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CHAPTER 7

A Paraxylene Simulated Moving Bed Whose Purities Exist Only as Cycle Averages

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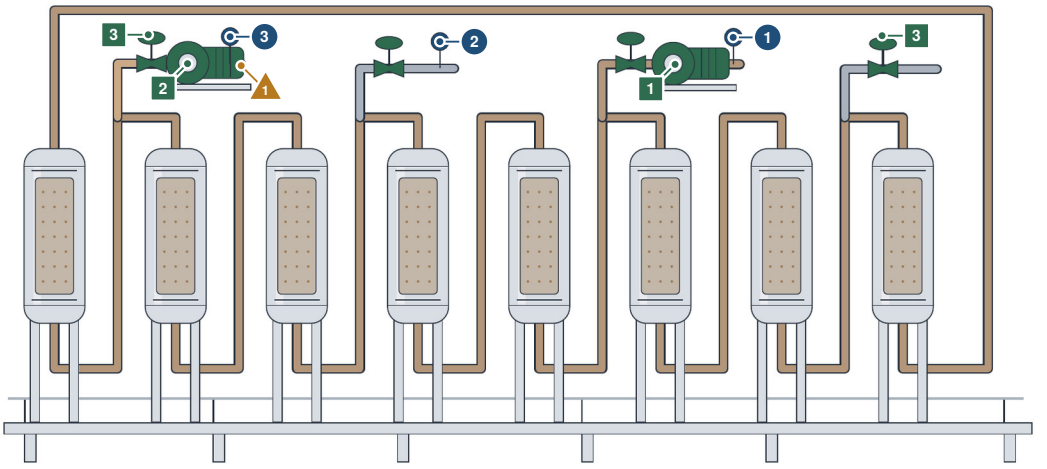
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CHAPTER 7

A Paraxylene Simulated Moving Bed Whose Purities Exist Only as Cycle Averages



The controller moves 1 extract pump, for the purity of the extract 2 feed pump, for the paraxylene lost to the raffinate 3 port valves, stepped one bed every switch by the sequencer

The controller reads 1 extract purity analyzer, one report a cycle 2 raffinate purity analyzer, one report a cycle 3 feed analyzer, which the predictive controller reads

What disturbs it 1 a feed that turns richer in paraxylene ▲ an adsorbent that slowly loses capacity

Notice that the three analyzers report once a cycle from the streams entering and leaving the ring, while the port valves move the four streams one bed forward every switch, two beds apart in the chapter's model. Illustration, not to scale.

IN PLAIN TERMS A Purity That Exists Only as an Average

The main idea. A solid holds paraxylene, the raw material of polyester, a little more tightly than the look-alike liquids around it. The solid fills a ring of beds, and the inlets and outlets step one bed on at set times, as if the solid moved.

The challenge. So the liquid that leaves keeps changing, and its purity is known only as an average over a full turn. The flows can be set right only once a turn, while the feed changes and the solid wears out.

Why it matters. In the simulated plant a change made once a turn keeps the product pure, and no fixed setting does.

THREE WAYS TO READ THIS CHAPTER

Explore	12 min	This page, the Did you know? box in Section 7.1, the History boxes in Section 7.2, the Try it boxes in Sections 7.4 and 7.6, the Did you know? box in Section 7.6, and Key points in Section 7.9. No equations.
Study	45 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
Practice	15 min	This page, Section 7.6 with Figure 7.5, Section 7.7, and Section 7.8 with its Open challenge box.

The control question A simulated moving bed has no steady state, and its purities exist only as twelve-minute averages reported once a cycle. Which flow-rate ratios keep both outlets on specification, and how much can a correction made once a cycle hold through a richer feed and an aging adsorbent?

Learning objectives

- Compute the zone flows, the port flows and the desorbent ratio of the ring from its flow-rate ratios and switching time.
- Construct the ideal triangle from the isotherm and explain why the simulated unit needs a margin from its edges.
- Explain the cyclic steady state and why a purity exists only as a cycle average.
- Compare cycle-to-cycle PIs on the logarithm of each impurity with a repetitive MPC through a feed step and an aging adsorbent.
- Name the pump that delivers off its meter from the pattern of the two purity analyzers.

Prerequisites Sections 1.4.7 (cyclic units and cycle-to-cycle control), 1.6.2 and 1.6.4. Section 1.6.3 only for the predictive controller. Chapter 5 runs a cycle-to-cycle loop on another cyclic unit.

The app https://apmonitor.com/apps/smb-paraxylene/

See also Volume 8, Chapter 11 for an adsorbent whose capacity is not measured, Volume 8, Chapter 9 for corrections made while results are still in flight, and Volume 8, Chapter 10 for learning from one layer to the next. Volume 9, Chapter 2 for a step-response predictive controller behind a dead time.

7.1 Introduction

No reading of the extract stream of a simulated moving bed is its purity. In the eight-bed ring simulated here, every 90 s the four ports that admit desorbent and feed and withdraw extract and raffinate move one bed forward, and the liquid leaving at the extract port comes from a different bed after each move. Ten cycles after a start-up, when every switch repeats the previous one shifted by one bed to better than one part in a million, the paraxylene content of the extract (desorbent-free) still runs from 99.40 to 99.98 % inside a single switch, while its average over the twelve-minute cycle is 99.89 %. Only that average is steady, only that average is sold, and only that average can be measured as a composite sample once a cycle.

DID YOU KNOW? Most of the Feed Comes Back

A classical paraxylene plant drawn in a 2010 study makes 250 thousand tonnes a year. The other isomers that leave its adsorber go to an isomerization reactor and return, and that recycle loop makes up the major part of the adsorber's feed [1].

Two beliefs that a block diagram leaves in place are the simulator's targets. The first is that a quality variable has a value at every instant that a controller can track. Here a purity exists only over a whole cycle, it arrives 2 min after the cycle ends, and a move of a flow shows fully only several cycles later. The second is that being inside a design region means being on specification. The triangle of equilibrium theory, which turns an isotherm into the two flow-rate ratios that decide both purities [2, 3], is drawn for an ideal unit with no dispersion and no mass-transfer resistance. With the dispersion of thirty mixing cells per bed, the left edge that protects the extract sits at $m_2 = 0.422$ on the triangle at $m_3 = 0.82$, while the simulated unit needs $m_2 \geq 0.568$ to reach 99.7 %. Processes that are corrected once per run, batch, lot or cycle from the measured outcome of the last form a class of their own, treated as run-to-run, iterative learning and repetitive control [4, 5], and a repetitive model predictive controller has been applied to a simulated moving bed [6]. Section 1.4.7 sets out the integral loop that such a unit closes once a report, and Volume 8, Chapter 10 learns in the same way from one layer of a part to the next.

However, a student rarely meets that class on a plant whose cycle can be watched. Models of industrial paraxylene units are written to study design, revamping and aging [7–9], controllers for simulated moving beds are reported on sugar and pharmaceutical separations [10–12], while the standard examples of run-to-run control come from batch reactors and semiconductor lots [4]. This chapter follows one simulated eight-bed paraxylene ring whose sequencer, cycle composites, triangle and purity controllers can be watched switch by switch. It asks what fixed ratios, cycle-to-cycle feedback and a repetitive predictive controller can hold through a richer feed, an aging adsorbent and a sixty-cycle challenge, and how much of the answer belongs to the bed's declared dispersion. The mixing-cell model, the triangle, the velocity-form PI law and the linear predictive controller are standard. What the chapter adds are measurements on one synthetic unit, among them that the challenge's verdicts hold at the shipped thirty cells per bed at five seeds and with the step halved, but change at 20, 45 and 60 cells. The model has 973 states, its paraxylene balance closes to 1.9×10^{-14} of the feed per cycle, its triangle matches an independent derivation to 2×10^{-16}, and its controllers read the analyzers and meters only. Nine graded cases judge both the learner's actions and the condition of the ring.

Section 7.2 follows the process from the patent to equilibrium theory. Section 7.3 sets out the ring as modeled: mixing cells, pumps and flow-rate ratios, cycle averages, the triangle and the instruments. Section 7.4 shows how the ring reaches its cyclic steady state, where the simulated unit meets its specification against the triangle, and which ratio moves which purity. Section 7.5 describes the fixed ratios, the cycle-to-cycle PIs and the repetitive MPC, and the design choices behind them. Section 7.6 reports the nine cases, Section 7.7 names the hardware and the practice behind the model, and Section 7.8 states what the model leaves out. The exercises at the end of the chapter run the cases in the app.

7.2 Moving the Ports Instead of the Solid

A true countercurrent of adsorbent and liquid would separate two components continuously, but it requires moving the solid. The arrangement that avoids it, told in the first History box below, keeps the beds still and advances the ports, so that relative to the ports the solid moves the other way. One of the first industrial applications was the recovery of paraxylene from mixed xylenes, and the units known publicly as UOP's Parex, IFP's Eluxyl and Toray's Aromax run in the liquid phase near 180 °C and 9 bar [8]. Paraxylene is the raw material of terephthalic acid, which is made into polyethylene terephthalate [1].

> ⧖ HISTORY **Fixed Beds With Moving Ports, 1957**
>
> A patent filed by Broughton and Gerhold in 1957 and issued in 1961 kept the sorbent still in a series of fixed beds and moved the inlets and outlets instead, shifting them downstream in equal steps so that the liquid met the sorbent as in a countercurrent. The patent aims the method at sorbents too fragile to be carried from zone to zone without losing their activity to attrition. To shift the ports it offers either a manifold of valves opened and closed by timed electric switches or a circular valve whose plug turns in a housing ringed with ports, two inlet passages alternating with two outlet passages [13]. In 1989 an article analyzed counter-current and simulated counter-current adsorption separation processes together [14].

Design moved from trial to equilibrium theory, as the second History box below tells, and its construction for nonlinear isotherms in simulated moving bed units [3] is the triangle in the plane of the zone II and zone III ratios that the simulator draws. Models of the industrial paraxylene unit followed [7], and a later study built one on measured xylene equilibria and kinetics on ion-exchanged faujasite as a tool to train operators and to choose operating conditions [8], while the loss of adsorbent capacity over a unit's life became a modeling question of its own [9]. A study of an industrial-scale unit states the specification the simulator adopts, paraxylene in the extract above

99.7 % with recoveries around 97 %, and models each bed with forty finite volumes to stand for its axial dispersion [1].

> ⧖ HISTORY **Drawing the Region in Advance, 1993**
>
> In 1993 a design procedure for the four-section unit was built in the frame of equilibrium theory, for a binary mixture with a desorbent of intermediate strength and a constant-selectivity isotherm, with mass-transfer resistance and axial mixing neglected. Requiring complete separation gave explicit bounds on the flow-rate ratios of the four sections, a region that can be drawn in advance from the adsorption constants and the feed composition. The same work analyzed the disturbances a unit meets, set criteria for a robust design and compared the theory with experiments on a six-port simulated moving bed run in the vapor phase [2]. In 1997 the construction was carried to nonlinear chromatographic separations [3].

Control came later than design. Model-based control of a simulated moving bed was reported for the separation of fructose and glucose [10], a repetitive model predictive controller that corrects the unit from one cycle to the next was applied to a simulated moving bed chromatography system [6], and automatic control of simulated moving beds was developed alongside [11]. The optimization and control of chromatography have been treated together [12]. Simulated moving beds serve the sugar, petrochemical and pharmaceutical industries, and their systematic optimization on the fully discretized cyclic model has been demonstrated [15]. Model predictive control in general is widely applied in the process industries [16]. The records read for this chapter do not describe the purity control of a commercial paraxylene unit, and the simulator's loops are offered for teaching, not as a description of how industrial units are run.

7.3 The Ring as Modeled

The unit is generic, taken from no licensor's design or operating plant, as shown in Figure 7.1, and its composition profile is unrolled in Figure 7.2. Eight beds of 20 m^3 and void fraction $\varepsilon = 0.40$ stand in a closed ring, numbered 1 to 8 in the direction the liquid flows. With the ring shift s $(0,\dots,7)$ the desorbent D enters at the inlet of bed s, the extract E leaves at the outlet of bed $s+1$, the feed F enters at the inlet of bed $s+4$ and the raffinate R leaves at the outlet of bed $s+5$ (bed numbers modulo 8), which makes four zones of two beds each. Zone I strips the paraxylene off the solid, zone II pushes the other C_8 back from the extract port, zone III holds the paraxylene back from the raffinate port and zone IV cleans the liquid that recirculates to zone I. Every switching time t_s the shift advances by one, and eight switches make a cycle. The engine's clock is the minute, flows are in m^3/s internally and reported in m^3/h, and compositions are liquid volume fractions. The feed is the C_8 cut with a paraxylene fraction x_F of 22 % at design, and the rest of the liquid is desorbent.

Table 7.1 gives each variable's role, its value at the design point, $m = (1.40, 0.62, 0.82, 0.30)$ at $t_s = 90$ s, and its range.

7.3.1 Mixing Cells, Mass Transfer and the Isotherm

Each bed is $N_c = 30$ mixing cells in series of volume $V_c = V/N_c$. In each cell the liquid fractions of paraxylene (A) and of the other C_8 aromatics lumped as one component (B) and their adsorbed amounts are states, as shown in Equation (7.1).

$$\begin{aligned} \varepsilon \frac{\mathrm{d}c_i}{\mathrm{d}t} &= \frac{Q_z}{V_c}\,(c_{i,\mathrm{in}} - c_i) - (1-\varepsilon)\frac{\mathrm{d}q_i}{\mathrm{d}t} \\ \frac{\mathrm{d}q_i}{\mathrm{d}t} &= k\,(q_i^{*} - q_i), \qquad q_i^{*} = \frac{N K_i c_i}{1 + K_A c_A + K_B c_B} \end{aligned} \tag{7.1}$$

where $i = A, B$, Q_z is the liquid flow of the zone the bed is in, $c_{i,\mathrm{in}}$ is the outlet of the upstream cell (or a port node), q is the adsorbed amount as the liquid volume it would make per volume of solid, k is the linear-driving-force coefficient and q^{*} the competitive Langmuir equilibrium with the desorbent's

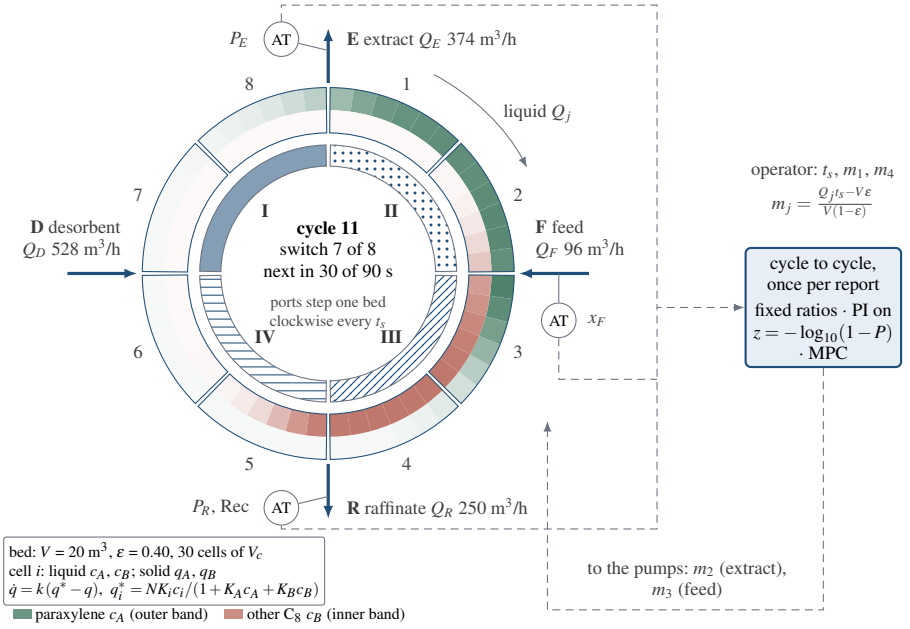


Figure 7.1 The eight-bed ring as modeled, redrawn from the Ring view of case 1 at $t = 130$ min, cycle 11, switch 7 of 8, with the unit at its cyclic steady state since cycle 10. Each bed's wedges are shaded by the paraxylene (outer band) and the other C_8 (inner band) in their liquid, the zones carry their own patterns, and the four ports sit where the sequencer places them at ring shift $s = 6$. The analyzers (AT) report cycle composites of the extract, the raffinate and the feed to the cycle-to-cycle layer, which sets m_2 and m_3. Not to scale.

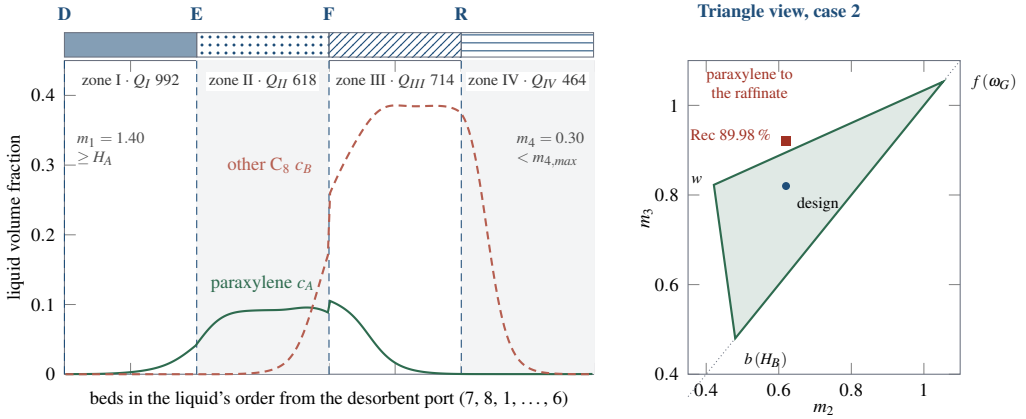


Figure 7.2 Left, the profile of the ring of Figure 7.1 unrolled from the desorbent port, paraxylene solid and other C_8 dashed, with the zone flows in m³/h. Right, the Triangle view of case 2 with m_3 held at 0.92 (square), above the upper edge wf, where the recovery over cycle 11 is 89.98 %. The dot is the design point. Left of the edge wb the other C_8 reaches the extract.

competition folded into the saturation capacity N and the affinities K_i. The Henry constants are $H_i = NK_i$, so $H_A = 1.20$, $H_B = 0.48$ and the selectivity K_A/K_B is 2.5 at design. Temperature and

Table 7.1 Variables, Their Roles and Design Values

Variable	Role	Design	Range
P_E	CV, extract analyzer	99.893 %	SP 99.00–99.95
P_R	CV, raffinate analyzer	99.868 %	SP 98.50–99.95
m_2	MV, extract pump	0.62	0.30–0.90
m_3	MV, feed pump	0.82	0.50–1.20
t_s	set, switching time	90 s	45–150
m_1, m_4	set, zones I and IV	1.40, 0.30	1.0–1.8, 0–0.6
x_F	DV, feed paraxylene	22 %	15–30
T	DV, adsorber temperature	177 °C	167–187
—	DV, aging rate	0	0–2 %/h
$c_{D,B}$	DV, other C_8 in desorbent	0	0–0.5 %
b	DV, one pump's meter bias	0	±5 %
σ	DV, analyzer noise	0.01 point	0–0.05
Rec, $\dot{m}_{PX}$	outputs	99.53 %, 18.10 t/h	—
c_A, c_B, q_A, q_B	states, per cell (960)	—	—
a	state, capacity (fresh = 1)	1	0.5–1

aging enter as shown in Equation (7.2).

$$\begin{aligned} K_i(T) &= K_{i,0}\exp\Big[-\frac{\Delta H_i}{R}\Big(\frac{1}{T}-\frac{1}{T_0}\Big)\Big] \\ k(T) &= k_0\exp\Big[-\frac{E_k}{R}\Big(\frac{1}{T}-\frac{1}{T_0}\Big)\Big] \\ N &= N_0\,a, \qquad \frac{\mathrm{d}a}{\mathrm{d}t} = -r_{age} \end{aligned} \tag{7.2}$$

where $T_0 = 177\,^\circ\mathrm{C}$, $\Delta H_A = -18\,\mathrm{kJ/mol}$, $\Delta H_B = -14\,\mathrm{kJ/mol}$, $E_k = 20\,\mathrm{kJ/mol}$, a is the capacity as a fraction of fresh and r_{age} the aging rate, held above $a = 0.5$. At 187 °C H_A falls to 1.081, the selectivity to 2.44 and k rises to $0.337\,\mathrm{s^{-1}}$, and at 167 °C they are 1.339, 2.56 and $0.266\,\mathrm{s^{-1}}$. The thirty cells stand for the bed's axial dispersion, the same device as the forty volumes per bed of an industrial model [1]. They are a declared physical choice rather than a converged grid, and the purities depend on them strongly. At the design point the extract purity is 97.18, 99.12, 99.89 and 99.98 % with 10, 15, 30 and 60 cells per bed.

7.3.2 Ports, Pumps and Flow-Rate Ratios

Four pumps realize the four zone flows. The desorbent, extract, feed and recycle pumps deliver Q_D, Q_E, Q_F and Q_{IV}, and the raffinate is what is left, as shown in Equation (7.3).

$$\begin{aligned} m_j &= \frac{Q_j\,t_s - V\varepsilon}{V(1-\varepsilon)}, \qquad j = I,\ldots,IV \\ Q_I &= Q_{IV} + Q_D, \qquad Q_{II} = Q_I - Q_E \\ Q_{III} &= Q_{II} + Q_F, \qquad Q_R = Q_{III} - Q_{IV} \\ Q_p &= (1+b_p)\,Q_{p,SP} \end{aligned} \tag{7.3}$$

where m_j is the ratio of zone j's liquid flow to the solid's apparent flow of one bed per switch, $Q_{p,SP}$ is the setpoint a pump's meter reads and b_p is a meter bias that makes one pump deliver more than its meter shows. The zone flows the beds see are rebuilt from what the pumps deliver, so a bias moves the true m while every meter still reads its setpoint. At design the zone flows are 992, 618, 714 and 464 $\mathrm{m^3/h}$, with 528 $\mathrm{m^3/h}$ of desorbent and 96 $\mathrm{m^3/h}$ of feed in and 374 and 250 $\mathrm{m^3/h}$ of extract and raffinate out. At each port node the incoming streams mix, as shown in Equation (7.4).

$$\begin{aligned} c^{I}_{i,\mathrm{in}} &= \big(Q_{IV}\,c_i^{IV,out} + Q_D\,c_{D,i}\big)/Q_I \\ c^{III}_{i,\mathrm{in}} &= \big(Q_{II}\,c_i^{II,out} + Q_F\,c_{F,i}\big)/Q_{III} \end{aligned} \tag{7.4}$$

where $c_F = (x_F, 1-x_F)$ and $c_D = (0, c_{D,B})$. The extract is drawn at the outlet of zone I and the raffinate at the outlet of zone III, each at the composition of the last cell there. A switching time entered during a switch takes effect at the next one, so every switch is whole and the flows, which follow t_s, never change inside it.

7.3.3 Cycle Averages and the Cyclic Steady State

Purity, recovery and production are integrals over each whole cycle of eight switches, as shown in Equation (7.5).

$$\begin{aligned} P_E &= \frac{\int Q_E c_A \, dt}{\int Q_E (c_A + c_B)\, dt}, \qquad P_R = \frac{\int Q_R c_B \, dt}{\int Q_R (c_A + c_B)\, dt} \\ \mathrm{Rec} &= 1 - \frac{\int Q_R c_A \, dt}{\int (Q_F x_F + Q_D c_{D,A})\, dt} \\ \dot{m}_{PX} &= \rho_{PX} \int Q_E c_A \, dt \,/\, \Delta t_{cyc} \end{aligned} \tag{7.5}$$

where the compositions are those at the extract and raffinate ports, $\rho_{PX} = 861\,\mathrm{kg/m^3}$ and $\Delta t_{cyc} = 8 t_s$. The recovery counts the paraxylene the raffinate did not take. At the cyclic steady state it equals the extract's paraxylene over the feed's, while after a change it does not count what the ring takes up or gives back. The extract-based definition read 73.15 % in the cycle after case 3's feed step, purely from the ring filling, while the loss-based one read 98.43 %, which is why the app uses the latter. The unit is declared at its cyclic steady state when, at every switch of a whole cycle, the profile differs from the one a switch earlier shifted by one bed by less than 10^{-6} in any liquid fraction, as shown in Equation (7.6).

$$\max_{b,n,i} \left| c_i(b+1, n, t_k) - c_i(b, n, t_{k-1}) \right| < 10^{-6} \tag{7.6}$$

where b is the bed, n the cell and t_k the instant of switch k.

Pause. Try Exercise 7.2 before reading on.

7.3.4 The Triangle

For the competitive Langmuir isotherm and a feed of fractions c_A^F and c_B^F, an ideal unit with no dispersion and no mass-transfer resistance gives both outlets pure inside a triangle in the (m_2, m_3) plane [3]. Its vertices $b = (H_B, H_B)$ and $f = (\omega_G, \omega_G)$ lie on the diagonal and w above it, where $\omega_G > \omega_F$ are the roots of Equation (7.7), with $\kappa_A = K_A c_A^F$ and $\kappa_B = K_B c_B^F$.

$$(1+\kappa_A+\kappa_B)\,\omega^2 - \left[H_A(1+\kappa_B) + H_B(1+\kappa_A)\right]\omega + H_A H_B = 0 \tag{7.7}$$

The two edges through w, wb and wf, are the lines of Equation (7.8), in that order.

$$\begin{aligned} \left[H_A - H_B(1+\kappa_A)\right] m_2 + \kappa_A H_B m_3 &= H_B(H_A - H_B) \\ \left[H_A - \omega_G(1+\kappa_A)\right] m_2 + \kappa_A \omega_G m_3 &= \omega_G(H_A - \omega_G) \end{aligned} \tag{7.8}$$

Left of wb the other C_8 is not pushed back in zone II and reaches the extract, and above wf the paraxylene is not held in zone III and reaches the raffinate. Zone I needs $m_1 \geq H_A$, and zone IV needs $m_4 < m_{4,max} = \frac{1}{2}\{\Theta - (\Theta^2 - 4H_B m_3)^{1/2}\}$ with $\Theta = H_B + m_3 + \kappa_B(m_3 - m_2)$. At design $\omega_G = 1.05280$, the base runs from 0.480 to 1.053, the vertex is $w = (0.421, 0.823)$, the upper edge at $m_2 = 0.62$ is $m_3 = 0.895$, the left edge at $m_3 = 0.82$ is $m_2 = 0.422$ and $m_{4,max} = 0.416$.

The app's triangle was re-derived by hand, and the vertex found as the intersection of the two lines agrees with the app's closed form to 2.2×10^{-16}. The construction is used here only for the competitive Langmuir case its source names in its title [3] and in the standard form given above. In the linear limit w falls on (H_B, H_A). The simulation itself reproduces the edges when it is made nearly ideal. With 60 cells per bed and $k = 3\,\mathrm{s^{-1}}$ the raffinate impurity at $m_2 = 0.62$ jumps from 0.003 % at $m_3 = 0.890$ to 0.50 % at 0.900, bracketing the line's 0.895. Zone IV fails between $m_4 = 0.41$

Table 7.2 Parameters. A: Adjustable in the Parameters Panel. V: Fixed and Stated in the Model Dialog

Symbol	Meaning	Value	
V, ε	bed volume, void fraction	20 m^3, 0.40	V
N_c	mixing cells per bed	30	V
N_0	saturation capacity, fresh	1.2 (0.9–1.5)	A
$K_{A,0}$, $K_{B,0}$	affinities at T_0	1.0, 0.4	A
ΔH_A, ΔH_B	heats of adsorption	−18, −14 kJ/mol	V
T_0	reference temperature	177 °C	V
k_0	mass transfer at T_0	0.30 s^{-1} (0.2–0.4)	A
E_k	its activation energy	20 kJ/mol	V
ρ_{PX}	paraxylene density	861 kg/m^3	V
—	analyzer delay after a cycle	2 min	V
—	cyclic-steady-state tolerance	10^{-6}	V

(0.096 % extract impurity) and 0.42 (3.1 %) against the limit 0.416. The left edge is a desorption wave and is smeared by dispersion, but it converges as the bed sharpens. At $m_2 = 0.42$ the extract impurity is 0.97 % with 60 cells and $k = 3\,\mathrm{s}^{-1}$ and 0.22 % with 150 cells and $k = 8\,\mathrm{s}^{-1}$, against the line's 0.4216.

7.3.5 Instruments, Initialization and Numerics

Composite samplers on the extract, the raffinate and the feed fill over each whole cycle, and three analyzers report the extract's paraxylene purity, the raffinate's other-C_8 purity (both desorbent-free) and the feed's paraxylene 2 min after the cycle ends, with 0.01 point of noise, holding between reports. An independent trapezoid integral of the outlet streams over 20 cycles of case 3 under PI control agrees with the plant's cycle records to 6.7×10^{-5} points for the extract and 4.8×10^{-5} for the raffinate, and with zero noise each report equals its record exactly, 2.008 min after the cycle (the first step past the delay). The recovery estimate uses the analyzers and the metered flows, so a meter bias biases it. The four flow meters read the pumps' setpoints, and the adsorber temperature and the sequencer's state are known. Every case except the start-up begins on the cyclic steady state that its settings produce, solved at load by integrating the ring switch by switch with the engine's own step until the profile repeats to 10^{-11}. Integration is fourth-order Runge–Kutta with a step of 0.5 s, the controller runs every 5 s and a log row is written every 15 s, on the engine of Section 1.6.1. Halving the step moves the cyclic steady state's purities by less than 10^{-7} points. Twelve ledgers integrate every port stream inside the integrator, and the paraxylene balance closes to 1.9×10^{-14} of the feed per cycle at the cyclic steady state. The state vector holds 960 cell states, the capacity and the twelve ledgers, 973 in all. Table 7.2 lists the parameters.

7.3.6 Assumptions

Three pseudo-components stand for the liquid. Metaxylene, orthoxylene and ethylbenzene are one lump with one selectivity, and the desorbent is folded into the isotherm, so the triangle is the one for a non-adsorbing solvent while a real desorbent adsorbs and competes. The isotherm and mass-transfer constants serve teaching, set so that the eight-bed unit reaches 99.7 % at 90 s, and N is an effective capacity rather than a pore volume. Liquid volumes are additive and the liquid incompressible. The ports switch in one step, so the rotary valve's flushing and the line volumes are left out. The bed temperature is uniform and set, the heat of adsorption is not balanced, and aging lowers the capacity only, compressed from years into the run. Industrial units have more beds and a longer cycle than eight beds of 20 m^3 at 90 s. The specification of 99.7 % and the recovery target of 97 % are the figures of an industrial-scale study [1], and the limits on m_2, m_3 and the 0.05 feed-pump minimum are teaching values, because real ones come from the downstream customer, the licensor's design and the equipment.

The desorbent ratio is the clearest consequence of the teaching isotherm. At the point the PIs settle at the unit uses $(m_1 - m_4)/(m_3 - m_2) = 3.79$ cubic meters of desorbent per cubic meter of

feed. The industrial-scale study uses 264.14 against 220.15 t/h of feed, 1.20 by mass, and calls a desorbent consumption below 1.5 classical, with a paraxylene Langmuir constant of 5.865 m^3/kg against 1.777 m^3/kg for meta- and orthoxylene, a selectivity of 3.3 [1]. At a selectivity of 2.5 even the ideal unit at the vertex w, with $m_1 = H_A$ and m_4 at its limit of 0.375, needs $(1.20 - 0.375)/(0.823 - 0.421) = 2.05$, and the dispersion of eight short beds and the margins on m_1 and m_4 need the rest.

7.4 How the Ring Responds

7.4.1 From a Ring of Desorbent to the Cyclic Steady State

Case 1 starts the ring full of desorbent at the design point. The feed's components spread round it cycle by cycle, and the paraxylene produced rises from 1.8 t/h in cycle 1 to 12.7 in cycle 2 and 18.1 t/h by cycle 6. The extract over cycle 1 carries only 10.0 % of the paraxylene fed, 92.6 % by cycle 3, while the loss-based recovery already reads 99.98 % because almost none reaches the raffinate. The largest profile change at a switch falls from 1.0×10^{-1} in cycle 1 to 4.1×10^{-7} in cycle 10, by a factor of 2.7 to 3.8 per cycle from cycle 5, and the cyclic steady state is declared at the end of cycle 10, 120.00 min. Inside the first switch of cycle 11 the extract still runs from 99.40 to 99.98 % around its cycle average of 99.89 %. The approach is a ring that fills, not a time constant, and any change of a flow, the switching time or the adsorbent starts it again.

> **TRY IT IN THE APP** **1 · Start-up: From a Ring of Desorbent to the Cyclic Steady State (Manual)**
> Load the scenario, press Run and watch the Cycle badge and the status strip. The paraxylene produced climbs from 1.8 t/h in cycle 1 to 18.1 t/h by cycle 6, and CYCLIC STEADY STATE appears at the end of cycle 10, at 120.00 min. Even then the extract inside one switch runs from 99.40 to 99.98 %.

Pause. Try Exercise 7.1 before reading on.

7.4.2 The Triangle Against the Simulated Unit

The triangle locates the edges, but not where the simulated unit meets its specification, as shown in Figure 7.3. Each curve is found by bisection on the cyclic steady state at fixed $m_1 = 1.40$, $m_4 = 0.30$ and $t_s = 90$ s. With the shipped thirty cells the recovery reaches 97 % at $m_3 = 0.8828$ for $m_2 = 0.62$, below the ideal upper edge at 0.8951, and the extract reaches 99.7 % only for $m_2 \geq 0.568$ at $m_3 = 0.82$, far to the right of the ideal left edge at 0.422. The specification therefore holds in a narrow wedge near the triangle's upper edge, and its corner lies close to the point the PIs settle at, $(0.564, 0.854)$, where the unit makes 25.81 t/h at a recovery of 97.87 %. With 60 cells the recovery edge moves up to 0.8945 at $m_2 = 0.62$, nearly on the ideal line, and the extract edge to 0.518, while with 15 cells the extract edge needs $m_2 \geq 0.74$ at $m_3 = 0.82$, and with 10 cells at $m_1 = 1.40$ and $m_4 = 0.30$ no point reaches 99.7 % at all. The case 2 point above the upper edge, $(0.62, 0.92)$, holds the extract at 99.938 % while the recovery settles at 89.98 %, as shown in the right panel of Figure 7.2.

7.4.3 Which Ratio Moves Which Purity

Each ratio sits on the edge that protects one outlet, so the extract purity answers mostly to m_2 and the raffinate purity mostly to m_3. From steps of $+0.01$ in the cyclic steady state, measured in decades of impurity, the relative gain of the pairing of extract with m_2 is 0.872 at the design point and 0.914 at the PIs' point. Central differences give 0.857 and 0.907, and step tests on the running engine read ten cycles later give 0.882 and 0.927 in percent. The crossed pairing would have relative gains near 0.13 and 0.09, and each of its loops would see its gain change seven- to elevenfold as the other closed. The raffinate purity's gain to m_3 changes 8.4-fold in percent between the design point and the PIs' point (-2.5 to -21.0 points per unit of m_3 by central differences) but only 1.9-fold in decades of impurity (-8.1 to -15.2), which is why both loops act on $z = -\log_{10}(1 - P)$.

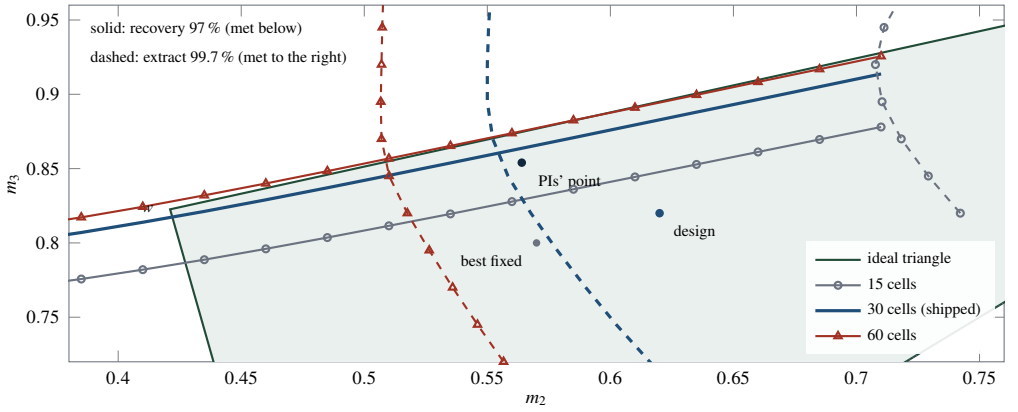


Figure 7.3 Where the simulated unit meets its specification, at three cell counts per bed, against the ideal triangle. Solid curves, recovery of 97 %, met below each curve. Dashed curves, extract purity of 99.7 %, met to the right. Circles mark 15 cells, triangles 60 cells, and the thickest curves the shipped thirty. Cyclic steady states at $m_1 = 1.40$, $m_4 = 0.30$, $t_s = 90$ s, fresh adsorbent and a 22 % feed. The shipped thirty cells leave a narrow wedge whose corner lies near the PIs' point.

7.5 Purity Control as Implemented

One Manual and Auto switch governs the ring. In Manual, m_2 and m_3 are the operator's stations, and m_1, m_4 and t_s are the operator's in every mode. In Auto the *Purity control* setting chooses *Fixed ratios*, which holds the stations where the operator put them and reads no analyzer, the *cycle-to-cycle PI*, or the *repetitive MPC*. Each controller execution builds a measurement packet from the analyzers, the meters, the sequencer and the temperature transmitter, and a test of the app fails if the packet carries anything else. Whatever the architecture, m_2 is clamped to 0.30–0.90, m_3 to 0.50–1.20, and m_3 is held at least 0.05 above m_2, the feed pump's minimum. The PIs track whatever is applied when they are not in charge, so a change of architecture or a return to Auto is bumpless.

7.5.1 The Cycle-to-Cycle PIs

Both loops are the velocity-form PID routine of Section 1.6.2 with the derivative set to zero, called only when a report arrives, as shown in Equation (7.9). The regeneration loop of Chapter 5 has the same structure.

$$
\begin{aligned}
e_k &= \pm\left(z_{SP} - z_k\right), \qquad z = -\log_{10}(1-P) \\
S_k &= S_{k-1} + K_c\left(e_k - e_{k-1}\right), \qquad \hat{u}_k = u_0 + S_k + I_{k-1} \\
u_k &= \min\left(u_{max}, \max\left(u_{min}, \hat{u}_k\right)\right) \\
I_k &= I_{k-1} + \left[\left(K_c/\tau_I\right) e_k + \left(u_k - \hat{u}_k\right)/\tau_I\right]\Delta t_k
\end{aligned}
\tag{7.9}
$$

where u is m_2 for the extract loop (direct acting, +) and m_3 for the raffinate loop (reverse acting, −), Δt_k is the time since the last report, one cycle in normal running, and S accumulates the proportional moves without clamping. The anti-windup is the back-calculation of Equation (1.17) with the tracking time τ_I, and a move cut by the feed-pump minimum is tracked as well. The defaults are $K_c = 0.06$ per decade and $\tau_I = 24$ min, two cycles, for both loops, with setpoints of 99.75 and 99.40 %. The integral used at report k was accumulated through report $k-1$, so its contribution lags the error that causes it by one report. Section 1.4.7 treats such a loop on a plant that answers reports late. An integral time at its slider's maximum of 600 min makes a loop proportional only.

7.5.2 The Repetitive MPC

The MPC plans m_2 and m_3 at every report over $N = 9$ cycles in three move blocks of 1, 1 and 7 cycles, on finite step responses of both purities in decades, as shown in Equation (7.10).

$$\begin{aligned} z_k &= \beta + \textstyle\sum_{j=1}^{9} \left[h_j^{(2)} \tilde{m}_{2,k-j} + h_j^{(3)} \tilde{m}_{3,k-j} \right. \\ &\quad \left. + h_j^{(F)} \tilde{x}_{F,k-j} \right] \\ \min\ & \textstyle\sum_k 20\, w_P \,(m_{2,k} - m_{3,k}) + \sum_j \frac{w_{\Delta u}}{0.01^2} \|\Delta m_j\|^2 \\ &\quad + \textstyle\sum_{o \in \{E,R\}} (400\, s_o^2 + 40\, s_o) \\ \text{s.t. } & z_{o,k} \geq z_{o,SP} - s_o, \quad s_o \geq 0, \quad m \text{ within its limits} \end{aligned} \tag{7.10}$$

where a tilde marks the deviation from the value in force over the last cycle, Δm_j is the move of block j, h_j are the increments of step responses identified on this model at commissioning with steps of $+0.01$ in m_2 and m_3 and $+2$ points of feed paraxylene from the PIs' point, x_F is the feed analyzer's report held over the horizon as a measured disturbance, β is the offset between the latest report and the model's prediction of it, renewed at every report, and $w_P = w_{\Delta u} = 1$. The final gains are 9.35 decades per unit of m_2 for the extract and -15.26 per unit of m_3 for the raffinate. Re-identified on the present model, the step responses reproduce the stored ones to four decimals for m_2 and m_3 and to 10^{-4} for the feed. The linear cost pushes the feed $m_3 - m_2$ up until both purities sit on their setpoints, which the soft constraints treat as floors. The plan is computed as a quadratic program by the shared linear MPC code of Section 1.6.3, with the dual algorithm of Goldfarb and Idnani [17], and a plan that comes back infeasible, not finite or out of range hands m_2 and m_3 to the tracked PIs without a bump. The model is not re-identified as the plant ages or warms, and those changes are left to β, as the step-response controller of Volume 9, Chapter 2 leaves its model error to a bias. The feed history starts from the feed analyzer's first report, which fills it, and not from the simulated feed composition.

7.5.3 Design Choices

Ten decisions taken while the app was built depart from its plan or settle what the plan left open, and each was measured. The beds carry 30 cells instead of 10, because ten reach 99.7 % at a 97 % recovery only with m_1 at its 1.8 limit and a feed of at most $m_3 - m_2 = 0.09$, 45 % of the design feed. The pairing is extract with m_2 and raffinate with m_3 rather than the crossed pairing the plan proposed, on the relative gains above, and the loops act on the logarithm of the impurity. The recovery is loss based, for the accumulation reason given with Equation (7.5). The feed step is 22 to 30 % paraxylene, because 26 moves the PIs' point only to 97.34 % recovery at its cyclic steady state. Case 4 teaches a production peak in the switching time rather than a region that closes, because the region does not close inside the stable range of $t_s \geq 45$ s and $m_1 \leq 1.8$. The honest infeasible case is the dirty desorbent of case 8. The MPC is identified once with an offset updated every cycle. The challenge adds a 30 t/h production floor, because without it a point far inside the triangle passes by making less. The sequencer, the composite samplers and the analyzers are written for this app, since the series' shared stage sequencer runs a bank of on and off stages against a demand and its analyzer samples an instant, while here the whole ring moves on a clock and the analysis is a cycle composite. Fixed ratios exists so that the challenge can ship in Auto with the suggested setting a control value.

The start-up logs nothing it has not measured. Before the first whole cycle and the first analyzer report at 14.01 min, the cycle averages, the recovery estimate, the production, the feed analysis and the profile change are logged blank, so their trends begin with a gap. The two loop measurements are the exception. They repeat their setpoints until the first report, because the series' loop metrics need a finite measured value, and the logged report count of zero marks those rows. The plant (the ring of Section 7.3), the gains and delays a student fits to the cycle records, and the MPC's step responses, which know neither the cell count nor the capacity, are three different models.

Table 7.3 The Nine Cases

#	Case and events	Teaching point
1	Manual, start from a ring of desorbent	the cyclic steady state
2	Manual at design, m_3 to 0.92, then m_2 to 0.44	which edge protects which outlet
3	Manual at the PIs' point, feed 22 to 30 % at 36 min	cycle-to-cycle feedback
4	PIs on, t_s 90 to 60, then 45 s	production against purity margin
5	Manual, capacity −5 % at 24 min	the triangle shrinks
6	Manual, extract pump +3 % off its meter at 24 min	a fault's signature
7	Manual, adsorber +10 K at 24 min, later 167 °C	temperature moves the region
8	PIs on, m_1 to 1.30, m_4 to 0.34, dirty desorbent	desorbent and infeasibility
9	Challenge, 60 cycles, aging, feed step at cycle 20	the whole problem

Table 7.4 Case Outcomes Measured on the Engine

Case and condition	Result
1, start-up	1.8 / 12.7 / 18.1 t/h in cycles 1, 2, 6; steady at 120.00 min
2, m_3 0.92	Rec 96.84 (cycle 3), 90.07 % (cycle 11); 24.5 t/h
2, m_2 0.44	P_E 99.47 to 96.04 %
3, Fixed	Rec 98.43 (cycle 4), below 97 % from cycle 8, 96.21 %
3, PI / MPC at 98 min	cycles 8–11 / 8–9 below 97 %; 36.1 t/h
3, PI / MPC / blind MPC from $t = 0$	lowest Rec after the step 97.63 / 98.41 / 97.90 %
4, t_s 120 / 90 / 75 / 60 / 45 s	21.2 / 25.8 / 28.2 / 29.0 / 18.9 t/h
5, aged, Manual / PI	Rec 93.20 % (cycle 10) / inside from 63.0 min
6, biased, Manual / PI	P_E 99.489, P_R 99.65 % / $P_E \geq$ 99.7 at 98 min
7, +10 K / 167 °C	Rec 87.65 % / P_E 98.95 %
8, m_1 1.30 / m_4 0.34	D/F 3.59, 24.96 t/h / D/F 3.73, 22.91 t/h
8, dirty desorbent	P_E 95.97 % (cycle 36), m_2 0.899, 4.35 t/h

7.6 Nine Cases on the Running Ring

The cases are listed in Table 7.3 and the principal measurements in Table 7.4. All values come from the app's own engine, stepped outside the browser at the browser's 0.5 s step and default seed, from the case as loaded. Settings a case asks for after the first cycle are entered at 13 min, and every number in the app's own texts was regenerated twice by script with identical output. Cycle values are the true cycle averages of Equation (7.5), and report times are those of the analyzers.

DID YOU KNOW? A Shorter Switch Can Make Less

From the simulator: with the PIs holding both purities, the ring makes 25.8 t/h of paraxylene at a switching time of 90 s and 29.0 t/h at 60 s, but only 18.9 t/h at 45 s, less than the 21.2 t/h at 120 s (Table 7.4).

7.6.1 Crossing the Edges

Case 2 runs at the design point and raises m_3 from 0.82 to 0.92 after the first cycle, above the upper edge. The extra feed raises the paraxylene produced from 18.1 to 24.5 t/h, but zone III no longer holds the paraxylene, the recovery falls to 96.84 % in cycle 3 and 90.07 % by cycle 11, and the raffinate purity to 97.28 %. Back at $m_3 = 0.82$ with m_2 lowered to 0.44, the extract purity falls from 99.47 to 96.04 %, although the point is still inside the ideal triangle, whose edge there is at 0.422. Case 7 moves the region instead of the point. Ten kelvin hotter, the vertex moves from $(0.421, 0.823)$ to $(0.392, 0.760)$, the point is left above the upper edge and the recovery falls to 87.65 % by cycle 10 while the extract stays at 99.872 %. At 167 °C the triangle grows past the point the other way, $w = (0.454, 0.892)$, the recovery returns to 98.22 % and the extract falls to 98.95 %, because zone II at the same m_2 no longer pushes back the more strongly held other C_8.

7.6.2 Feedback Once a Cycle

Case 3 enriches the feed from 22 to 30 % paraxylene at 36 min with the flows fixed at the PIs' point. The recovery first rises to 98.43 % in cycle 4 as the ring takes up the extra paraxylene, then the report at 98.0 min reads below 97 % for cycle 8 and the recovery falls to 96.21 % by cycle 13 (96.10 % at the new cyclic steady state), while the extract becomes purer, 99.915 %. Handed the ratios at that report, the PIs lower m_3 to 0.821 and m_2 to 0.526, cycles 8 to 11 stay below 97 %, both analyzers hold within 0.05 and 0.1 point of their setpoints from 194 min, and the richer feed yields 36.1 t/h. The MPC switched at the same report leaves only cycles 8 and 9 below 97 % and settles at the same time. Running from the start, the MPC never lets the recovery below 98.41 % after the feed step, against 97.63 % for the PIs. The same MPC with its feed analyzer frozen holds 97.90 %, so about two thirds of its advantage comes from the measured feed and one third from its plan.

TRY IT IN THE APP 3 · A Richer Feed and the Cycle-to-Cycle PI

Press Run and watch the Cycle view through the feed change at 36 min. When the report at 98 min shows the recovery below 97 %, switch to Auto with Cycle-to-cycle PI chosen under Purity control. The PIs lower m_3 to 0.821 and m_2 to 0.526, both analyzers hold close to their setpoints from 194 min, and the richer feed yields 36.1 t/h.

Case 5 removes 5 % of the capacity at 24 min. A resin whose capacity nobody measures is the subject of Volume 8, Chapter 11. Every Henry constant falls with it, H_A from 1.200 to 1.140, and the vertex moves to $(0.400, 0.781)$. The point leaves the region at 24.01 min and the recovery falls to 93.20 % by cycle 10. Switched to the PIs at 48 min, m_3 falls to 0.817 and m_2 to 0.547, the point is inside again from 63.0 min, the recovery is above 97 % from cycle 9, and the aged unit makes 24.0 t/h against 25.8 fresh. Case 6 makes the extract pump deliver 3 % more than its meter reads, 12.0 m^3/h, which lowers the true m_2 and m_3 together by 0.025. The extract purity falls to 99.489 % while the raffinate purity rises to 99.65 %, a pair that a recycle pump delivering 3 % too much (all four m up by 0.029) would reverse. In Auto the PIs command $m_2 = 0.590$ and $m_3 = 0.879$, so the beds see 0.565 and 0.855, and the extract analyzer reads 99.7 % again at 98 min. The fault is now hidden in the setpoints, and the recovery estimate from the meters reads 97.78 % against a true 97.88 %.

Pause. Try Exercise 7.3 before reading on.

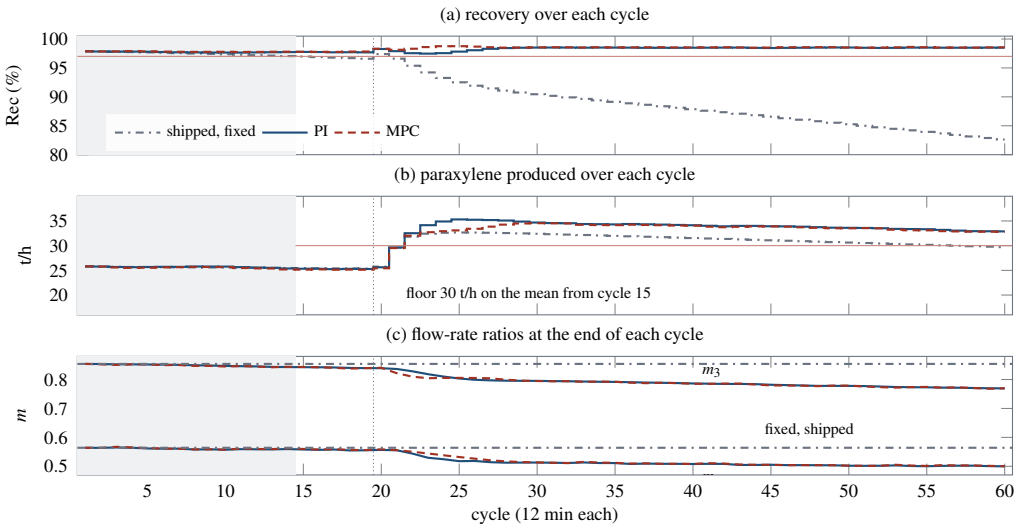


Figure 7.4 The challenge cycle by cycle. True cycle averages for the shipped fixed ratios (dash-dotted), the suggested PIs (solid) and the MPC (dashed), with the adsorbent aging 0.6 %/h throughout and a 30 % feed from cycle 20 (dotted). The shaded cycles 1 to 14 are not judged. The fixed point loses its recovery to aging while the PIs and the MPC walk m_2 and m_3 down.

7.6.3 Switching Time and Desorbent

At a fixed m every flow scales with $1/t_s$, so a shorter switch passes more feed per hour. With the PIs holding both purities, case 4 at 60 s first pushes the paraxylene to 37.4 t/h in cycle 3 while the extract falls to 99.38 %, the extract PI raises m_2 to 0.636, and the unit settles at 29.0 t/h against 25.8 t/h at 90 s. The switching time of 75, 120 and 45 s gives 28.2, 21.2 and 18.9 t/h. At 45 s the extract PI needs $m_2 = 0.744$, which leaves a feed of $m_3 - m_2 = 0.106$ and a desorbent ratio of 10.42. The triangle does not move with t_s, because equilibrium theory has no mass-transfer rate in it. What shrinks is the wedge of Figure 7.3, and the extract PI finds its edge.

Case 8 cuts the desorbent with the PIs on. Lowering m_1 to 1.30 dips the recovery to 97.43 % in cycle 4, the raffinate PI trims m_3 to 0.843, and the desorbent ratio falls from 3.79 to 3.59 for 24.96 t/h. Raising m_4 to 0.34 lets the other C_8 through zone IV, the extract PI raises m_2 to 0.594, and the ratio returns to 3.73 for 22.91 t/h. The desorbent then returns from its recovery column carrying 0.1 % of the other C_8, which enters zone I upstream of the extract port. The extract falls to 98.58 % within two cycles and 95.97 % by cycle 36 while the extract PI drives m_2 to 0.899, against its 0.90 limit, and the production to 4.35 t/h. No setting of the five handles can restore it. A grid of 1500 points followed by a pattern search over m_1 to m_4 and t_s from 45 to 150 s finds at best 99.284 % (at a recovery of 58.6 %) and 98.973 % with the recovery at 97 % or more, while the same best point with a clean desorbent exceeds 99.7 %. The cure is the desorbent column.

7.6.4 Sixty Cycles on an Aging Adsorbent

The challenge runs sixty cycles of 12 min. The adsorbent loses 0.6 % of its capacity every hour from the start and the feed changes to 30 % paraxylene at 228 min, the start of cycle 20. It is met when every cycle from cycle 15 has a true extract purity of at least 99.7 % and a recovery of at least 97 % and the paraxylene produced over those cycles averages at least 30 t/h. The configurations are compared in Table 7.5 and the cycles in Figure 7.4. As shipped, fixed ratios at the PIs' fresh point lose the recovery to aging from cycle 15, down to 82.62 % by cycle 60. The PIs pass with a lowest extract purity of 99.745 % (cycle 51), a lowest recovery of 97.47 % (cycle 23, just after the feed change) and

Table 7.5 Challenge Configurations Scored Over Cycles 15 to 60

Configuration	P_E min (%)	Rec min (%)	Mean (t/h)	Verdict
shipped, fixed 0.564 / 0.854	99.798	82.62	30.55	fails
fixed at design 0.62 / 0.82	99.912	97.57	23.39	fails
best fixed 0.57 / 0.80	99.735	97.95	27.00	fails
PI at half gain (0.03)	99.756	96.84	32.72	fails
suggested, PI	99.745	97.47	32.78	passes
MPC	99.745	97.77	32.44	passes
20 cells, PI / MPC	99.732 / 99.740	97.80 / 97.77	25.03 / 24.49	fail
45 cells, PI / MPC	99.746 / 99.746	97.17 / 97.77	36.36 / 36.11	pass
45 cells, fixed 0.54 / 0.80	—	—	30.48	passes
60 cells, PI	99.746	96.9976	37.87	fails
60 cells, MPC	99.745	97.77	37.65	passes
60 cells, fixed 0.52 / 0.79	—	—	31.83	passes

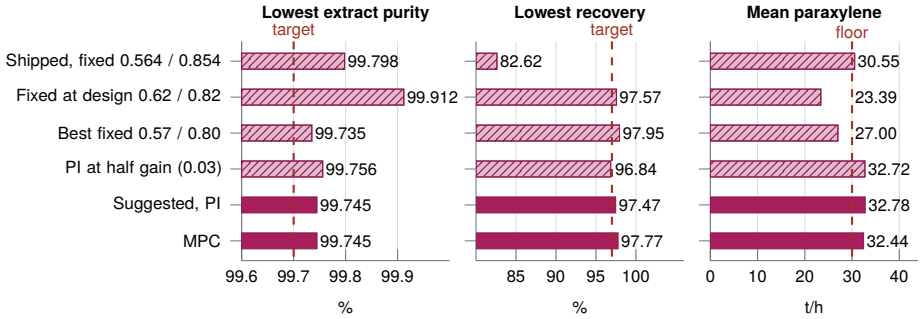


Figure 7.5 The configurations of the upper block of Table 7.5, at the shipped thirty cells per bed, against the three targets of the challenge: the lowest extract purity and the lowest recovery over cycles 15 to 60 and the mean paraxylene made. Solid bars pass, hatched bars fail, and the dashed line in each panel is the target. Notice that every fixed point fails on one target, the shipped point on the recovery and the two others on production, and that the PI at half gain misses the recovery by a fraction of a point. The lower block, with other cell counts, is not drawn.

32.78 t/h, walking m_3 from 0.854 to 0.769 and m_2 from 0.564 to 0.500. The MPC passes with 99.745, 97.77 and 32.44 t/h, holding the recovery at 98.14 to 98.76 % through cycles 21 to 28 against 97.47 to 98.44 % for the PIs, and solves 59 plans with none rejected. No fixed point on a 0.01 grid passes. The best, $(0.57, 0.80)$, holds both purities for all sixty cycles with only 27.00 t/h. At five seeds (default and 0 to 3) the PIs' lowest recovery lies between 97.34 and 97.47 %, always in cycle 23, and the MPC's between 97.75 and 97.77 %, the shipped run fails identically, and halving the step changes no verdict. Figure 7.5 sets the configurations of the table's upper block against the three targets.

The lower block of Table 7.5 repeats the challenge with the cells per bed changed in a copy of the source. At 20 cells nothing reaches the 30 t/h floor. At 45 cells the PIs and the MPC pass and so does the fixed point $(0.54, 0.80)$. At 60 cells two fixed points pass, the best making 31.83 t/h, the MPC passes, and the PIs as tuned miss the recovery by 0.0024 points in cycle 23, identically at half the step. The lesson that no fixed point passes, and the margin by which the PIs pass, therefore belong to the shipped dispersion. The ring at the instant Figure 7.1 redraws is shown in Figure 7.6.

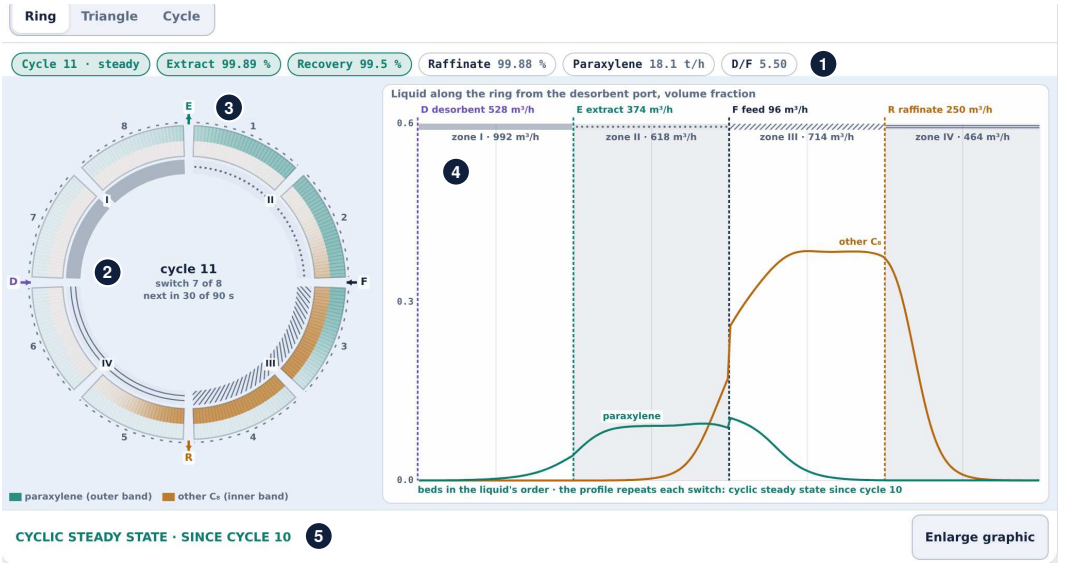


Figure 7.6 Case 1 at $t = 130$ min on the Ring view, in Manual at the design point. (1) The badges give the last cycle's extract purity of 99.89 %, recovery of 99.5 %, raffinate purity of 99.88 %, 18.1 t/h of paraxylene and a desorbent ratio of 5.50. (2) The ring's center reads cycle 11, switch 7 of 8, next in 30 of 90 s. (3) The four ports D, E, F and R sit where the sequencer has put them, with the zones I to IV between them. (4) The profile carries the zone flows of 992, 618, 714 and 464 m^3/h and the port flows of 528, 374, 96 and 250 m^3/h. (5) The status strip reads CYCLIC STEADY STATE SINCE CYCLE 10.

7.7 Technology in Practice

What Measures It

Figure 7.7 draws the ring of Section 7.3 with the hardware of a simulated moving bed in place of the schematic's symbols and the control system above it. The purities that the controllers correct come from analyzers behind composite samplers that fill over each cycle, and the model gives them a report 2 min after the cycle with 0.01 point of noise. Plant analyzers such as gas chromatographs and near-infrared spectrometers suffer from large measurement delays and high investment and maintenance costs [18], so the model's analyzers are faster and cleaner than a plant's, as Section 7.8 says. The four flow meters read the pumps' setpoints, and the meter bias of case 6 is the one fault the model gives them. An analyzer that reads the liquid inside the adsorber, rather than a composite of what has left it, is the subject of the box below.

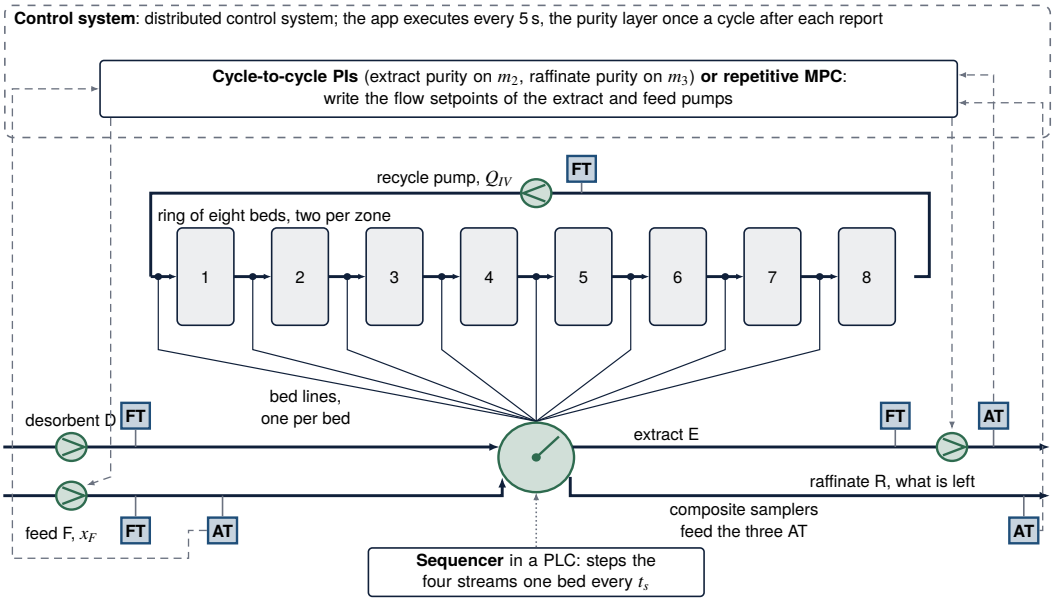


Figure 7.7 The ring's loops with their hardware. Blue boxes are sensing devices: the flow transmitters FT on the pumps and the three analyzers AT behind their composite samplers. Green symbols are final elements: the desorbent, feed, extract and recycle pumps and the rotary valve, which joins every bed line to the four streams. Dashed arrows are signals, the dotted one the sequencer's step command. Notice that the purity layer acts once a cycle, and only through the flow setpoints of the extract and feed pumps. The desorbent and recycle flows, which set m_1 and m_4, and the switching time are the operator's. Not to scale, and not a piping diagram.

TECHNOLOGY **Sensor: A Raman Analyzer on the Adsorber**

Raman scattering shifts the frequency of a small part of a monochromatic beam through coupling with the vibrations of the molecules it meets. The effect is so weak that it came into wide use only after powerful lasers arrived in the 1960s [19]. One paraxylene process design monitors the concentration profiles in its adsorber by on-line Raman spectroscopy for advanced dynamic control [20]. An optical analyzer can fail quietly. Its window must be kept clean of dust and condensation, and an analyzer fed stale liquid from a plugged sample line has no way of knowing it and reports a value that no longer follows the process [21].

What Moves It

Two kinds of final element act on the ring. Four pumps set the zone flows, and in the model each delivers its setpoint times one plus its meter bias, with the raffinate taking what is left. Only the extract and feed pumps belong to the purity loops, through m_2 and m_3. The ports move through the sequencer and its valve, not through a controller, at the switching time the operator sets.

TECHNOLOGY **Final Element: The Rotary Valve That Moves the Ports**

A typical industrial unit has 24 beds in two chambers of 12, each bed joined to one rotary valve by its own bed line, and pumps circulate the liquid between the chambers so that they act as a single unit [20]. At any moment only four bed lines carry the feed, the desorbent, the extract and the raffinate, and their positions are switched as the composition profile moves down the chamber [22]. A line that has just carried one stream holds its residue when it carries the next, which can contaminate the product. Designs answer with extra streams that flush the lines or with separate lines and individual on/off valves for each stream [23].

Where the Controller Runs

A distributed control system holds loops like these at a supervisory level that sends set points to field controllers, with loops nested or cascading and cycle times from milliseconds to minutes [24]. Programmable logic controllers (PLCs) serve such a system as local controllers within the supervisory scheme, programmed for logic, timing, counting and PID control [24]. The sequencer that steps the ports is a state machine, whose output depends on its position in the ring as much as on its inputs, and IEC 61131-3 names the Sequential Function Chart among its five languages for writing one [21]. In the app the controller executes every 5 s, while the cycle-to-cycle PIs are velocity-form PID blocks called only when a report arrives, once a 12 min cycle. The MPC sits above them as a supervisory layer that writes m_2 and m_3 and hands them back to the PIs when a plan fails.

IN PRACTICE **Keep the Desorbent Clean**

The desorbent leaves the adsorber in the extract and the raffinate, is recovered at the bottom of their two distillation columns and is recycled to the chambers. A slipstream goes to a small rerun column that rejects heavy components and desorbent degradation products, and filters may remove adsorbent fines. With these safeguards the desorbent stays good enough for the molecular sieve to last more than ten years. A very small amount of water may be injected into the feed to keep the adsorbent's selectivity high [22]. Case 8 shows the other side: with other C_8 in the desorbent, no setting of the five handles restores the extract.

What Is Modernizing It

Model predictive control has a solid foundation in refining and petrochemicals [16], and here it pays mostly through the feed analyzer it reads as a measured disturbance. Soft sensors estimate product quality from other process measurements where an online analyzer is not available, and they are also used to validate online analyzers [18], which would give the ring a second reading to hold against its analyzers. An analyzer that reads the concentration profile inside the adsorber, as in the box on the Raman analyzer above, gives a controller the profile that the chapter's composite samplers average away. New sorbents that would separate the xylenes with less energy are the subject of the Open challenge box in Section 7.8.

7.8 Limitations

Every size, rate and limit is a teaching value, and no operating unit supplied them. The isotherm, its heats and the mass-transfer coefficient were chosen so that eight short beds reach 99.7 % at 90 s, not fitted to any adsorbent, and the selectivity of 2.5 sits below the 3.3 of a published industrial-scale model. As a result the unit needs a desorbent ratio of 3.79 where that study uses 1.20 by mass and calls 1.5 or less classical [1]. The other C_8 are one lump, the desorbent does not compete in the triangle, and the heat of adsorption, the rotary valve and the line volumes are left out.

OPEN CHALLENGE **A Sorbent Beyond the Zeolite**

Paraxylene is separated industrially on faujasite-type zeolites, which need relatively high temperatures and pressures in a simulated moving bed and give a paraxylene selectivity usually below ten. Sorbents and membranes that would purify paraxylene with less energy are therefore sought [25], while a 2011 review of microporous materials found the number of satisfactory results still limited [26]. The bar is high, because a zeolite kept in clean desorbent lasts more than ten years [22]. Progress would be a sorbent more selective than the zeolite that survives years of cycling. It would lower the desorbent ratio that this chapter traces to its selectivity of 2.5.

The thirty cells per bed are a declared dispersion, and the purities move with them, from 97.18 % at 10 cells to 99.98 % at 60 at the design point. The challenge's verdicts move too. At 45 and 60 cells a fixed point passes, at 60 the PIs as tuned miss the recovery by 0.0024 points, and at 20 cells nothing reaches the production floor. At the shipped 30 cells every verdict holds at five seeds and at half the

step, and the student cannot change the cell count, but the lesson that fixed ratios cannot pass belongs to this bed and not to simulated moving beds in general. The PIs' margin on the recovery is 0.34 to 0.47 point. The MPC's advantage over the PIs comes mostly from the feed analyzer, and it was identified on the simulator's own model. The analyzers are faster and cleaner than real ones, and the protection of the unit is outside the model.

7.9 Conclusion

A simulated moving bed has no steady state to control, and this simulator puts its eight beds, its stepping ports, its cycle composites and its triangle on one clock. From a ring of desorbent the unit repeats itself to one part in a million after ten cycles, while its extract still saws from 99.40 to 99.98 % inside each switch. The triangle derived from the isotherm matches an independent derivation to 2×10^{-16} and the near-ideal simulation reproduces its edges, but with the shipped dispersion the extract needs $m_2 \geq 0.568$ where the triangle's edge is at 0.422. Paired extract with m_2 and raffinate with m_3 (relative gains 0.87 and 0.91) and acting once a cycle on the logarithm of each impurity, two PIs recover a richer feed, an aged adsorbent and a drifting meter, and they pass sixty cycles of aging at 32.78 t/h where the best fixed point makes 27.00. The repetitive MPC holds the recovery higher through the feed change, mostly because it reads the feed analyzer. The constants are teaching values, the desorbent ratio of 3.79 is about three times the 1.20 by mass of a modeled industrial unit, and the challenge's verdicts belong to thirty cells per bed. Further work would fit the isotherm to measured equilibria, add the competing desorbent and the rotary valve's flushing, and re-identify the MPC as the adsorbent ages. The simulator shows that in a cyclic process the controlled variable is a cycle and the controller is a correction from one cycle to the next.

KEY POINTS

- Nothing in a simulated moving bed settles inside a cycle: the extract still swings from 99.40 to 99.98 % within one switch, and only its cycle average is steady.
- The ideal triangle locates the edges, but with the shipped dispersion the extract needs $m_2 \geq 0.568$ where the triangle's edge is at 0.422.
- Paired extract with m_2 and raffinate with m_3 and acting once a cycle on the logarithm of each impurity, two PIs pass sixty cycles of aging at 32.78 t/h where the best fixed point makes 27.00.
- The repetitive MPC holds the recovery higher through the feed change, mostly because it reads the feed analyzer.

Where else this applies. Correcting the next cycle, run or layer from the measured result of the last is also the work of Chapter 5, Volume 8, Chapter 9 and Volume 8, Chapter 10.

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7.10 Exercises

7.1 Concept check · 2 min

Case 1 starts the ring full of desorbent, and the unit is declared at its cyclic steady state at the end of cycle 10. Inside the first switch of cycle 11 the extract still runs from 99.40 to 99.98 % paraxylene. Which statement is correct?

(a) The unit has not settled, and the profile still changes by more than the tolerance between switches

(b) The swing is the noise of the composite sampler, which the analyzer averages out over a cycle

(c) The swing comes from ports drawn between beds, which the sequencer corrects at the next switch

(d) What repeats is each switch shifted by one bed, so only the cycle average of 99.89 % is steady

7.2 Concept check · 2 min

The app defines the recovery as one minus the paraxylene that the raffinate takes over the paraxylene fed. In the cycle after case 3's feed step, a recovery defined as the extract's paraxylene over the feed's reads 73.15 %, while the loss-based one reads 98.43 %. Why does the app use the loss-based definition?

(a) The extract-based value falls while the ring takes up the extra paraxylene, though none of it is lost

(b) The extract analyzer reports 2 min late, so the extract-based value lags the cycle it describes

(c) The extract carries desorbent, which dilutes the extract-based value until the column recovers it

(d) The raffinate is the larger stream, so a loss-based value has the smaller measurement error

7.3 Concept check · 2 min

In case 6 one pump starts to deliver 3 % more than its meter reads. Over the next cycles the extract analyzer falls and the raffinate analyzer rises, while every flow on the screen still reads its setpoint. Which pump is it?

(a) The recycle pump, which raises every zone flow and so all four m_j together

(b) The extract pump, which takes more out ahead of zone II and lowers m_2 and m_3 together

(c) The feed pump, which raises m_3 alone and sends more paraxylene toward the raffinate

(d) The desorbent pump, which raises the flows of zones I to III and so m_1, m_2 and m_3

7.4 Theory and calculation · 6 min

The ring has eight beds of $V = 20\,\mathrm{m}^3$ with void fraction $\varepsilon = 0.40$, and switches every $t_s = 90\,\mathrm{s}$. Use Equation (7.3).

(a) Compute the four zone flows in m^3/h at the design point $m = (1.40, 0.62, 0.82, 0.30)$. Give one decimal. *Checkpoint:* 992.0, 617.6, 713.6 and 464.0 m^3/h

(b) Compute the desorbent, extract, feed and raffinate flows and the desorbent ratio Q_D/Q_F. *Checkpoint:* 528.0, 374.4, 96.0 and 249.6 m^3/h; 5.50

(c) The PIs settle at $m_2 = 0.564$ and $m_3 = 0.854$ with the same m_1 and m_4. Show that the desorbent ratio equals $(m_1 - m_4)/(m_3 - m_2)$, compute it and the feed, and compute the feed at the same m with $t_s = 60\,\mathrm{s}$. *Checkpoint:* 3.79; 139.2 and 208.8 m^3/h

7.5 Theory and calculation · 7 min

At the design point the Henry constants are $H_A = 1.20$ and $H_B = 0.48$, the affinities $K_A = 1.0$ and $K_B = 0.4$, and the feed fractions $c_A^F = 0.22$ and $c_B^F = 0.78$. Use Equations (7.7) and (7.8), and give three decimals.

(a) Compute κ_A, κ_B and the two roots $\omega_G > \omega_F$. *Checkpoint:* 0.220, 0.312; 1.053 and 0.357

(b) Compute the vertex w as the intersection of the edges wb and wf. *Checkpoint:* (0.421, 0.823)

(c) Compute m_3 on the upper edge at $m_2 = 0.62$ and m_2 on the left edge at $m_3 = 0.82$. The simulated unit reaches a recovery of 97 % at $m_3 = 0.8828$ for $m_2 = 0.62$, and an extract purity of 99.7 % only for $m_2 \geq 0.568$ at $m_3 = 0.82$. Compare. *Checkpoint:* 0.895 and 0.422

7.6 Theory and calculation · 7 min

Model each cycle-to-cycle PI as Equation (1.12) with a delay of $d = 2$ reports, one report per 12 min cycle. Ignore the proportional part and the tail of the real response, and use the final gains of the MPC's step responses as g: 9.35 decades of extract impurity per unit of m_2 and 15.26 decades of raffinate impurity per unit of m_3 (in magnitude). The integral part moves the handle by $K = K_c \Delta t / \tau_I$ per decade of error at each report.

(a) Compute K and gK for both loops at the shipped $K_c = 0.06$ per decade and $\tau_I = 24$ min. *Checkpoint:* $K = 0.03$; $gK = 0.281$ and 0.458

(b) Compute the magnitude of the closed-loop roots for each loop, and say where each sits against the double root and the edge of stability. *Checkpoint:* 0.530 and 0.677

(c) Repeat for both gains halved to 0.03. Which root is slowest, and what does the model predict for the recovery after the challenge's feed step? *Checkpoint:* 0.831 (extract) and 0.645 (raffinate)

7.7 App challenge · 8 min

Load case 1, Start-up: from a ring of desorbent to the cyclic steady state (Manual), at the default seed. Press Run at speed 2 (2 min of plant per wall second).

(a) Pause between 13 and 23 min and read the Paraxylene and Recovery (cycle) tiles. Pause again between 25 and 35 min and read them. *Checkpoint:* 1.81 t/h and 99.98 %; 12.67 t/h and 99.86 %

(b) The feed is 96 m^3/h of C_8 with 22 % paraxylene at 861 kg/m^3. What share of the paraxylene fed did the extract carry over cycle 1, and why does the Recovery tile read nearly 100 %? *Checkpoint:* 18.18 t/h fed; 10.0 %

(c) Run on at speed 10 and note the clock when CYCLIC STEADY STATE appears on the status strip. Pause at 130 min and read the Extract purity (cycle), Recovery (cycle) and Paraxylene tiles. Export the CSV and find the lowest and highest `truth_pe_now_pct` in the rows from 2.000 to 2.025 h (the file's time column is in hours for a run this long). Use a tolerance of 0.01 on every value. *Checkpoint:* 120 min; 99.893 %, 99.53 %, 18.10 t/h; 99.40 and 99.98 %

7.8 App challenge · 9 min

Load case 3, A richer feed and the cycle-to-cycle PI, at the default seed. It starts in Manual at the PIs' point, and the feed changes from 22 to 30 % paraxylene at 36 min.

(a) Run at speed 10 until the Recovery badge first reads below 97 %, near 98 min, and pause. Switch to Auto at any time before 110 min (Purity control is on Cycle-to-cycle PI), then run at speed 30 to 360 min. Read m_2 and m_3 on the two AIC cards and the Paraxylene tile. Export the CSV and list the cycles (`truth_cycle_of_record`) whose `truth_rec_cycle_pct` is below 97 %. *Checkpoint:* 0.526, 0.821, 36.11 t/h; cycles 8 to 11

(b) Reload the case with the reload button, and repeat (a) with Repetitive MPC chosen under Purity control before you switch to Auto. *Checkpoint:* 0.528, 0.821, 35.96 t/h; cycles 8 and 9

(c) Press Reset, which keeps your settings, so the run now starts in Auto with the MPC. Run to 360 min, export, and find the lowest `truth_rec_cycle_pct` from cycle 4 on. Choose Cycle-to-cycle PI, press Reset and repeat. Use a tolerance of 0.01 points. *Checkpoint:* MPC 98.41 %; PI 97.63 %

7.9 App challenge · 8 min

Load case 9, the Challenge (sixty cycles on an aging adsorbent), at the default seed. Run it as shipped at speed 300 (300 min of plant per wall second). The run pauses itself at 720 min.

(a) Read the So far tile and say which parts of the target the shipped fixed ratios meet. *Checkpoint:* 99.80 % · 82.6 % · 30.6 t/h

(b) Choose Cycle-to-cycle PI under Purity control, press Reset and run again. Read the So far tile and m_2 and m_3 on the AIC cards at the end. *Checkpoint:* 99.75 % · 97.5 % · 32.8 t/h; 0.500 and 0.769

(c) Set the Extract loop gain and the Raffinate loop gain to 0.030, press Reset and run again. Read the So far tile. Which part of the target fails? *Checkpoint:* 99.76 % · 96.8 % · 32.7 t/h

7.10 Application area · 4 min

Case 8 cuts the desorbent with the PIs on, at $t_s = 90$ s. At the PIs' point the desorbent ratio is 3.79 for 25.81 t/h of paraxylene. With m_1 lowered from 1.40 to 1.30 it is 3.59 for 24.96 t/h, and with m_4 then raised from 0.30 to 0.34 it is 3.73 for 22.91 t/h. The desorbent flow is $Q_D = (m_1 - m_4) \times 480\,\mathrm{m^3/h}$ at this switching time. Compute the desorbent per tonne of paraxylene at each step, say which cut an engineer should keep, and say what would lower the ratio toward the 1.20 by mass of an industrial unit.

7.11 Application area · 4 min

In case 6 the extract pump delivers 3 % more than its meter reads. In Auto the PIs restore the extract purity and command $m_2 = 0.590$ and $m_3 = 0.879$, while the beds see 0.565 and 0.855. The recovery estimate from the meters reads 97.78 % against a true 97.88 %. Every analyzer is now on its setpoint. Is the unit healthy? Check that the commanded offset fits a 3 % error on the extract flow, using $480\,\mathrm{m^3/h}$ per unit of m and $Q_E = (m_1 - m_2) \times 480\,\mathrm{m^3/h}$ with $m_1 = 1.40$, and say how an engineer could find the fault from plant data.

7.12 Review the agent · 5 min

An AI assistant asked how to make more paraxylene in case 2 writes: "At $m_3 = 0.82$ the left edge of the triangle is at $m_2 = 0.422$, and the design point is at 0.62. Lower m_2 to 0.44: the feed $m_3 - m_2$ rises from 0.20 to 0.38, the point stays inside the triangle, and equilibrium theory guarantees both outlets stay pure." Find the flaw and say how you would check it in the app.