98 percent at twenty-four, and it reaches 63 percent only at 312 min. In any window a student can watch, the record looks like a ramp. Fitting first order plus dead time to the first two hours returns a time constant of 3.1 h against the 5.2 h at which the step is 63 percent complete, and a gain 43 percent low, with a tuning to match. The application therefore reports the rate of change of distillate impurity in parts per million per hour, filtered over about five minutes, as an explicit indicator of whether an experiment has finished. Below about 20 ppm/h the column is as settled as it becomes inside a shift, and the design condition reaches that threshold 715 min after a three percent ratio step.

> **TRY IT IN THE APP 1 · The step test that does not finish (MANUAL)**
>
> Load the scenario, stay in Manual and raise the Reflux ratio from 14.17 to 14.60. Run at 200 min/s and watch the Drift badge rather than the purity trend. The badge climbs as the column starts to move and first reads under 20 ppm/h only at about 715 min, although one pass of liquid through the column takes eighteen minutes.

The tray temperature is not faster in open loop. Stage 70 moves half of its eventual change within ten minutes of the step, because the extra reflux reaches every rectifying stage at once, gives almost all of it back by twenty minutes as the liquid lag delivers the same reflux to the stripping section, and then follows the same composition front as the product. It is 36 percent complete at two hours and 63 percent complete at 312 min, exactly as the distillate is, and a first-order fit to its first two hours captures only the initial transient. What a shift-long window identifies on either signal is a slope. The inner loop is fast because feedback overdrives the ratio, as Section 4.6 shows, rather than because its measurement settles sooner. The outer analyzer loop is tuned from the requirement that it be slower than the inner loop by a wide margin, which is the standard cascade argument [15]. Volume 3, Chapter 2 shows the other half of that argument on a level loop: an inner loop rejects the disturbances that enter inside its own measurement path and few others.

4.4.2 Sensitivity Against Fidelity

The steady-state gain from reflux ratio to control tray temperature, for a one percent increase at constant boilup, is −0.047 °C at stage 70, which is as sensitive as any stage above the feed, and −0.016 °C at stage 25, roughly a third of it. Sensitivity is maximized in the stripping section, where the most sensitive stage is 127 at −0.39 °C, about eight times the sensitivity of stage 70. Sensitivity is not the criterion, however, because a stage far from the product responds to disturbances the product does not see. Section 4.6 reports the measured comparison.

4.5 Controller Design

4.5.1 Velocity Form PID

Every loop in the application uses the shared velocity-form PID of Section 1.6.2, Equations (1.14) to (1.17), executed every $\Delta t_c = 0.1$ min, with the derivative taken on the measurement through a first-order filter of time constant τ_f. The derivative path is configured ($\tau_f = 3.0$ min on TIC-401) but

$\tau_D = 0$ in every scenario, so every loop runs as PI. The bias is zero and the integral is seeded with the starting output at reset.

Anti-windup acts on the integral term alone, with the tracking time $T_t = \tau_I$, and the running sum of proportional and derivative increments is never truncated. The tracking time matters little here. In the uncompensated pressure case of Section 4.6 the demand reaches 27.3 while the ratio sits on its 24.0 stop, and a counterfactual run that absorbs the whole excess in one scan ($T_t = \Delta t_c$) leaves the ratio's later undershoot within 0.02 of the shipped value, although it arrives about 70 min sooner. No loop is slew limited. The reflux flow, R times the distillate flow filtered over 3 min, is clamped again to 3000–12 000 kmol/h after the PID, a limit TIC-401 does not know about, but it cannot bind within the ratio and boilup ranges. Transfer between Manual and automatic is bumpless in both directions, as Section 1.6.2 describes. The integration step is 0.02 min of fixed-step fourth-order Runge-Kutta, and every run, including its seeded noise, reproduces exactly (Section 1.6.1). The fastest run speed is 200 minutes of plant time per wall-clock second, so a twelve-hour settling time passes in a few seconds.

4.5.2 The Quality Control Settings

The quality control selector offers five configurations. The first four are described here and audited in Section 4.6, and the fifth, a model predictive controller, is the subject of Section 4.5.5.

The action a below is that of Equation (1.14). *Off* leaves the reflux ratio in manual. *Inferential* closes TIC-401 from the control tray temperature to the reflux ratio (limits 8 to 24), with $a = -1$ because more reflux ratio is a colder tray. *Cascade* adds AIC-401 from the product analyzer to the tray temperature setpoint (limits 44.0 to 50.5 °C), with $a = -1$ because a colder tray setpoint is more purity. *Analyzer only* removes the temperature loop and puts the analyzer straight on the ratio station, with $a = +1$ because more reflux ratio is more purity. Each scenario loads one of two tunings. The cautious set, used where the reflux is in manual and as the challenge's starting point, is $K_c = 0.6/°\mathrm{C}$ with $\tau_I = 400$ min on TIC-401 and $K_c = 0.15\,°\mathrm{C}$ per mol% with $\tau_I = 1200$ min on AIC-401. The tuned set, used in every closed-loop scenario, is $K_c = 5.0/°\mathrm{C}$ with $\tau_I = 60$ min (70 min on the differential) and $K_c = 0.9\,°\mathrm{C}$ per mol% with $\tau_I = 240$ min. The analyzer-direct case runs $K_c = 8$ per mol% of purity with $\tau_I = 240$ min.

Two further options change what the inferential measures. Pressure compensation subtracts the bubble-point pressure term arithmetically using a reference pressure, Equation (4.8), which is Equation (1.10) of Chapter 1.

$$T_n^{comp} = T_n - \frac{\mathrm{d}T}{\mathrm{d}P}\left(P - P_{ref}\right) \tag{4.8}$$

The differential option replaces the single tray with the difference between two trays, which removes the pressure term structurally because both trays move together. Section 4.6 reports where each option holds and where it fails.

4.5.3 Analyzer Validity

A frozen chromatograph republishes its last good result rather than failing visibly, so trends look calm while the outer loop integrates against an error nobody is measuring. The validity option inhibits the supervisory loop while the analyzer result is flagged bad, holding the tray temperature setpoint at its last value and tracking it so that the loop resumes without a bump. The measured consequence of omitting it is in Table 4.4.

4.5.4 Pressure, Levels and Floating Pressure

PIC-401 manipulates the cooling water valve, with $a = -1$ because more valve is a lower pressure, and $K_c = 12\,\%/\mathrm{bar}$ and $\tau_I = 1.2$ min in the tuned set (3 %/bar and 8 min in the cautious one). The two level loops are deliberately detuned so that the drum and sump absorb upsets rather than pass them downstream, with gains of 40 and 25 kmol/h per percent and integral times of 20 min in the tuned set (22 and 14 kmol/h per percent, 30 min, in the cautious one). Pressure minimization ramps

the pressure setpoint down at 0.006 bar/min while the valve command is below 92 %, toward a floor of 15.5 bar, and back up at three times that rate when the command exceeds 97.5 %, never above the operator's setpoint.

4.5.5 Model Predictive Control

The fifth quality setting replaces the single-number loops by a plan, built on the predictive control option of Section 1.6.3. Every $T_s = 5$ min, fifty controller scans, a quadratic program chooses the reflux ratio R and, under floating pressure, the setpoint P^{SP} of PIC-401 over $N = 48$ decisions, four hours, and the first move is held until the next decision [16, 17]. Three choices depart from the design first proposed, which named the cooling water valve as the second handle and reflux as the energy cost. The plan writes the pressure setpoint rather than the cooling water valve, because with the valve held at 65 % after the cooling water steps from 28 to 34 °C the pressure passes the 19.6 bar relief margin within a minute (19.65 bar). The pressure is a decision only under floating pressure, and otherwise stays at the operator's setpoint. Reflux is priced but is not an energy cost, because the boilup is an operator setpoint and unspent reflux leaves as distillate.

The controller's model is identified at the design point by steps of ± 0.15 in R, ± 0.25 bar in P^{SP} through PIC-401 and ± 0.02 in z_F, whose central differences over 48 h were fitted by Equation (4.9).

$$\begin{aligned} \Delta y(t) &= \Delta u \sum_{i=1}^{7} \left[a_i \, \phi_i(t) + b_i \, \psi_i(t) \right] \\ \phi_i &= 1 - e^{-t/\tau_i}, \quad \psi_i = 1 - \left(1 + t/\tau_i\right) e^{-t/\tau_i} \end{aligned} \tag{4.9}$$

Here Δu is the step, Δy the change in the compensated stage-70 reading of (4.8) or in $\ell = \ln(100 - x_D)$ with x_D in mol%, τ_i runs over 0.5, 2, 6, 20, 60, 200 and 700 min, and a_i and b_i are least-squares coefficients. The impurity is modeled in logarithms because its response is one-sided. With two states per lag and a random-walk disturbance d on the feed path the model has 43 states. Its gains on ℓ are -0.878 per unit ratio, $+0.646$ per bar and -26.6 per unit z_F, its residuals are 0.02 to 0.44 percent of each response, and an independent test with smaller steps agrees on the ratio response of ℓ to 0.6 percent at four hours. A steady-state Kalman filter reads the compensated tray once a minute, with a measurement variance of $(0.02\,^{\circ}\mathrm{C})^2$, and corrects the feed path and d, and at each new analyzer result a bias on ℓ moves as $b \leftarrow b + 0.3\,(\ell_{GC} - \hat{\ell} - b)$, which has the form of Equation (1.11) with $\lambda = 0.3$. Together they make the prediction offset free [18], as the fuel-bias estimator of Volume 9, Chapter 4 does for a drum boiler. The analyzer reaches the plan with its shipped cycle and sample age, noise, freeze and validity hold.

The plan minimizes Equation (4.10) over twelve move blocks whose lengths grow from one decision for the first four to fifteen, with a last block of three,

$$\begin{aligned} J = c_R \sum_{k=0}^{N-1} R_k + \rho_\sigma \sigma^2 + \mu_\sigma \sigma \\ + \sum_{j=1}^{12} \left[S_R \, \Delta R_j^2 + S_P \, (\Delta P_j^{SP})^2 \right] \end{aligned} \tag{4.10}$$

subject to Equation (4.11).

$$\begin{aligned} &\hat{\ell}_k \le \ln\left(100 - x_D^{SP}\right) + \sigma, \;\; k \ge 12, \;\; \sigma \ge 0 \\ &R_{lo} \le R_j \le R_{hi}, \quad |\Delta R_j| \le 0.5 \\ &P_{fl} \le P_j^{SP} \le P_{op}^{SP}, \quad |\Delta P_j^{SP}| \le r_f T_s \end{aligned} \tag{4.11}$$

Here $\hat{\ell}_k$ is the corrected prediction k decisions ahead, x_D^{SP} the purity target, Δ the move from the previous block or from the applied value, $c_R = 1$, $S_R = 300$, $S_P = 10$ per bar^2, and the one slack σ is

priced at $\rho_\sigma = 10^4$ and $\mu_\sigma = 10^3$, so it is zero whenever the band can be met. The purity row is soft and one-sided, so purity above the target is giveaway the reflux price removes. It starts one hour out, because a ratio move reaches only 9.9 percent of its effect on ℓ within 60 min. The ratio row is hard, $R_{lo} = \max(8, 3000/D_f)$ and $R_{hi} = \min(24, 12000/D_f)$ on the 3 min filtered distillate D_f, as the ratio station reads them. The pressure row is hard, with P_{op}^{SP} the operator's setpoint, $r_f = 0.006\,\mathrm{bar/min}$, and P_{fl}, never below the operator's floor, the pressure at which the valve would stand at $u_{lim} = 95\,\%$, from (4.7) at its declared values, Equation (4.12).

$$\begin{aligned} V_{SP} &= k_C\, u_{lim}\left(T_{C_3^{=}}^{sat}(P_{fl}) - \hat{T}_{cw}\right) \\ \hat{T}_{cw} &= T_{C_3^{=}}^{sat}(P_m) - V_{SP}/(k_C\, u_C) \end{aligned} \tag{4.12}$$

Here $\hat{T}_{cw}$ is the cooling water temperature the condenser behaves as if it had, from the boilup setpoint, the valve command and the measured pressure, filtered over 5 min. On scenario 11 this floor lies 0.001 bar above the true one on average. A dual active-set solver [19] handles the 24 block decisions, and S_R and the disturbance intensity were chosen once, on scenario 11, for the least quality IAE among settings that rejected no plan.

Under the plan the three PI loops track the applied ratio. When the solver reports anything but an optimum, or the first move is non-finite or outside the box, the plan is discarded and the inferential loop takes the reflux. Forced at four instants with the noise off, the hand-over steps the ratio by 7.1×10^{-4} to 2.2×10^{-3}, and a switch to manual leaves the ratio exactly where the plan put it. No plan was infeasible or rejected on any case of Section 4.6.7. The plant runs with the run's parameters, the instruments add lags, sampling and noise, and the model is the fit at the design point, so a plant edit is a mismatch, while an edit of $\mathrm{d}T/\mathrm{d}P$ or P_{ref} reaches the plan through the compensated reading. Solving one plan took 1.40 ms on average in Chrome on scenario 11, at a load average of 1.57.

4.6 Results

Twelve scenarios progress from an unfinishable step test to a graded challenge. Scenario 1 attempts the step test and finds that it does not finish, and scenario 2 finds that neither the tray temperature nor the purity settles inside a shift. Scenario 3 walks a thermometer along the temperature profile, scenario 4 closes the inferential and shows that a temperature is not a purity, and scenarios 5 and 6 break it with pressure. Scenario 7 chooses a tray and finds that the sensitivity rule is only half a rule, scenarios 8 and 9 audit the architecture, scenario 10 takes or fails to take the energy saving of floating pressure, and scenario 11 sets the predictive controller against the cascade. Scenario 12, the graded challenge, asks for the column to be restructured. Each case is credited separately when the learner performs the listed actions and the simulation reaches the listed state. Several ask for a rerun after Reset, which restarts the case from time zero and keeps the learner's own settings (Section 1.6.4), so the comparison a scenario teaches is also the condition for completing it. The challenge is judged on the case as given, and changing a model parameter or a disturbance setting voids the attempt. Credit accumulates toward certificates of progress and of completion for the module.

4.6.1 The Inferential Holds a Temperature

Stepping the tray temperature setpoint 0.09 °C down at 60 min moves the reflux ratio from 14.14 to 14.48, 2.4 percent, after overdriving it to 14.87, returns the temperature to within 0.005 °C of setpoint in 208 min, and raises the distillate from 99.527 to 99.614 mol% over the following hours, overshooting to 99.634 near eight hours. The loop has held a temperature, and the temperature corresponds to a purity only at the feed composition and pressure in force when the setpoint was written down.

4.6.2 Pressure Compensation and Its Limit

A 0.4 bar pressure setpoint move raises every bubble point in the column by about 1.25 °C, which is more temperature than the entire composition profile between the sensitive tray and the top. With an

Table 4.3 Feed Composition Change Held on Two Control Trays. Peak Departure From the Pre-Step Purity and Composition at 15 h.

Measure	Stage 25	Stage 70
Relative sensitivity	1	3
Peak departure (mol%)	+0.099	−0.373
Composition at 15 h (mol%)	99.489	99.298

uncompensated measurement the controller cannot win and tries anyway. The reflux ratio runs from 14.14 to its stop at 24.0 within 32 min of the step, and the distillate climbs to 99.89 mol% by 300 min against a specification of 99.5. When the compensation is switched on at 300 min with the pressure still high, the loop unwinds, undershoots to 13.56 near 750 min and settles at 14.37, 1.7 percent above where it started, with the distillate at 99.47 mol%. The residual is a process effect, because the higher pressure has lowered α from 1.1200 to 1.1170. Selected before the run instead, the compensated loop moves the ratio by at most 2.9 percent, after a dip to 12.48 in the first two minutes of the step, where the pressure transmitter (0.1 min filter) runs ahead of the thermowell (0.6 min lag) and the arithmetic briefly overcorrects.

The differential measurement removes the pressure term more completely at the measurement. A tenth of a bar moves a single tray by 0.312 °C and moves the difference between stages 90 and 70 by 0.0012 °C, which is 0.4 percent of it. Through a 0.6 bar pressure setpoint step held from 60 min, however, the compensated single tray lets the distillate fall by at most 0.092 mol% and settle at 99.44, while the differential, held near its 0.50 °C setpoint, lets it fall 0.63 mol% to 98.90 at 14.3 h, and it is still only 99.18 at 25 h. Pressure also changes relative volatility (1.1200 to 1.1155 here) and therefore changes the profile a given differential corresponds to. Compensating the measurement is not compensating the process.

🕮 **Pause.** Try Exercise 4.3 before reading on.

4.6.3 Tray Selection

Stage 70 has three times the sensitivity of stage 25 and loses. Table 4.3 reports the 72 to 78 percent feed composition step at 60 min held on each, with the stage-70 case run as the scenario directs, by moving the tray, resetting and taking the setpoint (46.71 °C) from the reading.

Stage 25 is nearer the product and is therefore a more faithful proxy for it. Its purity is still moving at fifteen hours and settles at 99.495 by 50 h, while stage 70 settles at 99.28. The most sensitive stage in the column is 127 at about eight times stage 70, and it is in the stripping section, which makes it an excellent inferential for the bottoms and a poor one for the distillate.

🕮 **Pause.** Try Exercise 4.2 before reading on.

4.6.4 Architecture Audit

Table 4.4 reports the architectures against the same feed composition step, with a healthy analyzer and then with the analyzer frozen, each on the scenario that runs it. In the frozen cases the chromatograph stops updating at 60 min with its last result 0.07 mol% high, and the feed steps a minute later. Figure 4.2 draws the five rows side by side.

Three results follow. With a healthy chromatograph the analyzer alone outperforms the cascade, which contradicts the usual recommendation. It departs 0.063 mol% against 0.143 and is back at 99.51 at fifteen hours while the cascade is at 99.47, although both reach 99.50 by thirty. The analyzer cycle time barely matters. Moving it from 5 to 60 min changes the peak departure only from 0.061 to 0.070 mol%. Against a response that is 63 percent complete at 5.2 h and settles in about twelve, a twenty-minute analyzer is a fast measurement. The far smaller column of Volume 5, Chapter 3 is the opposite case, where an analyzer lag of a few minutes already takes the loop out of its band.

Table 4.4 Architecture Comparison on the 72 to 78 Percent Feed Composition Step. Peak Departure From the Pre-Step Purity and Distillate Composition at 15 h and 30 h, All in mol%.

Architecture (scenario)	Peak	15 h	30 h
Inferential alone (7)	−0.373	99.298	99.283
Cascade (9)	−0.143	99.472	99.499
Analyzer only (8)	+0.063	99.512	99.499
Cascade, frozen, hold at 600 min (9)	−0.712	98.906	98.903
Cascade, frozen, hold from start (9)	−0.516	99.190	99.170

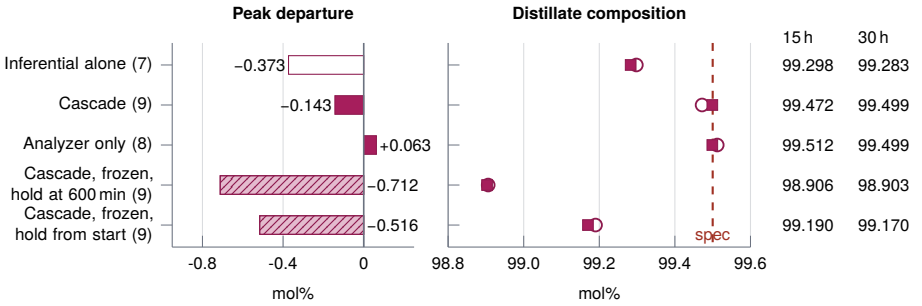


Figure 4.2 The architectures of Table 4.4 on the 72 to 78 percent feed composition step. (a) Peak departure from the pre-step purity: the open bar has no analyzer, solid bars a healthy one, hatched bars a frozen one. (b) Distillate composition at 15 h (open circles) and 30 h (filled squares) against the 99.5 mol% specification (dashed line). Notice that the analyzer alone departs least while the chromatograph is healthy, and that a frozen chromatograph left in the cascade until 600 min takes the column furthest below the specification.

Pause. Try Exercise 4.1 before reading on.

The inferential earns its place elsewhere. With the chromatograph frozen and the validity hold not armed until 600 min, the outer loop keeps integrating a stale error and walks the tray setpoint from 46.80 to 46.99 °C, the purity falls to 98.81 at 473 min and settles at 98.90, which is worse than the inferential alone. Arming the hold from the start freezes the setpoint at 46.80 °C, and the cascade then settles at 99.17, exactly where the inferential alone settles on the same case when its setpoint is 46.80 °C rather than the commissioned 46.71 °C. The remaining gap to the inferential row is the trim the analyzer applied before it failed. The case for the inner temperature loop on this column is therefore availability rather than speed.

TRY IT IN THE APP 9 · What the inferential is actually for

Run the case as loaded. The chromatograph freezes at 60 min and the feed goes richer a minute later. Watch the Tray temperature setpoint walk from 46.80 to 46.99 °C until the hold comes on at 600 min, while the purity falls to 98.81 and settles at 98.90 mol%. Press Reset, set Analyzer validity to Hold on bad quality before Run, and the cascade settles at 99.17.

4.6.5 Floating Pressure

Enabling pressure minimization on a cold night, with cooling water at 16 °C, walks the pressure setpoint to its 15.5 bar floor in 417 min and raises relative volatility from 1.1200 to 1.1388. At fixed boilup the improvement appears first as recovery. By 1000 min the cascade has lowered the reflux ratio to 13.86, against 14.11 on the same case at a fixed 18 bar, the distillate has risen from 494 to 504 kmol/h, and the bottoms carry 0.21 mol% propylene instead of 6.0. The reboiler duty does not

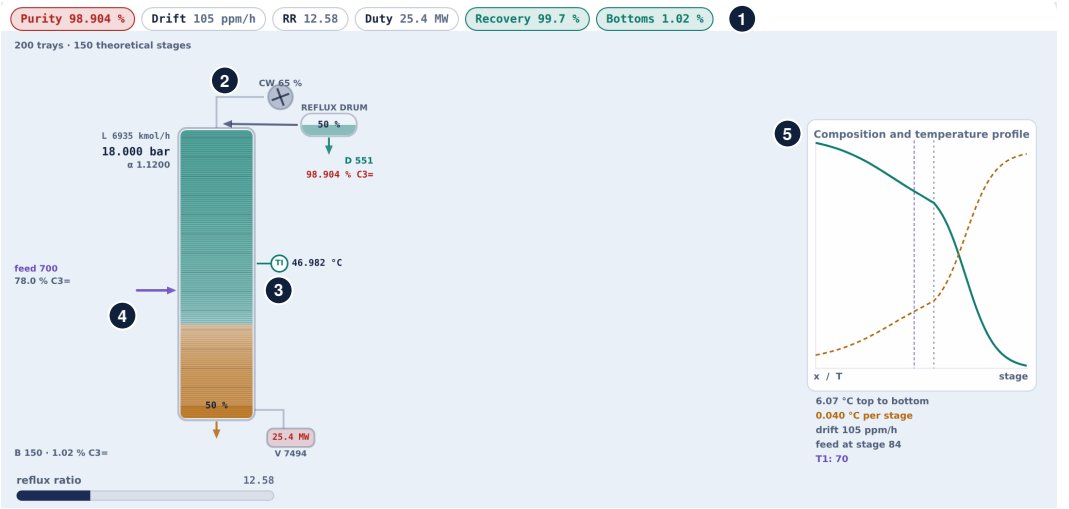


Figure 4.3 The propylene splitter application near the end of scenario 9, the analyzer validity scenario, at 1800 min with the quality cascade in automatic, cropped to the plant view. The chromatograph froze at 60 min reading 99.592 mol%, the feed went from 72 to 78 percent propylene at 61 min, and the validity hold was armed at 600 min. (1) The status chips read the true purity, the drift, the reflux ratio (12.58), the duty, the recovery and the bottoms. (2) The condenser, its cooling water valve and the reflux drum sit above the shell, which is drawn in elevation with its 150 theoretical stages colored by propylene mole fraction, and the reboiler and sump below it. (3) The control tray thermometer and (4) the feed sit on the side of the shell. (5) The inset plots the composition and temperature profiles against stage number with the control tray and the feed stage marked.

move. It stays at 25.40 MW, because the boilup is a number an operator typed and no loop is reducing it. Cutting the boilup to 7341 kmol/h at 1000 min takes the duty to 24.88 MW, half a megawatt, with the distillate still on grade. That cut collects a small part of what the lower pressure created. In the model the design split (494 kmol/h of distillate at 99.5 mol% with 6 mol% propylene in the bottoms) needs 6100 kmol/h of boilup at 15.5 bar against 7433 kmol/h at 18 bar, 20.67 MW against 25.19 MW, and the cascade settles there (ratio 11.35, bottoms 6.01 mol%) when the boilup is cut to 6100 kmol/h and the cooling water stays cold. The saving is rented from the weather. When the cooling water warms to 34 °C at 1200 min the valve saturates, the pressure touches 19.03 bar, and the minimization backs the setpoint up to 17.99 bar. A column cut to 6100 kmol/h settles at 17.4 bar, where that boilup is far too little, and its bottoms reach 27 mol% propylene by 2400 min. The distinction between creating a saving and collecting it is the point of the scenario, and it is why floating pressure is usually commissioned together with a duty minimization rather than alone [11, 12].

4.6.6 The Graded Challenge

The challenge runs 2400 min from the design point on a configuration that is wrong three ways, with an uncompensated stage-25 inferential, the cautious tuning and no supervisory loop. Four disturbances arrive: feed composition 72 to 77 percent at 120 min, cooling water 22 to 33 °C at 500 min, feed rate 700 to 790 kmol/h at 900 min, and feed composition 77 to 70 percent at 1200 min. It is met when the distillate is held within 0.12 mol% of the 99.5 mol% target from 1200 min to the end with propylene in the bottoms below 8 mol% at 2400 min. As loaded, the column never goes off specification. It gives purity away instead, up to 99.76 mol%, with a worst error after 1200 min of 0.259 mol%, while the bottoms reach 39.5 mol% propylene after the feed rate step and end at 23.8. The suggested configuration compensates the stage-70 measurement, closes the cascade with the

Table 4.5 Quality Structures Against Model Predictive Control on the Feed Composition Cases

Case (window)	Structure	IAE (mol% · min)	Giveaway (kmol)	Off-spec (min)	More than 0.01 below (min)	Lowest purity (mol%)	Propylene product (kmol)	Plans, fallbacks
F (900 min)	inferential	175.1	0.2	767.1	751.0	99.156	8193	—
	cascade	47.5	0.2	789.5	774.1	99.386	8037	—
	analyzer only	37.8	3.3	0.0	0.0	99.512	7904	—
	predictive	13.6	1.2	0.0	0.0	99.502	7954	180, 0
D, $\theta_{GC} = 60$ min (900 min)	inferential	175.1	0.2	767.1	751.0	99.156	8193	—
	cascade	48.3	0.2	792.0	777.9	99.375	8040	—
	analyzer only	37.5	3.3	0.0	0.0	99.510	7905	—
	predictive	13.3	1.2	0.0	0.0	99.504	7953	180, 0
Scenario 11 (1800 min)	inferential	220.4	13.6	452.1	407.1	99.269	15672	—
	cascade	123.3	8.1	355.8	327.8	99.364	15775	—
	analyzer only	144.0	6.9	817.0	778.6	99.323	15778	—
	predictive	23.2	1.0	942.3	324.2	99.459	15805	360, 0

IAE, giveaway and off-specification minutes (below 99.5 mol%) are the scorecard's, on the true distillate composition from $t = 0$, and the next column counts the minutes more than 0.01 mol% below over the same steps. The lowest purity follows the first event. The reboiler duty is 1371 GJ at 900 min and 2743 GJ at 1800 min in every row. Cases F and D are noise free, so their inferential and cascade rows differ in the third decimal from Table 4.4. Diagnosis runs on scenario 11, not part of the application: handed the true present purity, the predictive controller spends 689.3 min below specification, 192.2 of them more than 0.01 below, and with its band from the first step 797.0 min. With the target set above the specification it spends 336.1 min below with 1.78 kmol of giveaway at 99.51 mol%, 111.0 min with 4.26 kmol at 99.53, and none with 7.35 kmol at 99.55.

validity hold, applies the tuned set, floats the pressure to a 16.2 bar floor and raises the boilup to 8500 kmol/h. It passes with a worst error of 0.103 mol%, below target at 1208 min, inside the band with 0.017 to spare, and 5.72 mol% in the bottoms, although the condenser valve is saturated from the cooling water step onward. Every case starts its column at steady state on the case's own boilup and reflux ratio, so the higher boilup acts from the first scan through the reboiler lag and the configuration gives one run whether it is chosen before the run or carried through Reset. An automated check confirms that the suggested configuration meets the target, so the challenge cannot be set without a demonstrated solution.

4.6.7 Comparison With Model Predictive Control

Table 4.5 sets the closed-loop structures of Table 4.4 against the predictive controller. Case F is scenario 8's feed step, 72 to 78 percent at 60 min with a 20 min analyzer, and case D is the same with a 60 min cycle. Scenario 11 adds a step to 70 percent at 900 min, floats the pressure toward a 15.5 bar floor and carries thermowell noise of 0.01 °C and analyzer noise of 0.02 mol%. Every row has the same seed and instruments, the analyzer-fed structures work to the same 99.5 mol% target, the shipped structures keep their shipped tuning, the predictive controller keeps the settings of scenario 11 on every case, and none receives a preview.

The predictive controller has the least integrated error on every case, the least giveaway on scenario 11, and the least on cases F and D among the structures that hold the specification. The inferential loop and the cascade give away only 0.2 kmol on cases F and D because they spend more than 760 min below it. On case F the plan integrates 13.6 mol% · min against 37.8 for analyzer direct, because it reads the feed change in the tray. Its disturbance estimate passes 10^{-3} at 69.1 min, nine minutes after the step, and by 180 min it has cut the ratio from 14.02 to 13.29, while analyzer direct has taken 0.04 off its ratio. A 60 min analyzer cycle hardly matters to either (13.3 against 37.5), because the chromatograph samples rather than delays.

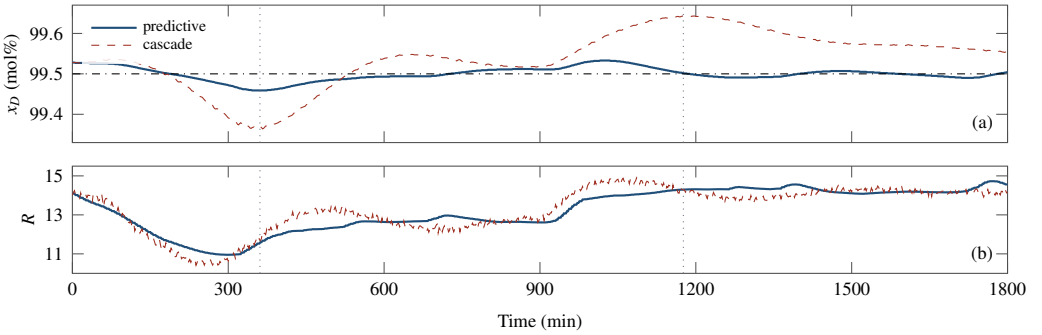


Figure 4.4 Scenario 11 under the predictive controller (thick solid line, blue) and under the cascade (dashed line, red). (a) True distillate composition against the 99.5 mol% specification (thin dash-dotted line). (b) Reflux ratio. The dotted verticals mark 361 min, the predictive controller's lowest purity, and 1176 min, the cascade's highest after the lean feed.

> **DID YOU KNOW? Hours Below Grade With a Fast Inner Loop**
>
> From the simulator (Table 4.5). On case F, the feed step with a 20 min analyzer, the cascade spent 789.5 min of the first 900 min below the 99.5 mol% specification. The analyzer working alone on the reflux ratio spent 0.0 min there.

On scenario 11 the plan's lowest purity is 99.459 mol% at 361 min against the cascade's 99.364 at 366 min, and after the lean feed the cascade carries the purity to 99.643 mol% at 1176 min while the plan stays at or below 99.533, as shown in Figure 4.4. The plan also walks the pressure setpoint onto its floor, about 16.26 bar, by 295 min, where the shipped minimization stops at 16.37 bar. The duty is 2743 GJ in every row, and the reflux the plan does not spend leaves as product, 15805 against 15 775 kmol of propylene.

The plan loses the off-specification minutes of scenario 11, 942.3 against 355.8 min, while the minutes more than 0.01 mol% below are level, 324.2 against 327.8. The root is that the target equals the specification for every structure and the reflux price holds the plan's prediction on that line, so errors of a few hundredths decide the side. Estimation error is only part of it, since with the true present purity the plan still spends 689.3 min below. The rest comes from the model's prediction, whose bias on ℓ reaches 0.304 here against 0.064 on case F, and from the first hour of each plan, which the band leaves free. With an exact estimate the plan still rides the line, 268.5 min below on case F run to 1800 min and 115.0 min on it with a 5 min cycle, all within 0.01 mol%. The free hour costs no start-up minutes, since no case has a predictive off-specification minute in its first hour, and a band from the first step still loses the tile, 797.0 against 355.8 min. The back-off in the note to Table 4.5 removes the loss at a price. Raised 0.01 mol% at a time, the target first keeps every minute within 0.01 of the specification at 99.53 mol%, with 4.26 kmol of giveaway, and at 99.55 mol% the plan spends no minute below while giving away 7.35 kmol, still less than the cascade's 8.07.

The model's reach ends where its inputs end. On the challenge with the suggested configuration and the plan in place of the cascade, the worst error after 1200 min is 0.038 mol% against 0.103, but the run spends 1166.1 min below specification against 811.5 and reaches 99.727 mol% after feed rate and cooling water steps the model does not contain.

4.7 Technology in Practice

Figure 4.5 draws the quality loops of Section 4.5, the pressure loop and the predictive option with the hardware of a splitter in place of the schematic's symbols.

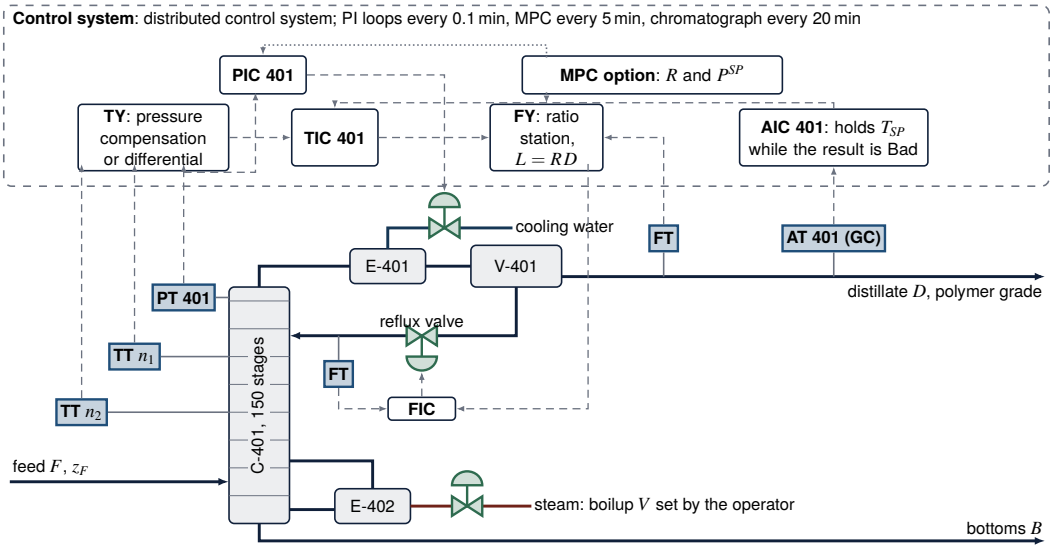


Figure 4.5 The splitter's loops with their hardware. Blue boxes are sensing devices: PT 401 on the overhead, the control and reference tray thermometers TT n_1 and TT n_2 in their thermowells, flow transmitters on the distillate and the reflux, and AT 401, the product chromatograph. Green symbols are final elements: the reflux valve in its flow loop, the cooling water valve and the steam valve, which the operator sets. Dashed arrows are signals, dotted arrows the moves that the MPC option writes. Notice that the only reading of the product arrives every 20 min, while everything the tray loop acts on is continuous. Not to scale, and not a piping diagram.

What Measures It

The controlled quality is the propylene in the distillate, read by a process chromatograph on the product line. Chromatographs are a very common choice for monitoring and controlling distillation columns [20]. Beneath it the tray loop reads a temperature in a thermowell and the overhead pressure. The chapter's chromatograph reports every 20 min, its thermowell lags by 0.6 min and its pressure transmitter is filtered over 0.1 min.

> **TECHNOLOGY** **Sensor: Resistance Thermometer in a Thermowell**
>
> A resistance thermometer is a fine wire of pure metal, usually platinum, whose resistance rises almost linearly with temperature, and 100 Ω at 0 °C is a common reference value. The measuring current warms the wire, so the reading errs high unless the current is small or pulsed [20]. Platinum elements span about −200 to 800 °C and are chosen for high accuracy and precision, best at the lower temperatures [21]. A thermowell lets the element be changed without opening the column, but its metal adds a first-order lag, and an air gap at the bottom of the well adds a second one, which can unsettle a loop. Transmitters close together on a column can disagree where the flow past them differs [20].

What Moves It

Two valves carry the loops. The reflux valve sets the internal traffic of the column through its flow loop and the ratio station, and the cooling water valve sets the overhead pressure. A third, the steam to the reboiler, is left to the operator, which is why the floating-pressure saving of Section 4.6 appears in megawatts only when someone cuts the boilup. The chapter's cooling water valve saturates on a warm afternoon.

TECHNOLOGY Final Element: The Reflux Valve Under a Ratio Station

The reflux is moved by a control valve inside a flow loop, and that loop's setpoint comes from a ratio station. The station measures a wild flow, here the distillate, multiplies it by an adjustable constant and hands the result to the captive flow's controller. Excess friction in the valve makes the stem stick and then jump, and leaves it deaf to small reversals of its signal. Poorly kept valves without positioners can show more than 10 % of this hysteresis, which up-and-down steps of the output in manual reveal [20]. The chapter's reflux is the ratio times the distillate filtered over 3 min, and a 0.09 °C setpoint step moves the ratio by 2.4 %.

Where the Controller Runs

A distributed control system has a supervisory level that sends set points to its field controllers, and its loops are sometimes cascaded, one loop's set point taken from another's process variable, at cycle times from milliseconds to minutes [22]. The app's PI loops execute every 0.1 min, the predictive controller every 5 min, and the chromatograph reports every 20 min. The structure maps onto standard blocks: an arithmetic block for the compensation or the difference, a PID block whose setpoint is written by the analyzer's PID, a ratio station, and a flow loop. The validity hold has a ready home in fieldbus function blocks, which pass each value with a status of Good, Bad or Uncertain. A smart device can flag its own data as Bad, and a block that receives a Bad input can be configured to hold its output at the last Good value [20].

What Is Modernizing It

The first development is the heat pump. In mechanical vapor recompression the overhead vapor is compressed so that it condenses hot enough to drive the reboiler. The practice is limited to mixtures whose relative volatility is close to one, which makes propane/propylene splitters important examples, and heat-integrated columns are projected to save up to 50 % more than recompression [23]. The same guide reports that floating pressure has cut winter energy use by up to 25 % in case studies. The second is the soft sensor. A 2009 survey counted 439 industrial soft-sensor applications, 331 of them on distillation, and one of their purposes is to validate an online analyzer against the estimate [24]. The compensated tray temperature of this chapter is a soft sensor of the plainest kind. The third is the layer above the loops. A 2003 survey found predictive control well founded in refining and petrochemicals [16], and the predictive controller of Section 4.5.5 removes giveaway at the price of minutes below the specification.

IN PRACTICE Giveaway Shows on the Shift Log

An energy guide for petrochemical plants advises a routine. Compare the design reflux with the ratios each shift runs, and compare the steam used with the reflux ratio and the purity every day. Many plants purify more than the specification asks, and the cure costs little: lower the reflux in small steps until the purity just meets it, which lowers the reboiler duty. In one reported case a debutanizer ran at maximum reflux and boilup to stay on grade through feed changes, and an online chromatograph kept it on specification so much more often that the energy saved paid for the analyzer in three months [23].

4.8 Limitations

The model is a teaching representation of a superfractionator and not a design tool. The separation is binary, so contaminant specifications cannot be studied. There is no energy balance and no hydraulic capacity limit, so the constraint that most often stops a real splitter, flooding before the reboiler runs out, is absent. Tray efficiency is constant, which removes a common way for a column to lose separation while every instrument reads normally.

The instrument chain is idealized. The chromatograph is a perfect sampler with a cycle time and two explicit fault modes, freeze and bias, and a real analyzer has more ways to be wrong than either. The thermowell is one lag, and matched high-resolution sensors on a real column drift relative to

one another, which is the practical reason a differential measurement is harder to maintain than its steady-state performance suggests.

Finally, the pressure-compensation coefficient is exact in the model. On a real column it is fitted at commissioning from a steady-state model, and a coefficient carried through two control system migrations without being re-derived is one of the more common quiet faults in this service. The application can show what a wrong coefficient does only by having a learner type one in.

The predictive controller's model was identified at the design point with stage 70 as the control tray, so another tray is a mismatch only the analyzer bias corrects, and beyond the horizon smaller steps fall 3.5 percent short of its ratio response and 20 percent short of its feed response at 48 h. The boilup, the feed rate and the cooling water reach it only through the tray and the analyzer. Its target is the specification, with no back-off by default.

> **OPEN CHALLENGE** **Keeping an Inferential True**
>
> Tray temperature control assumes that a temperature held at its setpoint keeps the product on specification. When the feed composition or rate of a multicomponent column changes, that assumption fails, and pressure moves the temperatures as well. Distillation is the main target of soft sensors, and in a 2009 survey of engineers that a 2013 review reports, accuracy lost to changes in the process was the problem named most often, at 29 %, which makes model maintenance the most critical issue. Progress means estimators that stay accurate without maintenance [24]. The compensation coefficient of this chapter is such a model.

4.9 Discussion

Three conclusions from this column generalize beyond distillation.

The first is that the speed of a measurement must be judged against the plant and not against a clock. A twenty-minute analyzer is slow on a heat exchanger and fast on a superfractionator, and on this column the measured penalty for moving the analyzer cycle from 5 to 60 min is 0.009 mol% of peak departure. Effort spent shortening that cycle would be effort wasted, while effort spent on validity logic is worth 0.27 mol% of settled composition when the chromatograph freezes.

The second is that a proxy measurement should be selected for fidelity rather than for sensitivity. The most sensitive tray in the column is a poor inferential for the distillate because it responds to a great deal the distillate does not see. The rule of thumb that selects the steepest point of the temperature profile answers a different question, which is where the signal-to-noise ratio is best, and the two answers coincide only when the sensor is near the product.

The third is that removing a disturbance from a measurement is not the same as removing it from the process. The differential temperature cancels pressure at the thermometer almost perfectly and still lets the distillate fall 0.63 mol% through a held 0.6 bar pressure change, because pressure enters the column twice, once through the bubble point and once through the relative volatility. A compensation scheme derived from the measurement equation alone cannot know that.

> **OPEN CHALLENGE** **Separating Propylene Without a Tall Column**
>
> Distillation needs more than 100 stages to make polymer-grade olefins, because the relative volatility of propylene and propane is low, and a 2020 review sees membranes as the promising alternative. A membrane with a selectivity above 10 could be paired with distillation to save energy, and one above 35 could work alone. Yet the carriers that make some membranes selective are unstable, through the reduction of silver ions, the disproportionation of copper ions and poisoning by sulfides, which limits long operation, and framework membranes still need ways to be made at large scale. Progress means membranes that stay selective in long operation and can be built at industrial scale [6].

4.10 Conclusion

A propylene splitter is a plant on which the first experiment a control course teaches cannot be performed. The simulated column of this chapter is 53 percent complete four hours after a three

percent reflux ratio step and needs 715 min to fall below 20 ppm/h of impurity drift, so the identification must be done on a secondary measurement and the primary measurement must arrive intermittently. The tray temperature that results is a bubble point, and its 3.10 °C/bar pressure term is large against a composition profile spanning 5.80 °C over 151 stages, which is why an uncompensated measurement runs the reflux ratio into its stop on a 0.4 bar excursion. Measured on the same feed disturbance, the analyzer placed directly on the ratio station departs 0.063 mol% against 0.143 for the cascade and 0.373 for the inferential alone, and the ordering reverses the moment the chromatograph freezes, where a cascade that keeps integrating the stale result until its validity hold is armed settles at 98.90 mol% and is worse than having no cascade at all. Selecting the control tray for sensitivity rather than fidelity costs 0.19 mol% of composition at fifteen hours. A model predictive controller, the fifth setting, cuts the giveaway of scenario 11 from 8.1 to 1.0 kmol and loses its off-specification minutes, 942 against 356 min, by riding the specification. A fuller model would add an energy balance so that reflux subcooling and feed enthalpy reach the internal traffic, a hydraulic capacity limit so that flooding can end an experiment the way it ends a real push, and a multicomponent feed so that a product can fail on something this separation does not address. The superfractionator is an accessible browser platform for learning what a soft sensor measures and what a supervisory layer is for.

KEY POINTS

- The column answers so slowly that a step test does not finish in a shift, so a tray thermometer stands in for a product analyzed every twenty minutes.
- A tray temperature is a bubble point, and its pressure term of 3.10 °C/bar is large against a profile of 5.80 °C.
- On the feed step the analyzer alone departs 0.063 mol% against 0.143 for the cascade, and with the chromatograph frozen the cascade without its hold settles at 98.90 mol%.
- Choosing the tray for sensitivity rather than fidelity costs 0.19 mol% at fifteen hours.

Where else this applies. A fast inferred measurement corrected by a slow assay returns in Volume 5, Chapter 11 and Volume 19, Chapter 10, and an inferential measurement carrying bias and noise in Volume 15, Chapter 3.

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4.11 Exercises

4.1 ○ Concept check · 2 min

On the feed composition step of scenario 8, moving the analyzer cycle time from 5 to 60 min changes the peak purity departure of the analyzer-only loop only from 0.061 to 0.070 mol%. Which explanation is right?

(a) The loop is tuned so slowly that it never acts on a single analyzer result

(b) The cycle is short against a response that is 63 percent complete only at 5.2 h

(c) The tray temperature carries the feed change to the loop before the analyzer reports

(d) The analyzer noise is larger than anything a shorter cycle could have detected

4.2 ○ Concept check · 2 min

The most sensitive stage in the column is stage 127, about eight times as sensitive to the reflux ratio as stage 70. Why is it a poor control tray for the distillate?

(a) Its thermowell noise is amplified eight times by the higher sensitivity

(b) It sits below the feed, so a change in the reflux ratio never reaches it

(c) It responds to a great deal that the distillate composition does not see

(d) Its temperature is fixed by the reboiler duty and does not move with reflux

4.3 Concept check · 2 min

The difference between stages 90 and 70 moves only 0.0012 °C when the pressure rises by a tenth of a bar, against 0.312 °C for a single tray. Held near its setpoint through a 0.6 bar pressure step, it still lets the distillate fall 0.63 mol%. Why?

(a) The differential loop drives the reflux ratio onto its limit of 24 after the step

(b) The two thermowells have different lags, so the difference reads the transient as composition

(c) The difference cancels the pressure term only while the pressure is changing, not after

(d) Pressure also lowers the relative volatility, which moves the profile the difference stands for

4.4 Theory and calculation · 6 min

The splitter separates propylene from propane at a relative volatility $\alpha = 1.12$ at 18 bar. For a binary pair, the Fenske minimum stage count and the Underwood minimum reflux ratio for a saturated liquid feed are

$$N_{min} = \frac{\ln\left[\frac{x_D}{1-x_D}\,\frac{1-x_B}{x_B}\right]}{\ln \alpha}, \qquad R_{min} = \frac{1}{\alpha - 1}\left[\frac{x_D}{z_F} - \frac{\alpha\,(1-x_D)}{1-z_F}\right].$$

(a) Find N_{min} for the design products, $x_D = 0.99528$ and $x_B = 0.05986$. *Checkpoint:* 71.5 stages.

(b) Find R_{min} for $x_D = 0.995$ and $z_F = 0.72$. *Checkpoint:* 11.35.

(c) Floating pressure takes the column to 15.5 bar. Use Equation (4.3) to find α there, repeat (a) and (b), and compare the design reflux ratio of 14.17 with R_{min} at both pressures. *Checkpoint:* $\alpha = 1.13875$, 62.4 stages, $R_{min} = 9.81$.

4.5 Theory and calculation · 5 min

The column boils up $V = 7494$ kmol/h at a reflux ratio $R = 14.17$, and the drum level holds $D = V - L$ under constant molar overflow.

(a) Use Equation (4.6) to find the distillate and the reflux flows. *Checkpoint:* 494.0 kmol/h and 7000 kmol/h.

(b) The reflux flow is raised by 1 % at constant boilup. Find the new distillate flow and its change in percent. *Checkpoint:* 424.0 kmol/h, −14.2 %.

(c) The reflux ratio is raised by 1 % instead. Find the new distillate flow and its change in percent, and explain why the manipulated variable is the ratio. *Checkpoint:* 489.4 kmol/h, −0.93 %.

4.6 Theory and calculation · 8 min

Stage 70 holds liquid at $x = 0.82$. Use Equations (4.4) and (4.5) with the parameters of Section 4.3, and take the steady-state gain of stage 70 as −0.047 °C per 1 % increase of the reflux ratio.

(a) Find the rise of the stage-70 temperature when the pressure goes from 18.0 to 18.1 bar at constant composition. *Checkpoint:* 0.312 °C.

(b) Express that rise as the change of reflux ratio, in percent, that an uncompensated tray loop would make to cancel it. *Checkpoint:* 6.6 %.

(c) The pressure goes from 18.0 to 18.4 bar. Find the error left in the compensated reading of Equation (4.8) with $P_{ref} = 18$ bar and $\mathrm{d}T/\mathrm{d}P = 3.10\,°\mathrm{C/bar}$, in °C and in percent of reflux ratio. Then name what makes the ratio settle 1.7 % above its starting value in scenario 5. *Checkpoint:* 0.0028 °C, 0.06 %.

4.7 App challenge · 8 min

Load scenario 1, "1 · The step test that does not finish (MANUAL)", at the default seed. The case starts in Manual. Before Run, set Reflux ratio to 14.60. Run at speed 200 (200 min per wall-clock

second) until the clock passes 900 min, pause and export the CSV. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from minutes.

(a) In column `settle_ppm_h`, the drift rises above 100 ppm/h soon after the step. Find the first later row below 20 ppm/h. *Checkpoint:* 715 min.

(b) In column `xD_pct`, read the rows at 120.0 and 240.0 min. The step finally takes the distillate from 99.528 to 99.638 mol%. What fraction of the change has arrived at each time? *Checkpoint:* 99.560 and 99.586, 29 and 53 percent.

(c) Explain what a first-order fit to the first two hours would report about this column, and why the drift column is the better guide. *Checkpoint:* A time constant too short and a gain too low.

4.8 App challenge · 8 min

Load scenario 5, "5 · The thermometer is a pressure gauge first", at the default seed with no change. The pressure setpoint steps from 18.0 to 18.4 bar at 60 min, and the measurement switches to Pressure-compensated at 300 min. Run at speed 200 until the clock passes 2400 min (about 12 s), pause and export the CSV. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from minutes.

(a) Column `reflux_saturated` turns to 1 when the ratio sits on a limit. Find the first such row after 60 min, and read the commanded ratio in column `reflux_ratio_cmd` of that row. *Checkpoint:* 91.8 min, 24.00.

(b) In the row at 300.0 min, read `xD_pct`, `tray_raw_C` and `tray_comp_C`, and explain the difference between the two temperatures. *Checkpoint:* 99.892, 47.410 °C and 46.170 °C.

(c) After 300 min, find the lowest `reflux_ratio_cmd` and its time, and read `reflux_ratio_cmd` and `alpha` in the row at 2400.0 min. *Checkpoint:* 13.56 at 750 min, then 14.37 and 1.1170.

4.9 App challenge · 10 min

Load scenario 11, "11 · The answer arrives tomorrow; the plan is made now", at the default seed. Quality control is on MPC. For each run below, run at speed 200 until the clock passes 1800 min (about 9 s), pause and export the CSV, and read `metric_giveaway_kmol` and `metric_offspec_min` in the row at 1800.0 min and the lowest `xD_pct` with its time. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from minutes.

(a) Run the case as loaded. *Checkpoint:* 0.98 kmol, 942.3 min, 99.459 at 361 min.

(b) Press Reset, set Quality control to Cascade before Run, and run again. *Checkpoint:* 8.07 kmol, 355.8 min, 99.364 at 366 min.

(c) Press Reset, set Quality control back to MPC and Propylene purity target to 99.53 mol% before Run, and run again. Explain why the minutes below specification fall. *Checkpoint:* 4.26 kmol, 111.0 min, 99.491.

4.10 Application area · 4 min

A site energy engineer commissions pressure minimization on this column. A month later the reboiler duty has not changed. Using the results of scenario 10, explain why, what must be added for the saving to appear as energy, and what that addition must do on a warm afternoon.

4.11 Application area · 3 min

An operations manager wants to use the simulator to decide how far the feed can be pushed above 790 kmol/h by raising the boilup. Name two things the model leaves out that decide that answer on a real splitter, and say what the app would show instead.

4.12 Review the agent · 5 min

An AI assistant reviewing this column writes: “Table 4.4 shows that the analyzer alone departs 0.063 mol% on the feed step against 0.143 mol% for the cascade, and is back at 99.51 at fifteen hours while the cascade is at 99.47. The TIC-401 inner loop therefore adds nothing. Put AIC-401 straight on the ratio station and retire the tray thermowells.” Find the flaw, and say how you would check it in the app.