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CHAPTER 5

Cyclic Propane Dehydrogenation Beds Whose Regeneration Sets the Next Cycle

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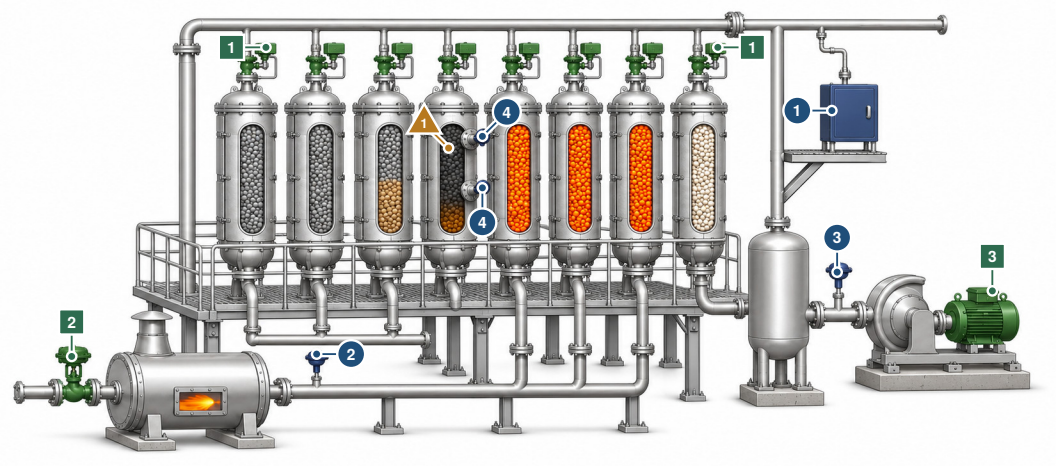
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CHAPTER 5

Cyclic Propane Dehydrogenation Beds Whose Regeneration Sets the Next Cycle



The controller moves 1 valves that switch each bed between its four phases, worked by the sequencer
2 fuel valve of the air heater, which sets the regeneration air temperature
3 compressor drive, whose speed holds the vacuum on the beds

The controller reads 1 product analyzer, one result for each three-minute slot 2 regeneration air thermometer
3 suction pressure transmitter, which reads the vacuum 4 bed thermocouples, which read every part of a bed

What disturbs it ▲1 coke on the catalyst, which grows as the catalyst ages ▲ a bed whose valves fail
▲ more propane fed to each bed

Notice that three beds make product while three others take the hot air, so a change to the air reaches only beds not yet on line, and that the beds of the model lie horizontal rather than upright. Illustration, not to scale.

IN PLAIN TERMS Beds That Run on Stored Heat

The main idea. Eight beds of catalyst take turns turning propane gas into propylene. While a bed makes product, nothing heats it. It spends heat it stored like a battery, then goes off line to be reheated with hot air.

The challenge. The only way to change what a bed makes is to heat it more before its next turn. So every correction arrives one or two turns late. When a bed breaks down, the order of the turns matters more than any controller.

Why it matters. The way the turns are set decides whether the plant keeps its output, its target or a steady flow of product.

THREE WAYS TO READ THIS CHAPTER

Explore	11 min	This page, the History boxes in Section 5.2, the Did you know? boxes in Sections 5.1 and 5.5, the Try it boxes in Section 5.5, and Key points in Section 5.8. 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 5.5 with Figure 5.5, Section 5.6, and Section 5.7 with its Open challenge box.

The control question A dehydrogenation bed on line spends heat it stored in its last regeneration, so no move reaches the beds now making propylene. How far can a regeneration temperature set once a slot hold the conversion through a lost bed and a feed step, and what does the schedule decide first?

Learning objectives

- Compute a bed's heat store, its cooling on line and the equilibrium conversion at the bed pressure.
- Explain why a regeneration move reaches the conversion one to two cycles late, and why a deeper vacuum buys selectivity rather than conversion.
- Tune a cycle-to-cycle PI for a delay of reports and compare it with a predictive controller that measures the feed.
- Choose a seven-bed schedule after a lost bed and price it in conversion, propylene and product ripple.

Prerequisites Sections 1.4.7 (cyclic units and cycle-to-cycle control), 1.4.3 (endothermic beds), 1.6.2 and 1.6.4. Section 1.6.3 only for the predictive controller.

The app https://apmonitor.com/apps/propane-dehydrogenation/

See also 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, and Volume 9, Chapter 4 for stored energy drawn down fast and restored slowly.

5.1 Introduction

Nothing heats a dehydrogenation bed while it makes propylene. In the generic unit simulated here, each of eight beds holds 33 t of chromia catalyst and inert material at 1.1 kJ/(kg K), 36.3 MJ for every kelvin, and receives 10 t/h of propane at 600 °C and 0.50 bar a. In its nine minutes on line the reactions absorb 2.44 GJ, the bed supplies 2.36 GJ of that from its own heat by cooling 65.0 K, and its conversion falls from 69.9 to 44.7 %. Steam purge, nine minutes of hot air that also burns the 10.1 kg of coke laid down, and an evacuation return it to the line at 622.6 °C after 24 min. Three beds are on line at every instant, staggered by one 3 min slot, and their product is compressed to a propylene splitter of the kind treated in Chapter 4.

+ DID YOU KNOW? The Third Source of Propylene

A 2023 review counts propane dehydrogenation as the third-largest source of propylene in the world, with 4.5 percent of the total capacity [1]. The bank simulated here sends 14.57 t/h of propylene to its splitter (Table 5.1).

The simulator addresses a belief that a block diagram encourages, that a controller corrects the conversion by acting on the reactor that makes it. In this plant no move reaches a bed on line. When the regeneration air is raised 10 K, the first bed to feel it comes on line 5 min later only 1.2 K warmer, and the bank's conversion has made 78 percent of its final rise of 2.93 points 26 min after the move. The correction is made on the next batch of stored heat, from a measurement of the last one, which is the structure of run-to-run and batch-to-batch control in semiconductor and batch chemical manufacture [2, 3]. A second belief is that a better equilibrium buys conversion. Lowering the suction from 0.45 to 0.35 bar a raises the equilibrium conversion of propane at 600 °C from 63.4 to 67.6 %, while the bank's conversion moves from 57.80 to only 58.15 % because the heat stored in the beds, not the equilibrium, sets how much propane they can convert. What the vacuum does buy is selectivity, 88.0 to 90.7 %. Fixed beds that store the heat of one period for the next are a class of their own, of which reverse-flow reactors [4] and the regenerative crackers and dehydrogenators of the refinery [5, 6] are members.

The literature on this process divides along disciplinary lines. Reviews treat the catalysts and the competing technologies [1, 7–9], kinetic studies fit transient rates on a single catalyst [10], and a dynamic model of a commercial reactor follows one bed through reaction and regeneration for

operational optimization [6], while the run-to-run literature draws its examples from batch and semiconductor processes [2]. This chapter works with one simulated bank whose beds, sequencer, regeneration air, vacuum and analyzer interact. It measures how far a regeneration temperature chosen once a slot can hold the conversion through a lost bed and a feed step, and what the schedule decides before any controller acts. The kinetics, the shared bed stack, the velocity-form PI law and the linear model predictive controller (MPC) are all established methods. The results are measurements on a single synthetic unit, and the most consequential is that no regeneration within the bed limit lets seven beds with three on line reach the 57 % target (52.6 % at 680 °C air), so that the schedule, not the loop, decides the twelve-hour challenge. The model has 114 states, its energy and carbon ledgers close to 4×10^{-12} GJ and 2×10^{-8} kmol over every case, each run starts on its own cyclic steady state, and the controllers read instruments only. Nine cases each carry a completion rule written against the state of the bank. The general picture of a cyclic unit corrected once a report is in Section 1.4.7.

Section 5.2 follows the regenerative fixed bed from catalytic cracking to dehydrogenation and places the control problem among run-to-run methods. Section 5.3 sets out the bank: the reactions and equilibrium, a bed on the shared cell stack, purge, regeneration and evacuation, the surge and the compressor, the sequencer and the measures of performance, the instruments and the assumptions. Section 5.4 describes the control layers, from the two regulatory loops to the cycle-to-cycle PI and the MPC. Section 5.5 runs the nine cases, from where the heat goes and the regeneration as the handle to a lost bed, aging, the vacuum and the twelve-hour challenge. Section 5.6 names the hardware and the practice behind the model, Section 5.7 states what the model leaves out, and Section 5.8 sums up.

5.2 Regenerative Fixed Beds, From Cracking to Dehydrogenation

The Houdry process cracked oil over fixed catalyst beds, and Eugene Houdry's contributions to catalytic cracking are reviewed in [11], while the History box below follows its first commercial unit and the equipment it relied on. The sequence of a modern cyclic dehydrogenation bed, reaction, purge, regeneration and evacuation, keeps the same elements, and the same reliance on valves and vacuum.

> ⧖ HISTORY **Valves on Timers, 1937**
>
> In the early 1920s the French engineer Eugene Houdry began looking for a catalyst that would make gasoline from lignite, and he later turned to petroleum. His process gained a way to regenerate the catalyst after only ten minutes of use, and in March 1937 the first fully commercial unit went into operation. It processed 15 000 barrels of petroleum a day with a molten-salt heat control technique and motor-operated valves controlled by timers [12]. A paper of 1947 turned to the equipment such fixed beds relied on: steam-jet ejectors that evacuated the air from the reactors, removed oil vapors during the purge periods and held a vacuum on the closed heat-transfer salt systems [5].

The chemistry of propane dehydrogenation suits this arrangement. The reaction absorbs heat and is limited by equilibrium, so it needs a high temperature and benefits from a low pressure, while selectivity is hard to hold at the temperatures the reaction needs [7, 9]. In a cyclic reactor the catalyst loses activity quickly to carbon deposits and is restored by periodic regeneration [6]. Alkane dehydrogenation over supported chromium oxide is reviewed in [13], the mechanisms by which catalysts deactivate, fouling by carbon among them, are reviewed in [14], and transient kinetic models of propane dehydrogenation have been fitted on a platinum–tin catalyst [10]. Reviews compare the commercial dehydrogenation technologies and their operating windows [8, 9]. A recent review tabulates the cyclic fixed-bed process known as Catofin against the continuous moving-bed alternative, with chromia on alumina, fixed beds, 600 °C to 700 °C, a cycle of 15 to 30 min and a propane conversion of 48 to 65 % [1]. A dynamic model of a commercial Catofin reactor for isobutane describes beds of chromia on alumina cycling through dehydrogenation, regeneration, evacuation,

purge and reduction every 18 to 30 min, and names the gradual loss of heat in the bed together with deactivation as the operating concern [6].

> ⧖ HISTORY **Chromia and the Heat Problem, From 1933**
>
> Chromium oxide on alumina became the commercial catalyst of choice for dehydrogenation after the work of Frey and Huppke, published in 1933. Companies that set out to build a process on it met three problems: supplying enough heat to the reactor, controlling the temperature closely enough to hold the conversion up and the degradation products down, and regenerating the catalyst. Every industrial process that followed uses the heat of burning the coke in the dehydrogenation step, and the cyclic version runs a series of adiabatic fixed beds that alternate quickly between reaction and regeneration. In the 1970s and 1980s the main interest was butane, dehydrogenated toward synthetic rubber. By 1999 propane and isobutane had become more important [13].

Control of such a unit is layered. The sequencer owns the valves, ordinary loops hold the regeneration air and the compressor suction, and the conversion is corrected once a cycle from an analyzer, which places it in the family of run-to-run, iterative learning and repetitive control, where each run is adjusted from the measured outcome of the last [2, 3]. Iterative learning on a part built layer by layer is the subject of Volume 8, Chapter 10. Model predictive control, widely applied as supervisory control in the process industries [15], fits the same cadence when its model is written slot by slot. The literature reviewed here does not describe a cycle-to-cycle loop on a commercial unit, and the simulator's loop is offered as a teaching design rather than as industrial practice.

5.3 The Bank as Modeled

The bank is generic and drawn from no plant or licensor, as shown in Figure 5.1. Eight horizontal adiabatic reactors A to H take turns in a fixed rotation. A bed on line receives propane F_{in} from a charge heater at T_{feed} and sends its effluent to a product header, a bed in regeneration receives hot air at T_{air}, a bed in purge receives steam, and an evacuated bed is drawn to the vacuum header with no flow. The product passes a surge volume V_s at the suction pressure P_s to a compressor at speed n_c, and the beds run ΔP above the suction. The regeneration air leaves an air heater at T_{ah} and is raised to T_{air} by fuel gas injected through a valve. The engine's clock is the minute, flows inside a bed are in mol/s, heats in GJ and temperatures in °C. The engine and its clocks are those of Section 1.6.1. Each bed carries twelve states, six cell temperatures T_i and six coke masses $m_{coke,i}$, and the plant adds five more and thirteen ledgers, 114 in all.

Table 5.1 gives each variable's role and its value in case 2 at $t = 0$, which is the design point.

5.3.1 Reactions and Equilibrium

Three reactions run on line, the dehydrogenation $C_3H_8 \rightleftharpoons C_3H_6 + H_2$, thermal cracking $C_3H_8 \rightarrow CH_4 + C_2H_4$, and coking $C_3H_6 \rightarrow 3\,C + 3\,H_2$, at the rates of Equation (5.1).

$$
\begin{aligned}
r_1 &= a\,k_1 \left(\frac{P}{P_0}\right)^{n-1} \left(p_{C_3H_8} - \frac{p_{C_3H_6}\,p_{H_2}}{K_p}\right) \\
r_2 &= f_{cr}\,k_2\,p_{C_3H_8}, \qquad r_3 = a\,f_{ck}\,k_3\,p_{C_3H_6} \\
k_j &= k_{j,0} \exp\left[-\frac{E_j}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \\
K_p &= \exp\left(\frac{\Delta S_1}{R} - \frac{\Delta H_1}{RT}\right), \qquad a = a_{cat} \exp\left(-\frac{m_{coke}}{c_D W}\right)
\end{aligned}
\tag{5.1}
$$

where p_k are partial pressures in bar at the bed pressure P, $P_0 = 0.5\,\text{bar}$, $T_r = 873.15\,\text{K}$, $n = 0.3$ is the order of the dehydrogenation in total pressure, a is a cell's activity, W its mass, $c_D = 1.6\,\text{kg}$ of coke per tonne of bed lowers the activity to 37 percent, and a_{cat}, f_{cr} and f_{ck} are the disturbance settings. Cracking is thermal and does not depend on the activity. With $\Delta H_1 = 129.5\,\text{kJ/mol}$ and

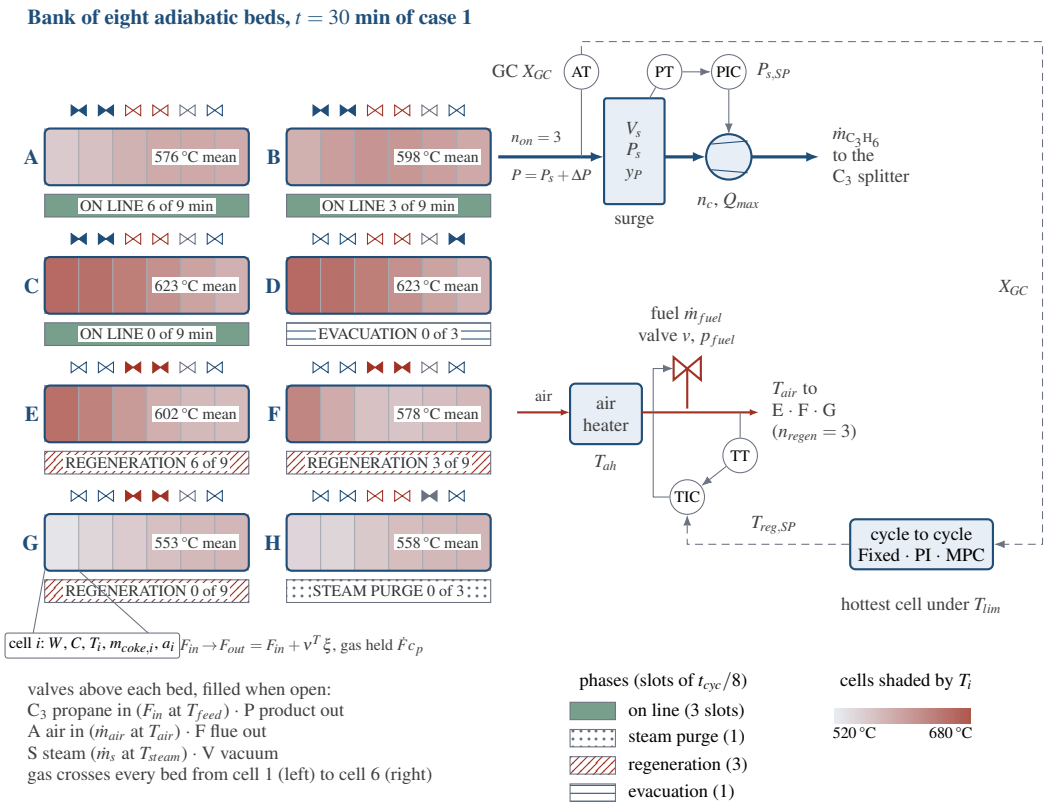


Figure 5.1 The eight-bed bank as modeled, redrawn from the Bank view of case 1 at $t = 30$ min with every station held in Manual. Beds A, B and C are on line (6, 3 and 0 min into their nine), D is evacuated, E, F and G regenerate in 660 °C air and H is purged with steam. Cells are shaded by temperature, from 523 °C at G's inlet to 658 °C at C's, and the valve sets show which gas each bed receives. The product side carries 14.35 t/h of propylene at a suction of 0.446 bar a, and the GC (AT) feeds the cycle-to-cycle layer, which writes the TIC's setpoint. Bed A's own chart over the same run is Figure 5.2. Not to scale.

$\Delta S_1 = 139.2\,\mathrm{J/(mol\,K)}$, $K_p = 0.334$ bar at 600 °C, and the equilibrium conversion of pure propane, $X_{eq} = \sqrt{K_p/(P+K_p)}$, is 63.3 percent at 0.5 bar a and 50.0 percent at 1 bar a. The thermodynamic polynomials of NASA Glenn [16] give $\Delta H_1 = 130.01\,\mathrm{kJ/mol}$, $\Delta S_1 = 139.28\,\mathrm{J/(mol\,K)}$ and $K_p = 0.315$ bar at 600 °C, or 62.2 and 48.9 %, so the app's equilibrium sits about one point high. The difference comes almost entirely from the app's ΔH_1, 0.5 kJ/mol under the tabulated value, and is kept as a teaching value.

5.3.2 A Bed on the Shared Cell Stack

Each bed is built on the packed-bed cell stack shared by the framework's reactor applications, which solves a cell's composition algebraically and carries its temperature as a state. The stack is assembled here as six one-cell beds per reactor so that each cell carries its own coke and activity. On line, cell i

Table 5.1 Roles and Design Values of the Variables

Variable	Role	Design	Range
X_{GC}	CV, bank conversion (GC)	57.8 %	SP 45–68
T_{air}	CV, air (TIC)	660.0 °C	SP 600–720
P_s	CV, suction (PIC)	0.450 bar a	SP 0.25–0.80
$T_{reg,SP}$	MV, cycle to cycle	660 °C	600–T_{lim}
v	MV, fuel valve	49.9 %	0–100
n_c	MV, compressor speed	74.8 %	0–100
t_{cyc}	set, cycle time	24 min	16–40
F	set, feed per bed on line	10 t/h	6–14
—	set, with a bed out	leave the gap	3 options
p_{fuel}	DV, fuel gas pressure	100 %	40–110
α_c	DV, compressor available	100 %	40–100
a_{cat}	DV, catalyst activity	100 %	50–100
f_{ck}, f_{cr}	DV, coke make, cracking	1, 1	0.5–3
S, $\dot{m}_{C_3H_6}$	outputs	88.0 %, 14.57 t/h	—
T_i, $m_{coke,i}$	states, per cell (96)	—	—
x_v, T_{air}, P_s	states, plant	—	—
n_c, y_P	states, plant	—	—

obeys Equation (5.2).

$$\begin{aligned} F_{out,i} &= F_{out,i-1} + \nu^T \xi_i, \qquad \xi_{j,i} = W\, r_j(T_i, F_{out,i}) \\ C\,\frac{\mathrm{d}T_i}{\mathrm{d}t} &= \dot{F} c_p\,(T_{i-1} - T_i) - \textstyle\sum_j \xi_{j,i}\,\Delta H_j \\ \frac{\mathrm{d}m_{coke,i}}{\mathrm{d}t} &= 3\,M_C\,\xi_{3,i} \end{aligned} \tag{5.2}$$

where $F_{out,0} = F_{in}$ is pure propane, the first cell's inlet temperature T_{i-1} is T_{feed}, $W = 5.5\,\mathrm{t}$, $C = 6.05\,\mathrm{MJ/K}$, ν holds the stoichiometry of the three reactions, $\Delta H_2 = 82\,\mathrm{kJ/mol}$, $\Delta H_3 = -20\,\mathrm{kJ/mol}$, M_C is the molar mass of carbon, and $\dot{F} c_p$ is the propane fed times 160 J/(mol K), held along the bed. Each cell's extents are found by six Newton iterations from zero with no convergence test, so a sweep of the bed depends only on its inputs and runs replay bit for bit. At 10 t/h, $F_{in} = 62.99\,\mathrm{mol/s}$ and $\dot{F} c_p = 10.08\,\mathrm{kW/K}$, so the gas would need 10.0 min to change a cell's temperature by itself, longer than the on-line period. The bed's temperature therefore follows its heat of reaction, and the cell nearest the inlet, where the propane is richest, cools first and furthest. The stack itself is checked apart from any plant, against the tanks-in-series answer, the plug-flow limit and its own energy closure, and its outlet error halves when the number of cells doubles.

5.3.3 Purge, Regeneration and Evacuation

Off line a different gas crosses the bed. In regeneration the coke laid down on line burns and releases its heat in the cell where it lies, so a bed that made more coke is reheated more, whatever the air temperature. Purge, regeneration and evacuation differ only in the gas, as shown in Equation (5.3).

$$\begin{aligned} C\,\frac{\mathrm{d}T_i}{\mathrm{d}t} &= \dot{m}_g c_g\,(T_{i-1} - T_i) + \Delta H_b\, k_b(T_i)\, m_{coke,i} \\ \frac{\mathrm{d}m_{coke,i}}{\mathrm{d}t} &= -k_b(T_i)\, m_{coke,i} \end{aligned} \tag{5.3}$$

where in regeneration $\dot{m}_g c_g$ is the air per bed, $\dot{m}_{air} = 40\,\mathrm{kg/s}$ at 1150 J/(kg K), the first cell's inlet is T_{air}, $\Delta H_b = 32.8\,\mathrm{MJ/kg}$ and $k_b = 1\,\mathrm{min}^{-1}$ at 650 °C with an activation energy of 100 kJ/mol, first order in the coke with the oxygen in excess. In purge the gas is $\dot{m}_s = 3\,\mathrm{kg/s}$ of steam at $T_{steam} = 450\,^{\circ}\mathrm{C}$ and nothing burns, and an evacuated bed, or one out of service, holds its state. The air's time constant on a cell, $C/(\dot{m}_{air} c_{air}) = 2.19\,\mathrm{min}$, is short against the nine-minute regeneration,

so the air front crosses the bed and leaves its inlet cells near T_{air}. One regeneration air header serves every regenerating bed, as shown in Equation (5.4).

$$\begin{aligned} T^{*}_{air} &= T_{ah} + \frac{\eta\,\mathrm{LHV}\,\dot{m}_{fuel}}{n_{regen}\,\dot{m}_{air}\,c_{air}} \\ \dot{m}_{fuel} &= x_v\,\dot{m}_{f,max}\sqrt{p_{fuel}} \\ \tau_{air}\frac{\mathrm{d}T_{air}}{\mathrm{d}t} &= T^{*}_{air} - T_{air}, \qquad \tau_v\frac{\mathrm{d}x_v}{\mathrm{d}t} = v - x_v \end{aligned} \tag{5.4}$$

where $T_{ah} = 600\,^{\circ}\mathrm{C}$, $\eta = 0.98$, $\mathrm{LHV} = 47\,\mathrm{MJ/kg}$, $\dot{m}_{f,max} = 0.36\,\mathrm{kg/s}$, p_{fuel} is the fuel gas pressure as a fraction of design, n_{regen} is the number of beds regenerating, $\tau_{air} = 0.1\,\mathrm{min}$ and $\tau_v = 0.05\,\mathrm{min}$. At design the valve stands at 49.9 % and burns 0.647 t/h, and with fewer beds regenerating the same fuel heats less air further.

5.3.4 Surge, Compressor and Vacuum

The beds' effluent mixes in the surge volume, whose pressure and propylene share follow the balances of Equation (5.5).

$$\begin{aligned} \frac{V_s}{RT_s}\frac{\mathrm{d}P_s}{\mathrm{d}t} &= \sum_{on} F_{out} - n_c\,\alpha_c\,Q_{max}\frac{P_s}{RT_s} \\ N_s\frac{\mathrm{d}y_P}{\mathrm{d}t} &= \sum_{on} F_{out}\,(y_{in} - y_P), \qquad N_s = \frac{P_s V_s}{RT_s} \end{aligned} \tag{5.5}$$

where F_{out} is a bed's total outlet flow, y_{in} the propylene share of the beds' combined effluent, $V_s = 1500\,\mathrm{m^3}$ at $T_s = 40\,^{\circ}\mathrm{C}$, $Q_{max} = 23.3\,\mathrm{m^3/s}$ at full speed, α_c the compressor's available capacity, and the speed follows its command with 0.1 min. The propylene to the splitter is the compressor's molar flow times y_P, and the bed pressure is $P = P_s + \Delta P$ with $\Delta P = 0.05\,\mathrm{bar}$. The surge holds 25.9 kmol at 0.45 bar a, about 1.4 min of the bank's 310.7 mol/s, and at design the compressor runs at 74.8 % speed. Because its capacity is a volume at suction, a deeper vacuum needs more speed for the same moles.

5.3.5 The Sequencer and the Measures of Performance

The cycle is cut into eight slots of $t_{cyc}/8$, and every phase lasts a whole number of them, three on line, one in purge, three in regeneration and one evacuated. Each bed in service holds a position in a ring, its position sets its phase, and at every slot boundary all beds move one position on, so the hottest bed comes on line and the one on line longest goes to purge. A bed taken out of service leaves an empty position. The setting *With a bed out* leaves the gap, so that for three slots of each cycle only two beds are on line, or removes the hole when it reaches a regeneration position (seven beds, three on line, regeneration of two slots) or an on-line position (seven beds, two on line). The sequencer belongs to the plant, moves on at the end of each integration step, and switches every valve at a slot boundary in one step.

The bank's conversion and selectivity are taken over each slot, $X = 1 - \int\sum F_{\mathrm{C_3H_8},out}\,dt \,/\, \int\sum F_{in}\,dt$ and $S = \int\sum F_{\mathrm{C_3H_6},out}\,dt \,/\, \int\sum (F_{in} - F_{\mathrm{C_3H_8},out})\,dt$, which equal one bed's averages over its whole on-line period. The product ripple is the peak-to-peak propylene to the splitter within a slot as a percentage of its mean. Catalyst life is a projection from a teaching wear law, as shown in Equation (5.6).

$$\mathrm{life} = \frac{L_{ref}}{\exp\left[\frac{E_w}{R}\left(\frac{1}{T_w} - \frac{1}{T_i}\right)\right]} \tag{5.6}$$

where the bar is the mean over every cell in service and the last cycle, $E_w = 340\,\mathrm{kJ/mol}$, $T_w = 923.15\,\mathrm{K}$ and $L_{ref} = 0.54\,\mathrm{years}$, so the life halves about every 14 K near 650 °C. The projection does not lower the activity within a run.

Table 5.2 Parameters. A: Adjustable in the Parameters Panel. V: Fixed and Stated in the App. H: Fixed and Not Displayed

Symbol	Meaning	Value	
—	bed mass, heat capacity	33 t, 1.1 kJ/(kg K)	V
ΔP	beds above the suction	0.05 bar	A
T_{feed}	charge heater outlet	600 °C	A
T_{lim}	bed temperature limit	680 °C	A
$k_{1,0}$, E_1	dehydrogenation	0.012 mol/(s kg bar), 120 kJ/mol	A, V
n	order in total pressure	0.3	V
ΔH_1, ΔS_1	dehydrogenation	129.5 kJ/mol, 139.2 J/(mol K)	V
$k_{2,0}$, E_2	cracking	8×10^{-4} mol/(s kg bar), 200 kJ/mol	A, V
$k_{3,0}$, E_3	coking	1.4×10^{-4} mol/(s kg bar), 150 kJ/mol	A, H
c_D	coke for activity $1/e$	1.6 kg/t	A
k_b, E_b	coke burn rate	1 /min at 650 °C, 100 kJ/mol	V, H
ΔH_b	heat of coke burn	32.8 MJ/kg	V
c_p	gas per mol of propane fed	160 J/(mol K)	H
$\dot{m}_{air}$	air per regenerating bed	40 kg/s	A
c_{air}	air heat capacity	1150 J/(kg K)	H
T_{ah}	air heater outlet	600 °C	A
LHV, η	fuel heating value, share	47 MJ/kg, 0.98	V, H
$\dot{m}_{f,max}$, τ_v	fuel valve, lag	0.36 kg/s, 0.05 min	H
τ_{air}	air mixing lag	0.1 min	V
$\dot{m}_s$, T_{steam}	purge steam	3 kg/s, 450 °C	V
—	steam heat capacity	2300 J/(kg K)	H
V_s, T_s	surge volume	1500 m^3, 40 °C	A, V
Q_{max}	compressor at suction	23.3 m^3/s	A
τ_c	compressor speed lag	0.1 min	H
E_w, L_{ref}	wear law	340 kJ/mol, 0.54 y	V

5.3.6 Instruments, Initialization and Numerics

A gas chromatograph (GC) analyzes a composite sample of each slot's product and reports X_{GC} 1 min after the slot ends, with 0.1 point of noise, holding between reports. The regeneration air thermocouple carries a 0.1 min lag and 0.3 K of noise, the suction transmitter 0.001 bar of noise, the bed thermocouples read every cell, and the sequencer's state and the feed are known exactly. Every run starts on the cyclic steady state of its own settings. One bed is integrated through the ring with the engine's own step until it repeats to 10^{-7} K, and each bed is placed at the state of its ring position, so a bank started this way is periodic to the integrator. From a uniform 620 °C a bed repeats to 0.1 K within four cycles. Integration is fourth-order Runge–Kutta with a 1 s step, which puts every slot boundary on the grid, the loops execute every 5 s and the historian logs every 10 s. At the top playback speed of 120 min per second the twelve-hour challenge needs 6 s, provided the browser sustains it. The exported file (Section 1.6.4) sets each GC report beside the true slot conversion, so an explanation can be checked against the simulator's own record. Halving the step moves the cyclic start by less than 10^{-6} K and the design conversion by 0.012 points. Over every case the bank's energy closes on its ledgers to 4.0×10^{-12} GJ and its carbon to 2.2×10^{-8} kmol. Table 5.2 lists the parameters.

5.3.7 Assumptions

The beds are adiabatic and lose no heat, and six cells stand for plug flow, which gives 57.8 percent conversion at design against 59.5 with twelve cells and 60.4 with twenty-four, while the start and end temperatures move less than 1.3 K. The gas's heat capacity flow is that of the propane fed, and the reactions' change of it is left out. Coke is carbon from propylene, burned first order with the oxygen in excess, the air bringing nearly 190 times the oxygen the coke needs. A real cycle also reduces the catalyst with hydrogen before it goes back on line, and its valve sequence takes tens of seconds, while here a bed is purged with steam and evacuated with no flow and its valves switch at once. The GC reports a slot 1 min after it ends, faster than a real analyzer and sample system. The rate order in

total pressure, the cracking and coking rates, the 88 percent selectivity at design and the wear law are teaching values. The design conversion of 57.8 percent and the 24 min cycle lie inside the 48 to 65 percent and 15 to 30 min tabulated for the Catofin process [1], while the selectivity has not been compared with a source. The bed temperature limit of 680 °C and the vacuum alarm are teaching values. Real limits come from the catalyst supplier and the licensor, and the trips that guard them from the plant's safety requirements under IEC 61511.

5.4 The Control Layers as Implemented

The sequencer owns the valves, and no controller moves a bed between phases. One Manual and Auto switch governs the whole bank. In Manual the fuel valve and the compressor speed are the operator's stations and every controller tracks what is applied, so a return to Auto, or a change of architecture, is bumpless. Each execution builds the measurement packet, runs the cycle-to-cycle layer when a GC report has arrived, then the two loops.

5.4.1 Two Regulatory Loops

Both loops use the framework's velocity-form PID law of Section 1.6.2, Equations (1.14) to (1.17), with the derivative set to zero and a direction $a = \pm 1$ on the error. Only the emitted output is clamped, and the integral is corrected toward it with a tracking time of τ_I. The TIC ($a = +1$) holds T_{air} by the fuel valve at 0.5 % per K and 0.3 min within 0 to 100 %. The PIC ($a = -1$) holds P_s by the compressor speed at 300 % per bar and 2 min. Both execute every 5 s. Either loop becomes proportional only when its integral time is set to the slider's maximum, 10 min for the TIC and 60 min for the PIC.

5.4.2 The Cycle-to-Cycle Layer

Above the TIC the regeneration setpoint $T_{reg,SP}$ comes from one of three architectures. *Fixed* holds the operator's setpoint, 660 °C as shipped. The *cycle-to-cycle PI* is the same routine called only when a GC report arrives, once a slot, with Δt the time since the last report, $a = +1$, 3 K per point of conversion and 15 min, and its output clamped to 600–T_{lim}. The integral used at report k was accumulated through report $k-1$, so the integral part of a move reaches the air one report after the error that caused it. The air it sets reaches the first bed two slots later, so the loop meets a delay of a cycle, not a time constant. Equation (1.12) gives the pure-delay form of such a loop. A correction computed from results that arrive while later runs are already under way is also the problem of the vial filler of Volume 8, Chapter 9, and the simulated moving bed of Chapter 7 is this volume's other unit whose quality is known only once a cycle.

The *MPC*, the predictive option of Section 1.6.3 written slot by slot, plans $T_{reg,SP}$ at every report over $N = 16$ slots in four move blocks of 1, 1, 1 and 13 slots, on a finite step response model of the slot conversion, as shown in Equation (5.7).

$$
\begin{aligned}
& y_k = b + \textstyle\sum_{j=1}^{16} h_j (u_{k-j} - u_0) + \sum_{j=1}^{16} g_j (w_{k-j} - w_0) \\
& \min \ \textstyle\sum_k w_X (y_k - X_{SP})^2 + w_{\Delta u} (\Delta u_k / 5\,\mathrm{K})^2 \\
& \qquad + 0.06\, \ell_{life}\, u_k \\
& \text{s.t. } 600 \le u_k \le T_{lim}, \qquad u_k + \delta \le T_{lim} - m + \sigma
\end{aligned}
\tag{5.7}
$$

where u is $T_{reg,SP}$, w is the measured feed per bed, held over the horizon, h_j and g_j are the slot-by-slot increments of step responses identified on the model with +5 K and +0.5 t/h steps, one set for each schedule (eight beds, seven with three on line, seven with two), $h_1 = h_2 = 0$ because the air reaches the bank two slots late, b is the last report less the model's value of it, δ is the last measured hottest regenerating cell less the setpoint then in force, $w_X = w_{\Delta u} = \ell_{life} = 1$, $m = 5\,\mathrm{K}$, and the slack σ is priced $50\sigma^2 + 5\sigma$. At eight beds the identified gains are 0.288 points per K and -2.66 points per t/h. The linear cost on u stands for catalyst wear. Each plan is a quadratic program, solved in the framework's linear MPC module with the Goldfarb–Idnani algorithm, a dual active-set method [17].

When a plan comes back infeasible, not finite or outside its bounds, the tracked PI takes the setpoint without a bump.

5.4.3 Alarms and Three Models

BED TEMPERATURE LIMIT flags any cell above T_{lim}, VACUUM LOST flags a suction more than 0.02 bar above its setpoint for 2 min, and SCHEDULE GAP and BED OUT OF SERVICE report the sequencer. None of them trips the unit. Three models are kept apart. The plant is the model of Section 5.3, a reader of the trends can identify a second one, such as the 0.29 points per K and the two-slot delay of case 3, and the controllers' own model is the MPC's step response, which knows the schedule and the feed but neither the coke on any cell nor the activity.

5.4.4 Design Choices

Eight decisions taken while the app was built either depart from its plan or settle a value the plan left open. First, the dehydrogenation is of order 0.3 in total pressure, a teaching value. From 0.45 to 0.35 bar a the design cycle's conversion moves $+0.35$, $+0.07$ and -0.67 points at orders 0.3, 0.5 and 1, so a law of first order in the partial pressures would make the vacuum lower the conversion, the reverse of why the process runs under vacuum. Second, case 8 therefore teaches that the vacuum buys selectivity, because the stored heat caps the conversion. The selectivity gain holds at every order tried, 2.70, 2.46 and 1.80 points, while the conversion's sign does not. Third, the phases are fixed whole slots, because a rotation with a fixed number of beds on line needs them. Fourth, the sequencer and the GC are written for this app rather than taken from the shared stage sequencer and analyzer, since the shared sequencer starts and stops stages against a demand with run and rest times instead of rotating a ring, and the GC's composite must follow the slot length. Fifth, one air header and one TIC serve all regenerating beds. Sixth, each reactor is six one-cell beds of the shared stack so that each cell has its own coke. Seventh, catalyst life is a projection that does not feed back on the activity, and aging is a disturbance. Eighth, the challenge's conversion target is a band, every hourly average within ± 2 points of 57 % with a fuel limit, rather than a floor. A fixed 660 °C with two beds on line meets "at least 57 %" in every hour from the second, at 57.85 to 64.89 %, with no control and 0.647 t/h of fuel, so a floor would grade burning fuel rather than control.

5.5 Nine Cases on the Running Bank

The cases are listed in Table 5.3 and the principal measurements in Table 5.4. All values were measured headlessly on the app's engine, at its default seed and with the 1 s step the browser uses. Changes a case requests are applied once the run is under way, at 4 min where a case says after the first slot, and the challenge was repeated at seeds 0 to 3 and at half the step. Slot conversions are the simulator's composite over each slot.

> **✦ DID YOU KNOW? Losing a Bed Can Raise the Conversion**
>
> From the simulator: when bed D fails in case 5 and the seven beds close up with two on line, the Fixed regeneration gives 64.8 % conversion, against 57.8 % with the gap left, because each bed now regenerates longer. The price is propylene, 10.66 t/h against 12.73 t/h (Table 5.4).

5.5.1 Where the Heat Goes

Case 1 follows bed A from the instant it comes on line, with both stations held in Manual. Its mean temperature falls from 622.6 to 557.6 °C in nine minutes, the inlet cell from 658.1 to 540.1 °C and the outlet cell only from 581.1 to 574.9 °C, while its conversion falls from 69.9 to 44.7 % and averages 57.8 % at a selectivity of 88.0 %. The equilibrium at its mean temperature falls with it, from 71.5 to 46.0 %, so the bed runs close to equilibrium throughout and its conversion is limited by the heat left in it, as shown in Figure 5.2. The stored-heat arithmetic closes independently. The reactions

Table 5.3 The Nine Cases

#	Case and events	Teaching point
1	Manual, bed A just on line	where the heat goes
2	Auto, Fixed 660 °C, Schedule view	the ripple and its averaging
3	Regeneration air 660 to 670 °C	the handle, a cycle late
4	Cycle 24 to 32 min (16, 40)	the temperature swing
5	Bed D out at 12 min	three ways to run seven beds
6	Feed +15 % at 12 min, then PI or MPC	tuning for a delay
7	Catalyst aged at 12 min	coke as fuel, selectivity lost
8	Suction 0.45 to 0.35, then 0.30 bar a	vacuum buys selectivity
9	Challenge, 12 h: bed D out at 3 h, feed +15 % at 7 h	schedule and loop together

Table 5.4 Case Outcomes Measured on the Engine

Case and condition	Result
1, bed A on line	622.6 to 557.6 °C, X 69.9 to 44.7 %
2, PIC 300 / 40 / 1000 %/bar	ripple 5.1 / 2.6 / 9.0 %
3, air +10 K	slot X 57.80 to 60.73 %, S 86.9 %
4, cycle 16 / 24 / 32 / 40 min	X 56.1 / 57.8 / 58.4 / 56.8 %
4, same	life 5.0 / 3.0 / 2.1 / 1.6 y
5, gap, Fixed	57.8 %, 12.73 t/h, ripple 56.6 %
5, three on line, Fixed / PI	48.0 / 52.6 % (air at 680 °C)
5, two on line, Fixed / PI	64.8 / 57.0 %, 10.66 / 9.68 t/h
6, Fixed / PI / MPC	53.95 % / holds from 76 / 49 min
7, aged, Fixed	start 625.1 °C, X 56.3, S 85.8 %
8, 0.45 / 0.35 bar a	X 57.80 / 58.15, S 88.0 / 90.7 %
8, 0.30 bar a asked	held at 0.337, VACUUM LOST in 2 min

absorb 2.443 GJ over the period, the bed gives 2.359 GJ (36.3 MJ/K × 64.98 K) and the 600 °C feed the remaining 0.084 GJ. Over the whole cycle the air brings 2.182 GJ, the burn of the coke 0.332 GJ, the feed 0.084 GJ, and the purge steam takes away 0.155 GJ, which again sums to the reaction heat. The steam cools the bed to 553.4 °C, the air returns it to 622.6 °C with its hottest cell at 658.1 °C, and 0.4 kg of coke is left unburned for the next period.

> **TRY IT IN THE APP** **1 · One Bed Through Its Cycle (Manual)**
>
> Load the scenario and press Run, then watch bed A on the Bed view. In its nine minutes on line its mean temperature falls from 622.6 to 557.6 °C and its conversion from 69.9 to 44.7 %. Keep running through the purge and the regeneration and see it come back on line at 622.6 °C, ready to spend the same heat again.

Case 2 puts the eight beds together. The three beds on line are 0, 3 and 6 min into their periods, so the bank's instantaneous conversion saws between 54.1 and 62.1 % every slot and the propylene to the splitter between 14.12 and 14.87 t/h, a ripple of 5.1 %. Loosening the PIC to 40 % per bar and 15 min halves the ripple to 2.6 % while the suction stays within 0.445 to 0.455 bar a, because the surge itself averages the flow once the speed stops following it, and tightening it to 1000 % per bar and 1 min passes the sawtooth on at 9.0 %. The price of the loose loop is speed. A setpoint step from 0.45 to 0.40 bar a settles within 0.005 bar in 2.3 min as shipped and 8.3 min at 100 % per bar, and not within 54 min at 40 % per bar. This is averaging control applied to a gas inventory under vacuum.

5.5.2 The Regeneration as the Handle

Case 3 raises the regeneration air from 660 to 670 °C at 4 min and follows the response, as shown in Figure 5.3. The first slot to move is the one ending at 12 min, 57.92 against 57.80 %, made in part by a bed that finished its regeneration in the hotter air. A bed comes on line above 629 °C at 18 min, the slot conversion passes 60 % at 27 min and has made 78 % of its final change by 30 min and 98 % by 54 min. A second, smaller rise arrives one cycle later, when the beds start their next

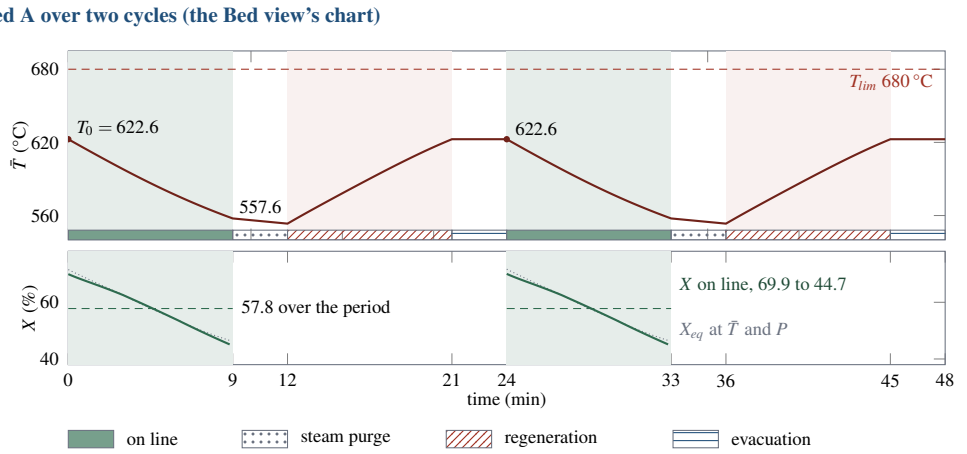


Figure 5.2 Bed A over two cycles, the Bed view's chart in case 1 with every station held in Manual. Top: its mean temperature (solid), falling on line from 622.6 °C and recovering in regeneration, against the 680 °C limit (dashed), over the phase strip. Bottom: its conversion while on line (solid) against the equilibrium at its mean temperature (dotted), with the average over each on-line period (dashed).

regeneration from a warmer end, and the bank settles at 60.73 % with every bed coming on line at 630.8 °C, 0.293 points per kelvin of air. The selectivity falls from 88.0 to 86.9 %, the fuel rises 0.106 t/h from 0.647 t/h, and the projected catalyst life falls from 3.0 to 2.0 years.

Pause. Try Exercise 5.1 before reading on.

> **TRY IT IN THE APP 3 · Regeneration Heat Is the Handle**
>
> Press Run and, after the first slot, raise the Regeneration air setpoint from 660 to 670 °C. Watch the Start of cycle badge: a bed comes on line above 629 °C at 18 min, and the slot conversion passes 60 % only at 27 min. The bank settles at 60.73 %, one to two cycles after the move.

Case 6 makes the delay a tuning problem. With the regeneration fixed, the first slot after the 15 % feed step reads 55.50 % and the bank settles at 53.95 %, the reactions now absorbing 2.633 GJ per bed and period against 2.443 GJ. Handed the setpoint at 18 min, the shipped PI raises the air step by step to 671 °C and holds the GC within 0.5 point of the target from 76 min, peaking at 57.06 %. The MPC holds from 49 min, peaking at 57.03 %. At its first report it moves the air to 668.7 °C against the PI's 661.9 °C, because its model knows both the delay of its own moves and the feed it has measured. Frozen so that it does not see the feed, it holds from 70 min, so the measured feed bought most of its lead. A tighter PI, 5 K per point and 12 min, holds from 52 min with a 0.44 point overshoot. Over a grid of gains from 2 to 8 K per point and integral times from 6 to 30 min, the most aggressive settings overshoot to as much as 58.6 % or never settle within the band, which is why the shipped tuning is slow.

5.5.3 Cycle Length, a Lost Bed, Aging and Vacuum

Lengthening the cycle in case 4 widens the swing at both ends. At 32 min a bed comes on line at 637.2 °C instead of 622.6 °C and its conversion runs from 76.4 down to 39.5 %, yet the average barely moves, 58.4 against 57.8 %, because the air puts in the same heat per minute. The selectivity falls from 88.0 to 87.8 %, the ripple rises from 4.6 to 8.4 % and the projected life falls from 3.0 to 2.1 years. At 16 min the bed starts at 608.0 °C and converts 56.1 % with 5.0 years of life, and at

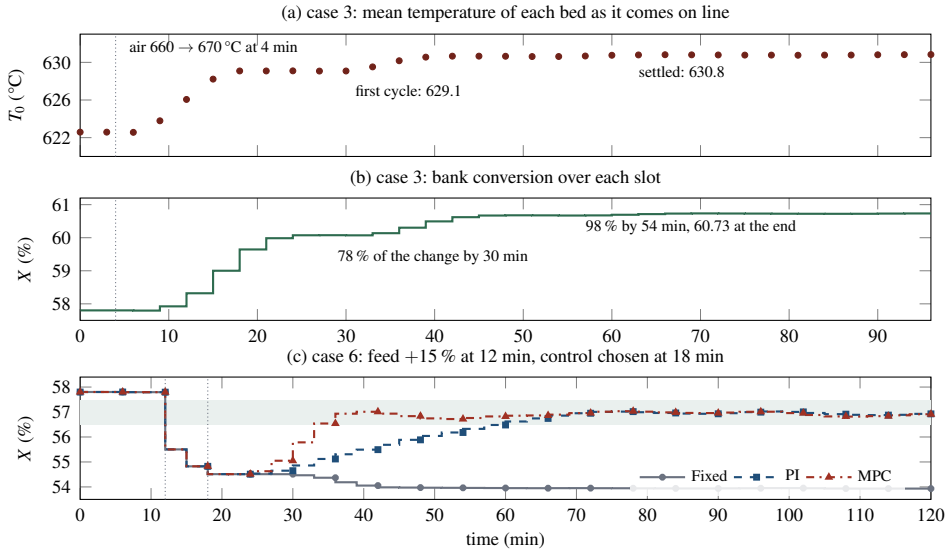


Figure 5.3 The regeneration acts a cycle late. (a) Case 3, the mean temperature of each bed as it comes on line after the air is raised 10 K at 4 min. (b) The bank's slot conversion in the same run, drawn over the slot it belongs to. (c) Case 6, the slot conversion after the feed per bed rises 15 % at 12 min, with the regeneration left Fixed (solid, dots) or handed at 18 min to the cycle-to-cycle PI (dashed, squares) or the MPC (dash-dotted, triangles). The shaded band is ±0.5 point of the 57 % target.

40 min the conversion itself falls to 56.8 % as the end of each period runs too cold. The model counts none of the costs of a short cycle, the valve strokes, purge steam and vacuum.

Case 5 loses bed D at 12 min. Leaving the gap keeps the conversion at 57.8 %, but the propylene falls from 14.57 to 12.73 t/h and ripples 56.6 % each cycle as the empty slot passes. Seven beds with three on line close up at 21 min and give a steady 12.39 t/h, but every bed now regenerates for two slots, starts at 596.9 °C, and the conversion falls to 48.0 %. Seven beds with two on line close up at 15 min, the conversion rises to 64.8 % on the longer regeneration, and the propylene falls to 10.66 t/h. The cycle-to-cycle PI holds 57.0 % with two on line at 636.6 °C air. With three on line it drives the air to the 680 °C limit and stops at 52.6 %. A sweep of the air temperature explains why. With three on line the conversion is 43.5, 45.7, 47.9, 50.3 and 52.6 % at 640, 650, 660, 670 and 680 °C air, so no regeneration under the limit reaches 57 % at 10 t/h per bed, and it would take a feed of 8.5 t/h (57.25 %). This infeasibility is deliberate, and the case states it.

The aged catalyst of case 7, at 75 % activity and 1.5 times the coke, lays down 88.6 instead of 80.9 kg of coke per cycle, whose burn releases 2.91 instead of 2.65 GJ, so the beds come on line hotter, at 625.1 °C. The conversion falls only from 57.8 to 56.3 %, because a slower catalyst draws less heat early, while the selectivity falls from 88.0 to 85.8 % and stays there. The PI restores 57.0 % with 662.5 °C air at a projected life of 2.6 instead of 2.9 years.

Pause. Try Exercise 5.3 before reading on.

In case 8 the suction setpoint is lowered to 0.35 bar a. The conversion rises only from 57.80 to 58.15 % while the selectivity rises from 88.0 to 90.7 % and the propylene from 14.57 to 15.11 t/h, as cracking and coking slow at the lower partial pressures, and the compressor needs 96.2 % of its speed. Asked for 0.30 bar a, it runs at full speed, holds 0.337 bar a, and VACUUM LOST appears 2 min after the request.

Pause. Try Exercise 5.2 before reading on.

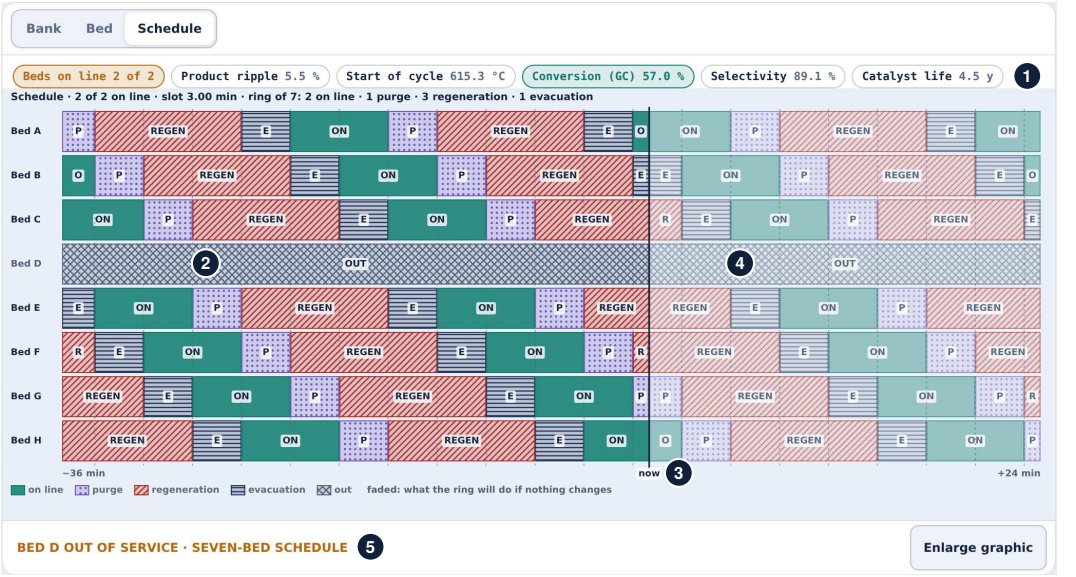


Figure 5.4 The challenge on its suggested settings, the cycle-to-cycle PI with seven beds two on line, at $t = 718$ min on the Schedule view, cropped to the plant. (1) The badges read 2 of 2 beds on line, a ripple of 5.5 %, a start-of-cycle temperature of 615.3 °C, a GC conversion of 57.0 %, a selectivity of 89.1 % and a projected life of 4.5 years. (2) Bed D, out of service since 3 h, while the seven-bed ring runs two on line, one in purge, three regenerating and one evacuated. (3) The present instant. (4) What the ring will do over the next 24 min, faded. (5) The status line that reports the bed out and the seven-bed schedule.

5.5.4 Twelve Hours With a Lost Bed and More Feed

The challenge runs 12 h. Bed D fails on line at 3 h and the feed per bed rises 15 % at 7 h. It is met when every clock hour's conversion from the second hour lies within ±2 points of 57 %, no cell exceeds 680 °C, the ripple stays at or under 10 % in every slot of the last two hours and the fuel averages at most 0.55 t/h, judged on the simulator's truth at every step. The configurations are compared in Table 5.5, and the suggested run is shown in Figure 5.4. As shipped, with Fixed regeneration and the gap left, the product ripples 58.6 % and the conversion drifts to 53.8 % after the feed rises, 3.19 points from the target at hour 11. The suggested settings pass, and the MPC on the same schedule passes too. Their margin is thin but steady. Over the default seed, seeds 0 to 3 and the halved step the worst hour lies 1.70 to 1.75 points from the target for the PI and 1.69 to 1.73 for the MPC, always hour 4, the close-up transient in which the bank's slot conversion briefly reaches 61.4 %. The MPC solves 239 plans with none rejected, and ties the PI at 1.72 against 1.73 points and 0.494 against 0.497 t/h. Its advantage is recovery speed after a measured feed change, not the graded outcome. Figure 5.5 sets the table's graded columns against their limits.

Three on line fails whatever the control, 8.14 points with the PI and 9.14 with the MPC, because the two-slot regeneration cannot reach the target under the limit. Even with the feed cut to 7.5 to 8.5 t/h per bed it misses by 2.89 to 3.08 points at hour 4. The PI with the gap holds the conversion within 1.10 points but fails the ripple and the fuel. The Fixed regeneration with two on line overshoots to 64.89 %. The tighter PI that settled case 6 sooner passes with 0.83 points, yet it overshoots case 6 by 0.44 point, and the shipped tuning was kept. The price of passing is throughput, 11.49 t/h of propylene on average against 13.66 t/h as shipped.

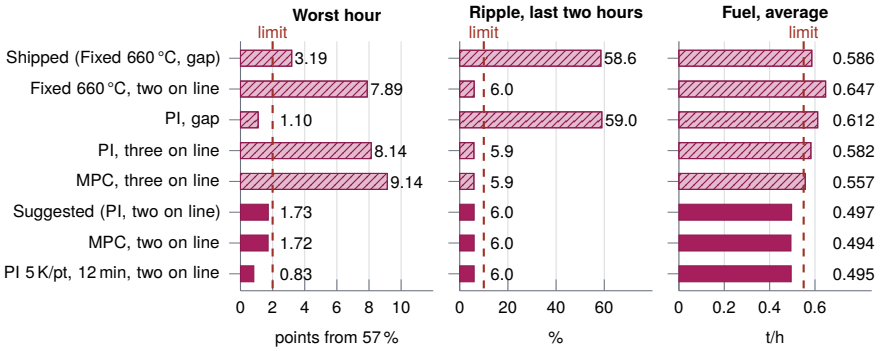


Figure 5.5 The challenge configurations of Table 5.5 against three of the four limits that grade them: the worst hourly conversion, the ripple in the last two hours and the average fuel. Solid bars pass the challenge, hatched bars fail it, and the dashed line in each panel is the limit. Notice that the gap fails on the ripple, three on line and Fixed regeneration fail on the conversion, and every failing configuration also burns more fuel than the limit allows. The fourth limit, no cell above 680 °C, holds in every row.

Table 5.5 Challenge Configurations Scored at 12 h

Configuration	Worst (pt)	Hottest (°C)	Ripple (%)	Fuel (t/h)	Verdict
shipped (Fixed 660 °C, gap)	3.19	659.6	58.6	0.586	fails
Fixed 660 °C, two on line	7.89	658.3	6.0	0.647	fails
PI, gap	1.10	674.0	59.0	0.612	fails
PI, three on line	8.14	671.3	5.9	0.582	fails
MPC, three on line	9.14	666.9	5.9	0.557	fails
suggested (PI, two on line)	1.73	658.1	6.0	0.497	passes
MPC, two on line	1.72	658.1	6.0	0.494	passes
PI 5 K/pt, 12 min, two on line	0.83	658.1	6.0	0.495	passes

5.6 Technology in Practice

Figure 5.6 draws the loops of Section 5.4 with the hardware of a cyclic bank in place of the schematic's symbols.

What Measures It

The conversion that the cycle-to-cycle layer corrects comes from a process gas chromatograph that analyzes each slot's product. Analyzers of this kind suffer from large measurement delays and high investment and maintenance costs [18], and the report a minute after each slot in this model is faster than a plant's. The regulatory loops read a thermocouple on the regeneration air header and an absolute pressure transmitter at the compressor suction. The model gives the thermocouple a 0.1 min lag with 0.3 K of noise and the transmitter 0.001 bar of noise, so neither a plugged impulse line nor a heavily damped signal appears in it.

> **TECHNOLOGY** **Sensor: An Absolute Pressure Transmitter on the Suction**
>
> An absolute pressure transmitter is a differential pressure instrument whose low side is sealed to a vacuum chamber, so any pressure above a perfect vacuum reads as a positive difference. It has no vent on the low side and a single impulse line to the process [19]. The impulse line can plug with debris, and where plugging is chronic the line is filled with a harmless fluid or purged with a steady flow. A transmitter damped too heavily draws a smooth trend that looks like tight control yet understates a real change [19].

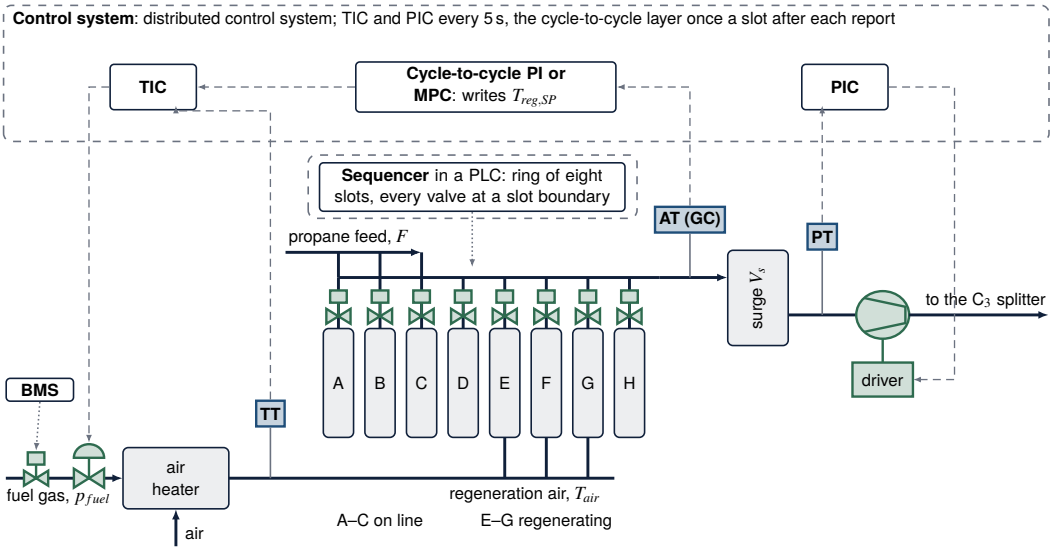


Figure 5.6 The bank's loops with their hardware. Blue boxes are sensing devices: TT on the regeneration air header, PT at the compressor suction and AT, the chromatograph on the product header. Green symbols are final elements: the fuel gas valve of the air heater, the compressor's driver and the on/off valves of the beds, one set drawn per bed. Dashed arrows are signals, dotted ones belong to the separate burner trip system and the sequencer. Notice that the cycle-to-cycle layer acts only through the air for beds that are not on line, and only once a slot. Purge steam, the vacuum header and the feed heater are left out. Not to scale, and not a piping diagram.

What Moves It

Three kinds of final element act on the bank. The fuel gas valve of the air heater is a throttling control valve, which the model follows with a 0.05 min lag and a flow that rises with the square root of the fuel gas pressure. The compressor's speed sets how deep the vacuum is, and its capacity, not the loop, ends case 8 at 0.337 bar a. The on/off valves of every bed belong to the sequencer, not to a controller. A real valve sequence takes tens of seconds, where the model switches every valve in one step.

> **TECHNOLOGY** **Final Element: On/Off Valves That Switch the Beds**
>
> A bed changes service through on/off valves, the fluid equivalent of an electrical switch, used to route a process fluid to different places. Ball, plug, butterfly, gate and globe valves serve this duty, and a large one opens to a nearly unimpeded path. A pair of pneumatic pistons on a rack and pinion can turn a butterfly valve, and a box of limit switches on its stem tells the control room where the valve stands. Tight shut-off is hard to keep in hot service, because bubble-tight seats usually need soft materials that limit the temperature range [19]. In the model every valve switches at once at a slot boundary, and a bed whose valves fail is taken out of service, as in case 5.

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 [20]. Programmable logic controllers (PLCs) serve such a system as local controllers within the supervisory scheme, programmed for logic, timing, counting and PID control [20]. The sequencer of this chapter is a state machine of that kind, whose output depends on its ring position as much as on its inputs, and IEC 61131-3 names the Sequential Function Chart among its five languages for writing one [19]. In the app the TIC and the PIC run every 5 s as velocity-form PID blocks. The cycle-to-cycle PI is

the same block called only when a report arrives, once a 3 min slot, and the MPC sits above both as a supervisory layer that writes $T_{reg,SP}$.

> **IN PRACTICE** **The Regeneration Air Heater Has Its Own Guard**
>
> The fuel valve that the TIC moves is a modulating valve. The burner it feeds is also watched by a burner management system, which purges the firebox with air for several minutes before ignition, lights the burner, and then watches for low fuel pressure, high fuel pressure and loss of flame. On any of them it halts the fuel with double block and bleed valves. Staff impatient to restart are often tempted to bypass its purge time. Such safety instrumented systems in the process industry are the subject of ANSI/ISA-84.00.01 [19]. The chapter's alarms trip nothing, and its fuel gas pressure disturbance is one of the inputs such a system watches.

What Is Modernizing It

Model predictive control has a solid foundation in refining and petrochemicals [15], and here it pays in recovery after a measured feed change, not in the graded outcome. 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 let a bank correct between chromatograph reports. Microprocessor burner controls time the purge more accurately, make it harder to override and connect to a network for remote monitoring [19]. On the catalyst side, a constant activity over the life of a chromia charge can be held by raising the reaction temperature gradually with time on stream [13], the slow drift that case 7 compresses into one step.

5.7 Limitations

No operating unit supplied the sizes, rates, heats or limits, all of which are teaching values. The kinetics have the standard forms with a rate order in total pressure chosen so that the vacuum helps, the equilibrium sits about one point above the NASA Glenn data, and the selectivity of 88 percent is not checked against a source. Six cells per bed leave the conversion 1.7 points under twelve, the heat capacity flow of the gas is fixed, and the reduction step and the valve sequence of a real cycle are left out. One air header serves every regenerating bed, so the regeneration of individual beds cannot be trimmed, and catalyst life is projected rather than fed back on the activity.

The control layers have their own simplifications. The GC reports a minute after each slot and its noise is 0.1 point, faster and cleaner than a real analyzer, so the cycle-to-cycle loop's information is better than a plant's. The MPC's step responses were identified on the model itself, so its model matches the plant's gain exactly at design, and it knows neither the coke nor the activity. The challenge's margin of 0.25 to 0.31 points is thin, although it held at every seed tried and at half the step. The MPC ties the PI on the graded outcome and wins only on recovery speed after a measured feed change.

> **OPEN CHALLENGE** **A Catalyst That Survives Its Cycles**
>
> Chromia catalysts lose activity over many cycles in ways that coke alone does not explain. Coke formation grows with the number of cycles, part of the chromium is reduced for good, and a spinel of chromium and alumina formed during cycling is linked to the loss. A 1999 review concluded that more characterization work was needed to understand this deactivation fully [13]. A 2023 review still names poor cycling performance and heavy carbon deposits as limits on industrial dehydrogenation, and the environmental risk of chromium as a limit on chromia catalysts [1]. Progress would be a measured law of activity against cycles, the piece this chapter's model replaces with a projected catalyst life.

5.8 Conclusion

A cyclic dehydrogenation bed spends heat it stored in the previous regeneration, and this simulator puts eight such beds, their sequencer, the regeneration air, the vacuum and the analyzer on one

clock. A bed on line cools 65.0 K and gives 2.36 GJ of the 2.44 GJ its reactions absorb, so 10 K more regeneration air raises the bank's conversion 2.93 points, first in the slot that ends 8 min after the move and fully one to two cycles later. A deeper vacuum buys 2.7 points of selectivity and 0.35 of conversion, because the stored heat, not the equilibrium, caps what a bed converts. With a bed lost, seven beds with three on line cannot reach the target under the bed limit (52.6 %), seven with two on line can, and a cycle-to-cycle PI or an MPC then holds every hour of the challenge within 1.73 and 1.72 points. The kinetics, the selectivity and the wear law are teaching values, and the analyzer is faster than a real one. A fuller model would add per-bed regeneration trim, the reduction step, a slower analyzer and catalyst aging that feeds back on the activity. Even without them, the bank shows control that acts on the next cycle rather than the present one.

KEY POINTS

- Nothing heats a dehydrogenation bed while it makes propylene: it spends heat stored in its last regeneration.
- 10 K more regeneration air raises the bank's conversion 2.93 points, but fully only one to two cycles later.
- A deeper vacuum buys 2.7 points of selectivity and 0.35 of conversion, because the stored heat caps what a bed converts.
- With a bed lost, seven beds with three on line cannot reach the target under the bed limit, while seven with two on line can, under a cycle-to-cycle PI or an MPC.

Where else this applies. Correcting the next run from the measured result of the last is also the work of Volume 8, Chapter 9, Volume 8, Chapter 10 and Chapter 7.

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5.9 Exercises

5.1 Concept check · 2 min

In case 3 the regeneration air setpoint is raised from 660 to 670 °C at 4 min. The TIC holds the new air temperature within a minute, yet the first slot conversion to move is the one ending at 12 min, and the bank reaches its final conversion only one to two cycles later. Why?

(a) The air heats only beds in regeneration, which come on line slots later, and the beds then start their next regeneration warmer

(b) The TIC is tuned slowly, so the air temperature itself takes most of a cycle to reach the new setpoint

(c) The gas chromatograph reports each slot late, so the conversion has moved long before the report shows it

(d) The surge volume holds the product for a cycle, so the splitter sees the higher conversion a cycle late

5.2 Concept check · 2 min

In case 8 the suction setpoint is lowered from 0.45 to 0.35 bar a. The equilibrium conversion of propane at 600 °C rises by about four points, but the bank’s conversion rises only from 57.80 to 58.15 %. What does the vacuum buy, and why?

(a) Nothing lasting, because the compressor cannot hold 0.35 bar a and the suction drifts back

(b) Selectivity, because the stored heat caps the conversion while cracking and coking slow at the lower partial pressures

(c) Conversion only after a cycle, because the beds must first cool to the new equilibrium temperature

(d) Throughput only, because the lower pressure lets the compressor pass more volume at the same speed

5.3 Concept check · 2 min

In case 7 the catalyst drops to 75 % of its fresh activity and makes 1.5 times the coke, with the regeneration fixed at 660 °C. Why does the bank’s conversion fall only from 57.8 to 56.3 %?

(a) The cycle-to-cycle PI raises the air to make up the lost activity

(b) The coke covers only the outlet cells, so the inlet cells convert as before

(c) A slower catalyst draws less heat early, and the extra coke burned in regeneration reheats the beds

(d) The equilibrium limits the conversion, so the activity matters only far from equilibrium

5.4 Theory and calculation · 7 min

Each bed holds 33 t of catalyst and inert at 1.1 kJ/(kg K) in six equal cells, and receives 10 t/h of propane (44.10 g/mol) at 600 °C. The gas carries 160 J/(mol K) per mole of propane fed, and in regeneration a bed receives 40 kg/s of air at 1150 J/(kg K).

(a) Compute the bed's heat capacity. Over its nine minutes on line in case 1 its mean temperature falls 64.98 K while the reactions absorb 2.443 GJ. How much of that heat does the bed give, and how much does the feed supply? *Checkpoint:* 36.3 MJ/K, 2.359 GJ and 0.084 GJ

(b) Compute one cell's heat capacity C, the molar feed F_{in}, the heat capacity flow $\dot{F}c_p$ and the time the gas alone would need to change a cell's temperature, $C/(\dot{F}c_p)$. Compare it with the time on line. *Checkpoint:* 6.05 MJ/K, 62.99 mol/s, 10.08 kW/K, 10.0 min

(c) Compute the air's time constant on a cell and compare it with the nine-minute regeneration. What does each comparison say about where a bed's temperature comes from on line and off line? *Checkpoint:* 2.19 min

5.5 Theory and calculation · 8 min

The app's dehydrogenation has $\Delta H_1 = 129.5\,\mathrm{kJ/mol}$ and $\Delta S_1 = 139.2\,\mathrm{J/(mol\,K)}$, with $K_p = \exp(\Delta S_1/R - \Delta H_1/(RT))$ in bar and $R = 8.314\,\mathrm{J/(mol\,K)}$. The equilibrium conversion of pure propane is $X_{eq} = \sqrt{K_p/(P+K_p)}$, and the bed pressure is $P = P_s + 0.05\,\mathrm{bar}$.

(a) Compute K_p at 600 °C. *Checkpoint:* 0.334 bar

(b) Compute X_{eq} at 600 °C for suction setpoints of 0.45 and 0.35 bar a. Give one decimal. *Checkpoint:* 63.3 and 67.5 %

(c) The NASA Glenn polynomials give $K_p = 0.315\,\mathrm{bar}$ at 600 °C. Compute X_{eq} at 0.50 bar with it. *Checkpoint:* 62.2 %

(d) In case 8 the same change of suction moves the bank's conversion from 57.80 to 58.15 %. What fraction of the rise in X_{eq} is that, and what caps the rest? *Checkpoint:* about 0.08

5.6 Theory and calculation · 7 min

Model the bank's cycle-to-cycle loop as Equation (1.12): the GC reports once a slot (3 min), the conversion answers the regeneration setpoint with $g = 0.293\,\mathrm{points/K}$ after $d = 2$ reports, and the integral law moves the setpoint by K kelvin per point of error at each report. Ignore the proportional part of the PI and the tail of the real response.

(a) Compute the integral gain K for the double root and at the edge of stability. *Checkpoint:* 0.853 K and 3.41 K per point

(b) The PI's integral part moves the setpoint by $K_c\,\Delta t/\tau_I$ per point of error at each report. Compute it, and gK, for the shipped 3 K per point and 15 min, the tighter 5 K per point and 12 min, and 8 K per point with 6 min. *Checkpoint:* gK = 0.176, 0.366 and 1.17

(c) Say what the model predicts for each tuning and compare with the chapter's case 6. *Checkpoint:* no overshoot, overshoot, unstable

5.7 App challenge · 8 min

Load case 3, Regeneration heat is the handle, at the default seed. Press Run at speed 1 (1 min of plant per wall second) and pause between 4 and 6 min. Set the Regeneration air setpoint on the TIC card to

670.0 °C, then run at speed 5 to 96 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) Read the Start of cycle badge and the Selectivity, Fuel and Catalyst life tiles. In the CSV, read the column `truth_x_slot_pct` in the 96.00 min row. Use tolerances of 0.1 K, 0.02 points and 0.01 t/h. *Checkpoint:* 630.8 °C, 86.9 %, 0.75 to 0.76 t/h, 2.0 y, 60.73 %

(b) Against the design values (start 622.6 °C, conversion 57.80 %), compute the conversion gained per kelvin of air and per kelvin of start-of-cycle temperature. *Checkpoint:* 0.293 and 0.357 points per K

(c) Use Equation (5.4) at steady state with three beds regenerating to compute the fuel at 660 and at 670 °C, and compare with the tile. *Checkpoint:* 0.647 and 0.755 t/h

5.8 App challenge · 8 min

Load case 5, A bed out of service, at the default seed. Before pressing Run, choose Cycle-to-cycle PI under Regeneration control and Seven beds, two on line under With a bed out. Run to 120 min at speed 5 and export the CSV. Then choose Seven beds, three on line, press Reset (it keeps your settings), run to 120 min again and export. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from minutes.

(a) For each schedule read `treg_C`, `treg_saturated` and `truth_x_slot_pct` in the 120.00 min row, and average `prod_c3h6_tph` over the rows from 99 to 120 min (one seven-slot cycle). Use tolerances of 1 K, 0.1 points and 0.05 t/h. *Checkpoint:* two: 636 to 637 °C, 0, 57.0 %, 9.68 t/h; three: 680.0 °C, 1, 52.6 %, 13.34 t/h

(b) Why does the PI hold the target with two on line and not with three? *Checkpoint:* three on line regenerates for two slots

(c) The chapter's sweep shows what feed per bed three on line would need. Which schedule gives more propylene at the target? *Checkpoint:* two on line, unless the feed drops to 8.5 t/h

5.9 App challenge · 8 min

Load case 9, the Challenge (twelve hours, a bed out and more feed), at the default seed. Run it as shipped at speed 120 (120 min of plant per wall second, about 6 s) to 12 h and read the So far tile. Then choose Cycle-to-cycle PI under Regeneration control and Seven beds, two on line under With a bed out, press Reset, and run again. Drop to speed 10 near 3.5 h and 4.5 h to read the tile, then finish the run.

(a) Give the four values on the So far tile at 12 h for each run. *Checkpoint:* shipped: ±3.2, 660, 58.6, 0.59; PI: ±1.7, 658, 6.0, 0.50

(b) What does the tile's worst hour read at 3.5 h and at 4.5 h in the second run, and which event made the worst hour? *Checkpoint:* ±0.1 then ±1.7 points; the ring closing up after bed D fails

(c) Which parts of the target does each run meet, and what does passing cost? *Checkpoint:* 11.49 t/h against 13.66 t/h

5.10 Application area · 5 min

A valve on bed D fails and the bed must stay out for a week. The splitter downstream needs a steady feed and the plan calls for 57 % conversion. Case 5 gives, against 14.57 t/h of propylene with eight beds: leave the gap, 57.8 % and 12.73 t/h rippling 56.6 %; three on line, 48.0 % and 12.39 t/h; two on line, 64.8 % and 10.66 t/h; two on line with the cycle-to-cycle PI, 57.0 % and 9.68 t/h. Compute the propylene each choice loses per day, and say which one an operator should run and what else could change.

5.11 Application area · 4 min

Case 4 runs the cycle at 16, 24, 32 and 40 min. The conversion is 56.1, 57.8, 58.4 and 56.8 %, and the projected catalyst life 5.0, 3.0, 2.1 and 1.6 years. Each bed runs one valve sequence a cycle, from reaction through purge and regeneration to evacuation. How many valve sequences does the bank make per day at 16, 24 and 32 min? Which costs of the cycle time does the model count, and which does it leave out?

5.12 Review the agent · 5 min

An AI assistant asked to make case 6 recover faster writes: “The bank’s conversion answers the regeneration setpoint within one slot, so treat it as a first-order lag of about 3 min. Lambda tuning then gives the cycle-to-cycle PI a gain of 8 K per point and an integral time of 6 min, which will hold the target within two slots of the switch instead of the shipped tuning’s hour.” Find the flaw and say how you would check it in the app.