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CHAPTER 7

A Hydrocracker Reactor Simulator for Open-Loop Instability and Layered Protection

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Edited by John D. Hedengren

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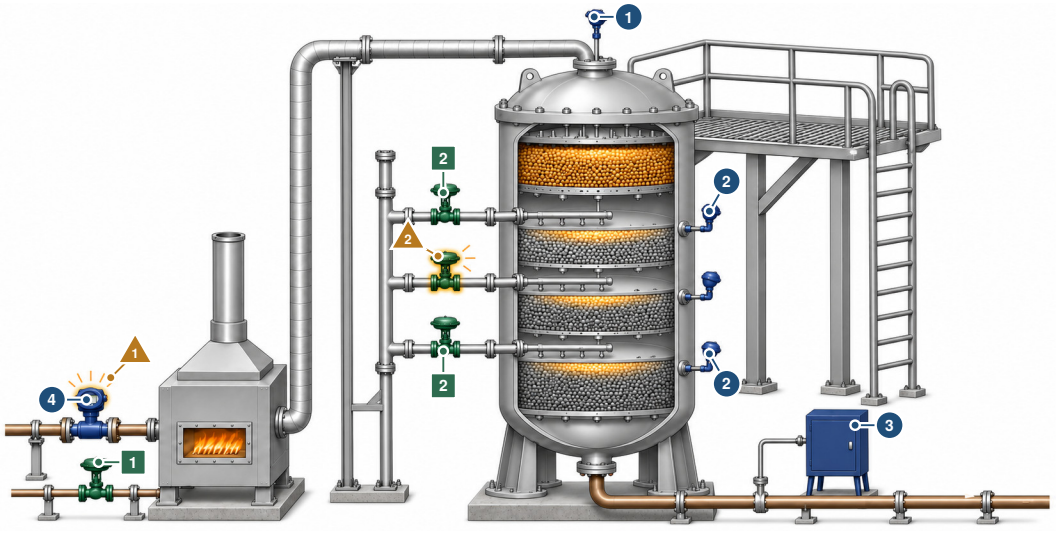
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CHAPTER 7

A Hydrocracker Reactor Simulator for Open-Loop Instability and Layered Protection



The controller moves 1 firing of the feed heater 2 three cold hydrogen valves between the beds

The controller reads 1 first bed inlet temperature 2 inlet temperatures of the three lower beds 3 conversion of the product 4 feed rate

What disturbs it 1 a feed cut 2 a stuck hydrogen valve ▲ a more active catalyst

The warm first bed at the top has no cold hydrogen valve above it, so only the slow feed heater at the lower left can cool it. Illustration, not to scale.

IN PLAIN TERMS A Reactor That Can Heat Itself Up

The main idea. A hydrocracker breaks heavy oil into lighter fuel as the oil passes down through four beds of solid grains. The breaking gives off heat, and hot oil breaks faster, so a bed can heat itself faster and faster.

The challenge. Cold gas blown in between the beds cools the lower three, but the first has only a slow heater. A guard that turns the heat down can be fooled, because its reading moves the wrong way for minutes after each cut.

Why it matters. Once a bed runs away no control is fast enough, and the reactor must be shut down.

THREE WAYS TO READ THIS CHAPTER

Explore	13 min	This page, the History boxes in Sections 7.2 and 7.3, the Did you know? boxes in Sections 7.1 and 7.6.4, the Try it boxes in Sections 7.5 and 7.6, and Key points in Section 7.10. No equations.
Study	50 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
Practice	20 min	This page, Section 7.6 with Figure 7.4, Section 7.7 and Section 7.8 with its Open challenge box.

The control question An adiabatic catalyst bed with an exponential rate law can be unstable before any controller is added, and one number decides it. How close is the first bed to that boundary, and which layers of control and protection can still act once a feed cut or a hotter catalyst pushes it there?

Learning objectives

- Compute the runaway index and the amplification of a bed from its rise and mean temperature.
- Explain why the interbed quench loops break the chain of amplifying beds, and why bed 1 has no fast handle.
- Explain why a feed cut at a fixed inlet makes the bed hotter.
- Show that an override reading a raw bed rise is positive feedback in the transient, and that one matched lag cures it.
- Compare one inlet setpoint cut by an override with a predictive controller that sets a target per bed.

Prerequisites Sections 1.4.4, 1.4.7, 1.6.2 and 1.6.3.

The app https://apmonitor.com/apps/hydrocracker/

See also Volume 7, Chapter 2 for a stirred tank at an ignition boundary. Volume 4, Chapter 2 for a protective override that rests at its clamp and Volume 4, Chapter 6 for a per-zone safety override that bounds the throughput.

7.1 Introduction

An adiabatic catalyst bed with an exponential rate law is one of the few plants a control course meets that can be unstable without a controller. Write the bed as a lumped stage reacting at the mean of its inlet and outlet temperatures, linearize, and a single dimensionless group appears: $r = \frac{1}{2} K \, \mathrm{d}x/\mathrm{d}T$, where K is the adiabatic temperature rise at complete conversion and x is the fraction converted in the bed. Below $r = 1$ the bed settles by itself and amplifies its inlet by $(1 + r)/(1 - r)$. Above it the operating point is unstable and only a controller can hold the reactor there. Section 1.4.4 derives the index on the running example of this volume, and Volume 7, Chapter 2 meets the same ignition boundary in a jacketed stirred tank.

Computed on the reactor modeled here, the first bed sits at $r = 0.538$ and turns a small inlet disturbance into 3.3 times as much outlet. An inlet 3.8 °C hotter, or eighteen percent more catalyst activity, crosses the boundary. Four beds at a gain of 3.3 in series would turn one degree at the feed heater into more than a hundred at the bottom of the reactor, which is why there is a quench valve between every pair of beds. The quench loops are not trimming. They are what breaks the feedback path three times, and a reactor with one bed of the same total catalyst would be inoperable.

> **DID YOU KNOW? Twenty Degrees Doubles the Rate**
>
> At normal pressure and flow, a rise of 20 °F, about 11 °C, almost doubles the rate of the hydrocracking reaction [1]. To hold it, each reactor has several catalyst beds with cool hydrogen injected between them [1]. The first bed of this chapter rises 23.9 °C from inlet to outlet at design.

The misconception the simulator corrects is that stability is a property of the control loop. On this reactor it is a property of the plant, it is a computable number, and it moves with every catalyst load and every feed cargo. A second misconception follows from the first. Bed 1 has no quench above it, so its only handle is a feed heater upstream with a 2.5 min lag, and once the first bed is past the boundary there is nothing in the control system fast enough. The answer is a trip. An actuator that can act only upstream of a fast instability is not a protection.

The class is general. Parametric sensitivity in fixed bed reactors, the property that a small parameter change produces a disproportionate change in the peak temperature, has a classical treatment from 1970 [2] and a general one later [3], and the safety literature on reactor runaway catalogs the mechanisms across chemistries [4]. This chapter works with an interactive hydrocracker that reports

the runaway index of every bed beside its temperatures. The index can be checked there against an amplification measured by experiment, the three protective layers can be built and audited, and an override turns out to be positive feedback when it reads the wrong measurement. The reactor has four beds with their quench mixing, an instrument chain, an override with a dynamically compensated measurement and a three-way trip, and the chapter gives them in the detail needed to rebuild them. An optional model predictive controller (MPC) of the four inlets is compared on measured runs with the shipped loops, and each of its gains is traced to its mechanism by a counterfactual run. The scenarios include an override that trips the reactor it was installed to protect, and a feed cut that makes the reactor hotter. The lumped bed model, the runaway index and override control are established, and the MPC takes the industrial form [5].

Section 7.2 gives the domain history. Section 7.3 states the model and its assumptions, and Section 7.4 derives the amplification of four beds in series and the transient sign of a bed rise. Section 7.5 describes the inlet loops, the override, the trip, the conversion loop and the MPC. Section 7.6 reports the measured results, Section 7.7 sets the hardware of a real unit beside the model, Section 7.8 gives the limitations, and Sections 7.9 and 7.10 draw the lessons that carry beyond this unit.

7.2 Background

Hydrocracking converts vacuum gas oil into distillate over a bifunctional catalyst at high hydrogen pressure. The cracking reactions are exothermic, the beds are adiabatic, and the heat released is proportional to the conversion, so a hydrocracker is among the highest-pressure, highest-value and most carefully protected units in a refinery.

The reactor is built as several beds in series with cold hydrogen injected between them, and the reason is thermal rather than chemical. Kinetic modeling of the conversion itself is a lumping problem, because the feed is a continuum and the products are a distribution. Discrete lumped kinetic models for vacuum gas oil hydrocracking and the discrimination between them have their own literature [6], and lumping approaches specific to dual bed reactors have been compared directly [7]. None of that is needed to state the control problem, which depends only on how much heat a unit of conversion releases and on how fast conversion rises with temperature.

The theory of what happens when a fixed bed exotherm outruns its cooling is older than the unit, and the History box below traces it. Modern treatments extend it to the maldistribution mechanisms that trigger runaway in trickle beds specifically [8], and the safety literature surveys the whole field [4]. A hydrocracker differs from the classical fixed bed case in one respect that matters for control: the cooling is not a wall, it is an injection between beds, so the protection is a valve rather than a heat transfer coefficient and it can be manipulated. Chapter 8 uses the same interbed hydrogen quench on a diesel hydrotreater.

> ⧖ HISTORY **1970: Runaway Gets a Criterion**
>
> The theory of a reactor that outruns its cooling is older than the modern hydrocracker, a process further developed in the early 1960s [9]. Semenov's balance of the heat an exothermic reaction releases against the heat removed laid the groundwork, and Bilous and Amundson did pioneering work on parametric sensitivity, showing how the peak temperature along a reactor varies with the coolant temperature [4]. In 1970 Van Welsenaere and Froment gave criteria for parametric sensitivity and runaway in fixed bed catalytic reactors [2], drawn from the locus of temperature maxima in the plane of temperature and conversion [4]. Morbidelli and Varma, whose work includes a 1986 paper on the same reactors [3], set the boundary of runaway where the sensitivity itself peaks and generalized the criterion to other parameters [4]. The runaway index of Section 7.3 asks the same question of one lumped bed.

Control developed in layers. The earliest arrangement is manual quench adjustment against bed thermocouples, with the operator reading the temperature rise across each bed as the visible

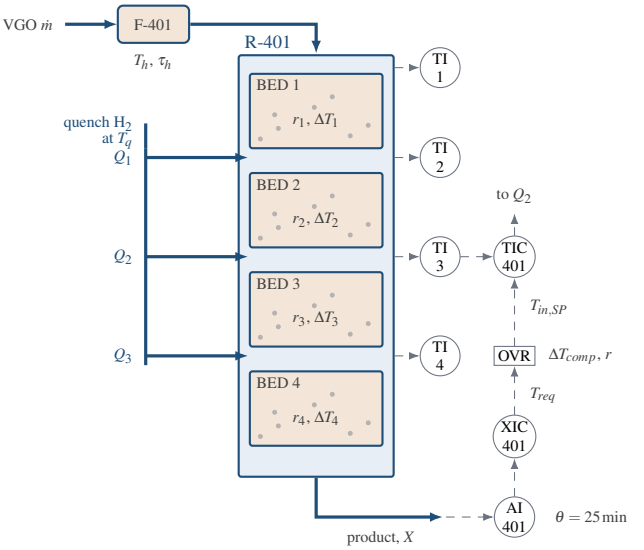


Figure 7.1 Hydrocracker reactor R-401. Vacuum gas oil $\dot{m}$ is heated in F-401 to T_h with lag τ_h and passes down through four adiabatic beds, each with its own runaway index r_i and temperature rise ΔT_i. Cold quench hydrogen at T_q is injected through valves Q_1, Q_2 and Q_3 between the beds. Bed inlet thermocouples TI-1 through TI-4 feed four inlet temperature loops, of which TIC-401, reading TI-3 and moving Q_2, is representative. AI-401 reports conversion X on cycle θ to the supervisory loop XIC-401, whose request T_{req} the override OVR can only lower before it becomes the common inlet setpoint $T_{in,SP}$. Bed 1 has no quench above it, and the trip is not drawn.

form of the reaction rate. Automatic inlet temperature control on the quench valves came next and is universal. A supervisory conversion loop on a product distillation became possible when the measurement did. Above that, the hydrocracker was among the first units in a refinery to receive a large multivariable controller, and the reason was precisely the constrained economics of an exothermic reactor with hard temperature limits: Cutler and Hawkins reported a dynamic matrix controller on a hydrocracker second stage reactor in 1988 [10], one of the earliest published industrial applications of the technology that became standard [5]. A recent study sets the reactor temperatures of an industrial hydrocracker with a feedforward model predictive controller driven by feed measurements, for constant diesel quality [11]. The regulatory layer underneath that controller is the subject of this chapter, together with the override and trip layers above it.

7.3 Process Model

Reactor R-401 processes 250 t/h of vacuum gas oil with recycle hydrogen at about 150 bar through four adiabatic catalyst beds. Every bed inlet is at 381 °C at the design condition, the bed rises are 23.9, 14.0, 11.1 and 9.3 °C for 51.2 % conversion, and the quench flows that return each inlet to 381 °C are 3.38, 1.99 and 1.57 t/h. Figure 7.1 shows the arrangement, and the variables are classified in Table 7.1.

Table 7.1 Classification of Variables at the Design Operating Point

Symbol	Role	Nominal	Range
$T_{in,i}$	CV, continuous	381 °C	340–400 °C SP
X (AI-401)	CV, analyzer	0.512	0.35–0.72 SP
ΔT_{max}	constraint	23.9 °C	alarm 33, trip 42
r_{max}	constraint	0.538	unstable above 1
T_h (F-401)	MV	381 °C	300–420 °C
Q_1, Q_2, Q_3	MV	3.38, 1.99, 1.57 t/h	0–30 t/h
$\dot{m}$	DV, measured	250 t/h	150–340 t/h
activity	DV, unmeasured	1×	0.6–1.6×
stuck valve	DV, unmeasured	off	on/off
$T_{out,i}$	states	profile	—

7.3.1 One Adiabatic Bed

Each bed is a lumped adiabatic stage reacting at the mean of its inlet and outlet temperatures, Equation (7.1), with the fraction converted in bed i given by Equation (7.2).

$$\tau \frac{\mathrm{d}T_{out}}{\mathrm{d}t} = T_{in} + K\,x\!\left(\frac{T_{in}+T_{out}}{2}\right) - T_{out} \tag{7.1}$$

$$x_i(T) = \min\left\{0.9,\; k_{ref}\,\frac{\dot{m}_0}{\dot{m}}\,a\,R_i \times \exp\!\left[-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]\right\} \tag{7.2}$$

where $\dot{m}_0/\dot{m}$ is the inverse space velocity relative to the design feed, a is the catalyst activity and R_i is the fraction of the feed still unconverted at the inlet of bed i, with $K = 90.0\,^{\circ}\mathrm{C}$ per unit of x, $E/R = 20\,000\,\mathrm{K}$, $T_{ref} = 392.5\,^{\circ}\mathrm{C}$ and $\tau = 3.5\,\mathrm{min}$. The unconverted fraction passes down as $R_{i+1} = R_i(1-x_i)$, and the reactor conversion is $X = \sum_i x_i R_i$. The remaining parameters are given in Table 7.2.

7.3.2 The Runaway Index

Linearizing Equation (7.1) about a steady state and collecting terms gives Equation (7.3), the result of Equation (1.6) with K in place of ΔT_{ad}.

$$\tau \frac{\mathrm{d}\,\delta T_{out}}{\mathrm{d}t} = (r-1)\,\delta T_{out} + (1+r)\,\delta T_{in}, \qquad r = \frac{K}{2}\frac{\mathrm{d}x}{\mathrm{d}T} \tag{7.3}$$

The bed is stable while $r < 1$ and unstable above it, and while stable it is an amplifier with the steady-state gain of Equation (7.4).

$$\frac{\partial T_{out}}{\partial T_{in}} = \frac{1+r}{1-r} \tag{7.4}$$

For an Arrhenius rate below the 0.9 ceiling, $\mathrm{d}x/\mathrm{d}T = xE/(RT^2)$ with T in kelvin, so $r = KxE/(2RT^2)$ and the index rises with conversion and with temperature together.

7.3.3 Quench Mixing

Cold hydrogen at 60 °C mixes with the bed effluent to set the next inlet, Equation (7.5).

$$T_{in,i+1} = \frac{\dot{m}\,c_{p,oil}\,T_{out,i} + \dot{q}\,c_{p,H_2}\,T_q}{\dot{m}\,c_{p,oil} + \dot{q}\,c_{p,H_2}} \tag{7.5}$$

Hydrogen has five and a half times the specific heat of the oil, so a few tonnes an hour moves an inlet temperature a long way. At design, 3.38 t/h takes bed 2 from 405 °C back to 381.

Table 7.2 Model Parameters

Symbol	Meaning	Value	Class
K	local heat-rise factor	90.0 °C	fixed
T_{ref}	reference temperature	392.5 °C	fixed
E/R	activation temperature	20 000 K	adjustable
k_{ref}	conversion per bed at reference	0.2600	adjustable
τ	bed thermal time constant	3.5 min	adjustable
τ_h	feed heater lag	2.5 min	adjustable
τ_q	quench valve lag	0.30 min	adjustable
τ_{TT}	thermocouple filter	0.15 min	adjustable
$c_{p,H_2}/c_{p,oil}$	specific heat ratio	5.5	adjustable
T_q	quench hydrogen temperature	60 °C	adjustable
θ	conversion analyzer cycle	25 min	adjustable
τ_{lab}	conversion analyzer averaging	3 min	adjustable
ΔT alarm	bed rise alarm	33 °C	visible
ΔT trip	bed rise trip	42 °C	visible
T trip	bed temperature trip	440 °C	visible
rate trip	rate of rise trip	28 °C/min	visible
τ_{rate}	rate of rise filter	0.8 min	visible

7.3.4 Why Less Feed Is Hotter

Conversion per bed scales inversely with space velocity, so cutting the feed at a fixed inlet temperature gives more conversion per unit of catalyst and the heat released has less mass to heat. At a fixed inlet of 381 °C, cutting the feed from 250 t/h to 220 t/h takes the steady first bed rise from 23.9 °C to 34.1 °C and the runaway index from 0.538 to 0.756. Below 212 t/h there is no cool steady state at all. A feed cut on a hydrocracker is a heat problem rather than a throughput problem, and it is one of the classic ways units have run away.

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

7.3.5 Assumptions

Each bed is one lumped adiabatic stage reacting at the mean of its inlet and outlet temperatures. A real bed has an axial profile whose peak is hotter than the outlet, so a real reactor is closer to its limits than its outlet thermocouples suggest.

One lumped cracking reaction carries one apparent activation energy. Real hydrocracking is a network and the hydrotreating reactions in the first bed release heat of their own, so the lumping literature exists for good reasons [6, 7].

The retained thermal surrogate is calibrated on local conversion rather than on whole-feed reaction enthalpy. Bed i releases Kx_i of heat while X credits it with x_iR_i, so the four design rises sum to 58.3 °C while KX is 46.1 °C. Bed 1, where $R_1 = 1$, is unaffected, and beds 2 to 4 run hotter than a constant whole-feed reaction enthalpy would imply. The local correlation preserves the calibrated amplification, fold and protective-layer lessons, but its temperature rises cannot be used as a reaction-duty balance.

Quench mixing is perfect and instantaneous. Maldistribution in a quench zone is one of the commonest causes of real hot spots and this model cannot show it [8].

Hydrogen partial pressure and recycle gas purity are fixed, and there is no catalyst deactivation. A real cycle is twelve months of slowly rising weighted average bed temperature to maintain conversion. The index also depends on conversion: temperature alone at fixed conversion slightly lowers it in this model. The application represents catalyst aging through the activity slider.

The trip is instantaneous. It drops the heater command to its 300 °C minimum and opens all three quench valves to 30 t/h at once, and the feed is not changed. A real emergency depressuring takes several minutes at a controlled rate and the beds keep reacting while it happens.

The conversion analyzer is a sample-and-hold on a 25 min cycle followed by a 3 min averaging lag, so its reading is between 0 and 25 min old and carries no dead time beyond that. Conversion on a real unit is inferred from a distillation and is both slower and less certain.

> ⧖ HISTORY **1997: A Runaway the Quench Could Not Stop**
>
> On January 21, 1997 a hot spot formed in the fourth of five catalyst beds of a hydrocracker reactor at a California refinery and spread to the bed below [1]. One bed outlet reading rose from 628 to 823 °F in 40 seconds. The operators distrusted readings that jumped between normal values and zero. They raised the quench and cut the furnace, and did not depressure the reactor as the written procedure required above 800 °F. The effluent pipe ruptured at a temperature likely above 1400 °F. One operator was killed and 46 people were injured. The investigators calculated that at least three times the maximum design quench flow would have been needed, and that only depressuring could have slowed the reaction. They asked for every bed temperature in the control room, backup indicators and tested emergency systems [1].

7.4 Dynamic Analysis

7.4.1 Four Beds in Series

Equation (7.4) gives the amplification of one bed. If each bed inlet followed the outlet above it one for one, four in series would multiply, Equation (7.6).

$$\frac{\partial T_{out,4}}{\partial T_h} = \prod_{i=1}^{4} \frac{1+r_i}{1-r_i} \tag{7.6}$$

At the design condition the four indices are 0.538, 0.321, 0.254 and 0.215, so the bed gains are 3.33, 1.95, 1.68 and 1.55 and the product is 17, and the first bed's gain alone repeated four times would give 122. With the three quench flows frozen at their design values the chain is weaker than the product, because each quench dilutes the effluent (by factors of 0.931, 0.958 and 0.967) and a hotter bed leaves less feed for the next, and the computed steady-state amplification from heater outlet to bed 4 outlet is 10 °C per °C. Either number is a reactor nobody can operate from a feed heater. A quench loop between each pair drives $\partial T_{in,i+1}/\partial T_{out,i}$ to zero at steady state, which reduces the chain to four independent beds of gain 3.33, 1.95, 1.68 and 1.55. The quench valves are not trimming the profile. They are the reason the vessel has four beds instead of one.

7.4.2 The Transient Sign of a Bed Rise

Take the bed as a first-order lag on the outlet and hold the reaction rise constant for the moment. Then $T_{out} = \mathcal{L}^{-1}\{T_{in}/(\tau s+1)\} + \Delta T_{rxn}$, and the measured rise responds to an inlet step of size a as Equation (7.7).

$$\Delta T_{meas}(t) = T_{out} - T_{in} = \Delta T_{rxn} - a\,e^{-t/\tau} \tag{7.7}$$

which for a negative step, that is a cut in the inlet, starts at $\Delta T_{rxn} + |a|$ and decays to ΔT_{rxn} with time constant τ. The measured rise therefore moves in the opposite direction to the steady-state answer for about $\tau = 3.5$ min after every correction. An override with gain K_o acting on that signal has an effective loop gain of $+K_o$ during that window rather than $-K_o$, which is the positive feedback reported in Section 7.6. Subtracting a lagged inlet, as in Equation (7.12), cancels the transient term in Equation (7.7) exactly and leaves ΔT_{rxn}.

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

7.5 Controller Design

7.5.1 Velocity Form PID

Every loop uses the shared velocity-form PID of Section 1.6.2 with the derivative on the measurement, restated in this chapter's symbols as Equations (7.8) to (7.10).

$$e_k = a\,(\mathrm{SP}_k - \mathrm{PV}_k) \tag{7.8}$$

$$P_k = K_c e_k, \qquad D_k = -K_c \tau_D\, a\, \frac{\mathrm{PV}^f_k - \mathrm{PV}^f_{k-1}}{\Delta t} \tag{7.9}$$

$$\begin{aligned} s_k &= s_{k-1} + (P_k - P_{k-1}) + (D_k - D_{k-1}) \\ c_k &= s_k + I_{k-1}, \qquad u_k = \mathrm{clamp}(c_k, u_{\min}, u_{\max}) \\ I_k &= I_{k-1} + \left[\frac{K_c}{\tau_I}\, e_k + \frac{u_k - c_k}{\tau_t}\right]\Delta t \end{aligned} \tag{7.10}$$

where a is $+1$ for direct and -1 for reverse action, PV^f is the measurement through the derivative filter, s_k accumulates the proportional and derivative increments without limit and c_k is the demanded output. The integral is seeded with the initial output, and anti-windup is back-calculation with tracking time $\tau_t = \tau_I$. No output carries a rate limit. In Manual a tracking routine sets I so that c_k equals the operator's value, and in Auto the manual stations follow the controller after every execution. The controller scan is 0.05 min and integration is fixed-step fourth-order Runge-Kutta at 0.01 min.

7.5.2 Three Layers

Regulatory. Four inlet temperature loops. The feed heater holds bed 1, direct acting, with $K_c = 2.5$ and $\tau_I = 3.0$ min. Three quench valves hold beds 2, 3 and 4, reverse acting because more quench is a colder inlet, with $K_c = 0.90$ t/h per degree, $\tau_I = 1.5$ min, $\tau_D = 0.35$ min and a 0.20 min derivative filter. A rate contribution on a loop holding an amplifying plant is worth more here than almost anywhere else. A stuck valve sits after the PID, so the quench loop above it does not see the fault and winds its own output to its 30 t/h limit, which is the signature a stuck valve leaves on a trend.

Override. A one-directional layer pulls the common inlet setpoint down when a bed rise approaches its alarm or the runaway index approaches its limit, Equation (7.11).

$$\begin{aligned} T_{in,SP} &= \mathrm{clamp}\big(T_{req} - \max\left(c_{\Delta T}, c_r\right), T_{\min}, T_{\max}\big) \\ c_{\Delta T} &= K_o\,[\Delta T_{comp} - \Delta T_{lim}]^+ \\ c_r &= K_r\,[\hat{r}_{\max} - r_{lim}]^+ \end{aligned} \tag{7.11}$$

where T_{req} is the conversion loop output, or the operator's setpoint with that loop in Manual, $T_{\min} = 340\,^\circ$C, $T_{\max} = 400\,^\circ$C, $K_o = 2.5$, $\Delta T_{lim} = 28\,^\circ$C (5 °C below the alarm), $K_r = 60\,^\circ$C per unit and $r_{lim} = 0.75$. The index is read from thermocouples, $\hat{r}_{\max} = \max_i \Delta T_{comp,i}\, E/(2R\bar{T}_i^2)$ with $\bar{T}_i$ the bed's mean temperature and the declared E/R, which is r at a steady state (to 2×10^{-15}) and lags it in a transient. Its 0.75 limit is a rise of 33.1 to 33.8 °C, above the 28 °C where the steeper $c_{\Delta T}$ starts, so it sets the cut in none of 351 runs. The cut is proportional and recomputed every scan. It can only pull down, on purpose. A layer that can also push up is a controller, and the value of an override is that it is not one. The protective override of Volume 4, Chapter 2 is built the same way, resting at its clamp while the machine is healthy. While the override cuts and the conversion loop is in automatic, that loop's integral is also back-calculated against the applied setpoint, each scan adding $(T_{in,SP} - u_k)\,\Delta t/\tau_I$ to I_k, so it does not wind up behind the cut and settles where the cut equals $K_c e$. In scenario 10 the conversion loop ends asking for 385.7 °C against an applied 382.8 °C, and the largest rise holds at 29.2 °C for as long as the run continues.

Trip. The trip fires on a bed rise of 42 °C, a bed temperature of 440 °C, or a rate of rise of 28 °C/min on the hottest bed, filtered with a 0.8 min lag. A rate trip is meant to fire first in a runaway, because

the other two are lagging indicators of an accelerating event, but on this plant it cannot. The bed time constant caps how fast an outlet can move. In scenario 9, run in Manual through an activity step to 1.45 at 10 min, the rise trip fires at 16.6 min with the hottest bed at 423.1 °C while the filtered rate peaks at 2.7 °C/min (4.1 °C/min at an activity of 1.6).

> **TRY IT IN THE APP** **9 · Which protection fires first**
>
> Load the case and press Run. Touch nothing: the reactor is in Manual, and at 10 min the catalyst activity steps to 1.45. Watch the three trip lines. The bed rise trip fires at 16.6 min with the hottest bed at 423.1 °C, while the rate of rise peaks at 2.7 °C/min against its setting of 28 °C/min.

7.5.3 The Rise the Override Reads

A bed rise is an outlet minus an inlet, and the two do not move on the same clock. The inlet answers a quench valve within the valve's 0.30 min lag and the outlet carries the catalyst time constant of 3.5 min. Cut the inlet quickly and the measured rise goes up for several minutes before it comes down, so the signal is inverted by the action meant to fix it, and a proportional override reading it is positive feedback.

The cure is one lag. Since the bed is $\tau\,\mathrm{d}T_{out}/\mathrm{d}t = T_{in} + \Delta T_{rxn} - T_{out}$, the compensated rise of Equation (7.12) equals the reaction rise seen through the same lag, $\Delta T_{rxn}/(\tau s + 1)$, so the thermal transient of the inlet is removed exactly.

$$\Delta T_{comp} = T_{out} - \frac{1}{\tau s + 1}\,T_{in} \tag{7.12}$$

The override reads the bed temperatures directly, without the 0.15 min thermocouple filter of the inlet loops. This is the same move as compensating a tray temperature for pressure or a flow for density. The measured consequence of omitting it is in Section 7.6.

7.5.4 Supervisory Conversion

XIC-401 holds conversion by setting the common inlet temperature, direct acting, with $K_c = 60\,^{\circ}\mathrm{C}$ per unit and $\tau_I = 120\,\mathrm{min}$. It is slow because the analyzer answers every 25 min through a 3 min average and because the plant beneath it is an amplifier.

7.5.5 Model Predictive Control

The inlet layer can instead be given to the MPC, an option that is never the default, which moves the feed heater and the three quench valves together. Section 1.6.3 describes the option in general, and what follows is specific to this reactor. The conversion loop still sets T_{req}, the override of Equation (7.11) still cuts it to $T_{in,SP}$ on the run's own settings, and the trip and the stuck valve act as they do above the loops, so the MPC takes the place of the four inlet loops and of nothing else. Every $T_s = 0.25\,\mathrm{min}$, five controller scans, it solves a quadratic program over $N = 40$ steps, a horizon of 10 min, for the heater command u_H and the quench commands $u_{Q,j}$ and keeps only its first move, held until the decision five scans later, as constrained receding-horizon control does [12].

The controller's model is the reactor of Section 7.3 written again inside the controller with the declared values of Table 7.2, the design feed $\dot{m}_0 = 250\,\mathrm{t/h}$ and unit activity, never the run's parameters, its feed or its activity, as shown in Equation (7.13).

$$\begin{aligned} \tau_h \frac{\mathrm{d}\hat{T}_h}{\mathrm{d}t} &= u_H + d_H - \hat{T}_h, \quad \tau_q \frac{\mathrm{d}\hat{q}_j}{\mathrm{d}t} = u_{Q,j} + d_{Q,j} - \hat{q}_j \\ \tau \frac{\mathrm{d}\hat{T}_{out,i}}{\mathrm{d}t} &= \hat{T}_{in,i} + K\hat{x}_i - \hat{T}_{out,i}, \quad \tau \frac{\mathrm{d}\hat{f}_i}{\mathrm{d}t} = \hat{T}_{in,i} - \hat{f}_i \end{aligned} \tag{7.13}$$

where the hat denotes the controller's own copy of a quantity, $j = 1, 2$ and 3 counts the quench valves, $\hat{T}_{in,1} = \hat{T}_h$, $\hat{T}_{in,i+1}$ follows from $\hat{T}_{out,i}$ and $\hat{q}_i$ by Equation (7.5) at the design feed, $\hat{x}_i$ is Equation (7.2)

at the design feed with the activity replaced by an apparent activity $\hat{a}_i$ of bed i, and d_H in °C and $d_{Q,j}$ in t/h are offsets on the actuator paths. The state $\hat{f}_i$ is the inlet seen through the bed's own lag, so $\Delta\hat{T}_{c,i} = \hat{T}_{out,i} - \hat{f}_i$ is the model's copy of the compensated rise of Equation (7.12). Four further states carry the inlets through the 0.15 min thermocouple filter, updated once per scan as the loops' filter is, which makes 16 states, and the eight measurements are those four filtered inlets and the four bed exits as the override reads them.

The model is written from the balances rather than identified by a step test, because at the design point bed 1 amplifies its inlet 3.33 times and sits 3.8 °C below its fold, so an open-loop step identifies a plant that is leaving its operating point. Driven open loop by the commands the shipped loops sent through common setpoint steps of ±2 °C, it reproduces the four filtered inlets within 6.6×10^{-6} °C and the four exits within 1.9×10^{-6} °C over 60 min on the declared plant. Linearized once at the design point it would miss the same responses by up to 44 % RMS and by 76 % at its largest error, on the bed 4 exit, so each plan relinearizes the model about the present estimate, by central differences, with an exact zero-order hold over T_s and the present rates as an affine term.

The estimator is a steady-state Kalman filter whose gain is computed once on the model linearized at the design point, sampled at the 0.05 min scan and augmented with the eight disturbances d_H, $d_{Q,j}$ and $\hat{a}_i$ as random walks. At every scan, whichever structure has the valves, the nonlinear model is integrated with the commands the controller sent and the gain corrects the 16 states and the eight disturbances from the eight thermocouple residuals, so selecting the MPC in the middle of a run finds its estimate up to date. Disturbances estimated on the model's inputs in this way are what make a predictive controller offset-free [13]. An output bias, the simpler choice, shifts the predictions of a model that keeps its design index of 0.538 on bed 1. After a feed cut or a more active catalyst it would therefore predict the design amplification of a bed whose true index has risen toward one, and on a bed past its fold a constant offset cannot follow a mode that diverges. The apparent activities carry the higher index into the relinearized model instead. The MPC is given no feed measurement, and the cut of scenario 11 to 220 t/h is read as an apparent activity of 1.136, which is 250/220, on every bed, moving the slowest pole of the planned model from -0.132 to $-0.109\,\mathrm{min}^{-1}$. A stuck valve is not reported to it either, and its unanswered requests appear as a growing quench offset. A bed converting less than 1 % holds its activity estimate, a quench offset is held where the model's flow would turn negative, the disturbances are frozen while the reactor is tripped, and after a reset the states are put back on the thermocouples with the disturbances at the declared plant.

Each decision minimizes the objective of Equation (7.14) over moves held in eight blocks, two of one step, two of two, then 4, 6, 9 and 15 steps, taken as changes from the commands applied now, 32 moves and eight slacks, a 40-variable program on the 12 states that reach a planned output.

$$
\begin{aligned}
\min_{\Delta u,\,\varepsilon} \; & \sum_{k=1}^{N}\sum_{i=1}^{4}\left(\hat{T}_{in,i,k} - r_i\right)^2 + 0.1N\sum_{i=1}^{4}\left(\hat{T}_{out,i,N} - T^{*}_{out,i}\right)^2 \\
& + \lambda\sum_{b=1}^{8}\left(\Delta u_{H,b}^2 + G_Q^2\sum_{j=1}^{3}\Delta u_{Q,j,b}^2\right) + \sum_{\ell=1}^{8}\rho_\ell\left(\varepsilon_\ell^2 + \varepsilon_\ell\right) \\
\text{s.t. } & 300 \le u_H \le 420, \quad 0 \le u_{Q,j} \le 30, \quad \varepsilon_\ell \ge 0 \\
& \hat{T}_{in,i,k} \le T_{in,SP} + \delta + \phi_{i,k} + \varepsilon_i \\
& \Delta\hat{T}_{c,i,k} \le \Delta T_{ceil} + \psi_{i,k} + \varepsilon_{4+i}
\end{aligned}
\tag{7.14}
$$

where k counts the steps and b the move blocks, the first move being taken from the command in force, r_i is the inlet target of bed i and $T^{*}_{out,i}$ the exit it settles to, $\lambda = 0.1$ per °C^2 is the move price, $G_Q = 6.5$ °C per t/h scales a quench move to the bed 2 inlet change it makes at design, the bounds are in °C and t/h, ε_ℓ are the slacks with prices ρ_ℓ, one slack per soft row over the whole horizon, and $\delta = 0.5$ °C. The funnels $\phi_{i,k} = [\hat{T}_{in,i,0} - T_{in,SP} - \delta]^{+}\mathrm{e}^{-kT_s/\tau_h}$ and $\psi_{i,k} = [\Delta\hat{T}_{c,i,0} - \Delta T_{ceil}]^{+}\mathrm{e}^{-kT_s/\tau}$, with $[\cdot]^{+} = \max(0,\cdot)$ and a subscript 0 for the model's present value, bring back a value already above

its limit. Tracking carries 1 per °C^2 at every step. The terminal weight of $0.1N$ per °C^2 on the exits keeps a plan from ending with a slow bed mode still away from its steady value, and the horizon's 10 min exceed the time constant of the slowest mode, $1/0.132 = 7.6$ min. The move price and the horizon were chosen once on scenario 11 and are never retuned per case.

The bounds on the commands are hard and are the limits the inlet loops clamp to. The ceiling is $\Delta T_{ceil} = \Delta T_{lim} - 0.5\,°\mathrm{C}$, where ΔT_{lim} is the override's threshold of Equation (7.11), the run's rise alarm less its override margin, so ΔT_{ceil} is 27.5 °C as shipped, half a degree inside the 28 °C at which the override starts on the same compensated rise. While the MPC holds the ceiling the override has nothing to do and remains the backup. Each rise row is soft, priced 10^3 per °C^2 and 10^3 per °C against 1 per °C^2 of tracking. Each inlet is capped softly at the setpoint after the override plus δ, so a plan never undoes a cut the override made. The caps on beds 2 to 4 carry the prices of the rise rows, and the cap on bed 1 carries 10^5. That separate price came from a restart. At 10^3, a warm-up after a trip reset traded bed 1's inlet for the cold beds below it, which are warmed only through the heater, and took that inlet to 384.0 °C at 220 t/h, 2.1 °C past the 381.87 °C fold of that feed, for 5.3 min, and to 392.6 °C with the stuck valve of scenario 6. At 10^5 the inlet peaks at 381.50 °C in all four restart cases measured, with no time above the fold, where the loops peak at 381.00 °C.

The targets are made consistent with the ceiling before each plan. Bed by bed down the reactor, r_i is the common setpoint after the override or, where lower, the inlet at which the model's steady rise at the present activity estimate equals ΔT_{ceil}, which follows from Equation (7.2) in closed form as Equation (7.15), and $T^{*}_{out,i}$ is the cool steady exit at r_i.

$$r_i = \min\left\{ T_{in,SP},\ \left[\frac{1}{T_{ref}} - \frac{R}{E}\ln\frac{\Delta T_{ceil}}{K k_{ref}\hat{a}_i R_i}\right]^{-1} - \frac{\Delta T_{ceil}}{2} \right\} \tag{7.15}$$

The bracket, in kelvin, is the mean bed temperature at which $K\hat{x}_i = \Delta T_{ceil}$, converted to °C before half the ceiling is subtracted, and R_i is the model's unconverted fraction at the targets of the beds above. After the cut of scenario 11, with $\hat{a}_1 = 1.136$, it gives 379.50 °C for bed 1.

Each condensed program goes to a dual active-set solver [14] with a ridge of $10^{-9}\left(1 + 2(100N + 0.1N + G_Q^2\lambda)\right)$ on its Hessian. At 16 min of scenario 11, with no limit row active, the shipped plan's first move equals a batch least-squares solution of the same problem to a relative 1.0×10^{-14}. A plan is kept only when the solver reports an optimum, its first move, whole plan, predicted outputs, objective value and slacks are all finite, no slack is negative and every move lies within its bound. A plan that fails is marked in the historian, and the four inlet loops, which track the applied commands at every scan with no preload, take the heater and the valves until the next valid plan. With the noise off, two rejections forced at 40 min of scenario 11 move the heater by less than 0.0001 °C and no quench valve by more than 0.0001 t/h on the hand-over scan, and none of the plans in the runs reported here was rejected. The first plan is solved on the priming call, so a run started under the MPC is under its control from $t = 0$, and while the reactor is tripped the MPC is idle. In Chrome a plan takes 0.95 to 1.20 ms, 0.38 to 0.48 % of a single core at the 1 min/s rung and 23 to 29 % at the top speed of 60 min/s, at which the page still draws 59.9 to 60.1 frames a second.

Three models are thus kept apart, the plant of Section 7.3 on the run's parameters, feed, activity and valve state, the instruments the loops also read, and Equation (7.13) on the declared values with eight estimated disturbances standing in for everything it is not told.

7.6 Results

Twelve scenarios run from a manual amplification measurement to a graded challenge. Each carries a completion rule that credits the listed actions and the state the simulation then reaches (Section 1.6.4), and the Exercises at the end of this chapter work through several of them. The challenge is judged on the case as given, so changing a model parameter or a disturbance voids the attempt.

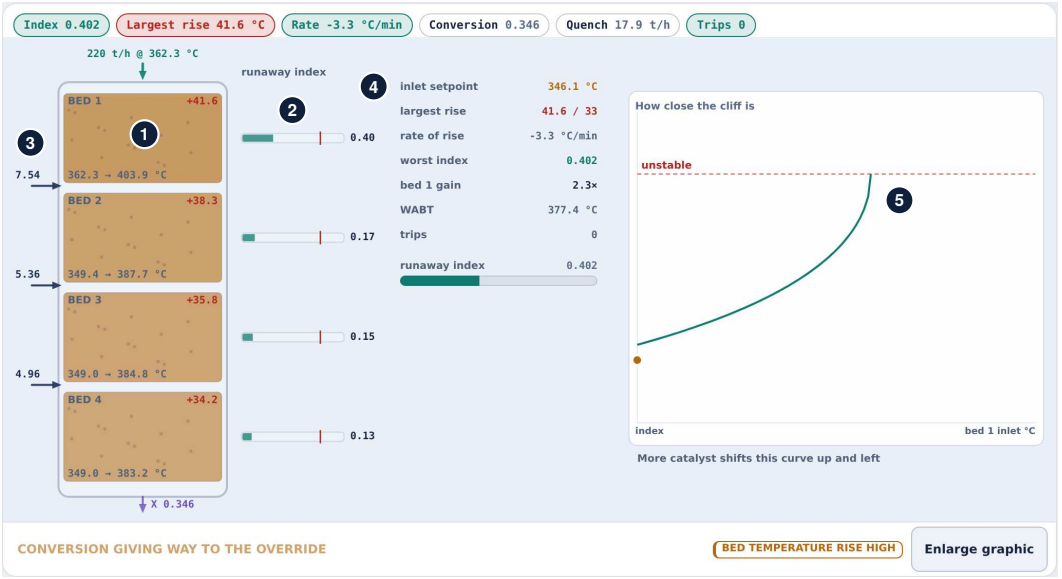


Figure 7.2 The hydrocracker application running scenario 8, the override measurement case, at 28.2 min with the conversion loop in automatic and the override reading the raw bed temperature rise, 8.2 min after a twelve percent feed cut and 0.05 min before the trip, cropped to the plant view with numbered callouts. (1) The reactor is drawn in elevation with its four beds, each shaded by its temperature rise and (2) carrying a runaway index bar against a line at one, and (3) with the quench flows between the beds. (4) The panel shows the inlet setpoint pulled down to 346.1 °C by the override, the largest rise at 41.6 °C against its 33 °C alarm, a rate of rise of −3.3 °C/min and a worst runaway index of 0.402. (5) The inset plots bed 1 runaway index against inlet temperature, solved from the model at the present feed and activity and ending at the fold (381.9 °C at 220 t/h), with the present operating point held at its left edge.

Table 7.3 Bed 1 Runaway Index and Rise Against Inlet Temperature

Inlet (°C)	r	Rise (°C)
380	0.493	21.7
381	0.538	23.9
382	0.592	26.4
383	0.662	29.8
384	0.763	34.7
384.5	0.848	38.9
384.8	0.961	44.4
385	no cool steady state	—

7.6.1 The Index and the Boundary

At the design condition the first bed sits at $r = 0.538$ and amplifies small inlet changes by $(1 + r)/(1 - r) = 3.33$, which the steady-state response to a ±0.5 °C inlet change reproduces to three figures. A whole degree moves it further. Stepping the heater from 381 to 382 °C in scenario 1 moves the bed 1 outlet from 404.86 to 408.45 °C in 120 min, a gain of 3.59, because the index rises with the step. Table 7.3 reports the index on the cool branch against inlet temperature.

The steps are not equal and they accelerate, which is what an exponential rate law does to a linear temperature increment. The last 0.8 °C, from 384 to the fold at 384.8 °C, moves the index

Table 7.4 Override Reading a Raw and a Compensated Bed Rise, on a Feed Cut From 250 t/h to 220 t/h at 20 min

Measurement	Engages (min)	Setpoint low (°C)	Peak rise (°C)	Outcome
Raw ΔT	25.8	344.7	42.2	trips at 28.25 min
Compensated ΔT	26.2	377.4	29.9	holds

almost as far as the three degrees before it (0.198 against 0.225). At the fold the cool steady state and the unstable one merge and vanish, and the only steady state left is an ignited bed held at the 0.9 conversion ceiling with a rise of 81 °C, far past every trip setting. The same fold is reached at a catalyst activity of 1.180 and at a feed rate of 212 t/h.

7.6.2 The Override That Trips the Reactor

Table 7.4 reports scenario 8, a twelve percent feed cut at 20 min with the conversion loop in automatic and the override armed, reading either the raw bed rise or the compensated one. The application gives one run whether the compensation is chosen before Run or carried through a Reset.

On the raw rise the override does nothing until the rise reaches its 28 °C threshold at 25.8 min, then takes the inlet setpoint from 380.2 to 344.7 °C in 2.5 min and trips the reactor on its 42 °C bed rise setting at 28.25 min, 8.25 min after the cut, and the state just before the trip is shown in Figure 7.2. Nothing is broken. The override is correctly signed for the steady state, the gain is reasonable and the measurement is accurate. It fails because the transient sign of the measurement is the opposite of its steady-state sign, so the loop cuts, the number gets worse, and it cuts harder. With the compensated measurement the same override engages at 26.2 min and never cuts more than 2.0 °C, the conversion loop and the override together take the setpoint no lower than 377.4 °C, and the largest rise peaks at 29.9 °C, far from a trip.

> **TRY IT IN THE APP** **8 · The number the override reads**
>
> Load the case and press Run. The feed is cut to 220 t/h at 20 min. Watch the Bed inlet setpoint trace. The override does nothing until 25.8 min, then takes the setpoint from 380.2 toward 344.7 °C in 2.5 min, and the reactor trips at 28.25 min. Press Reset, set Bed rise compensation to Compensated and run again. The rise peaks at 29.9 °C and nothing trips.

7.6.3 Bed 1 Has No Handle

With all four inlet loops in automatic and well tuned and the override Off, as scenario 4 ships, an activity step to 1.30 at 15 min puts bed 1 past the boundary and no inlet loop can save it, because bed 1's only handle is the feed heater with its 2.5 min lag. In scenario 4 the bed 1 index passes one at 26.5 min and peaks at 1.019, and the reactor trips on bed temperature rise at 27.3 min. The quench valves below protect beds 2, 3 and 4 from what bed 1 does, and they do, and with the override Off nothing protects bed 1 from itself. That is the structural reason a hydrocracker trips rather than controlling its way out of a real runaway. With the override On, a setting the scenario does not ship, the same loops do not trip, because the override pulls the common setpoint down to 374.3 °C and bed 1's index peaks at 0.769, at the price of 102.8 min with the compensated rise above 28 °C and a mean conversion of 0.5486. The override's index peaks at 0.692 while the true one passes 0.75 at 16.8 min, so the rise term alone cuts, from 17.25 min. The MPC of Section 7.5.5 holds the same step at a compensated rise of 27.52 °C, as Section 7.6.4 reports.

Pause. Try Exercise 7.3 before reading on.

Table 7.5 Inlet Loops Against the MPC, Default Seed, Full Duration of Each Case

Case	Structure	Rise, comp./raw (°C)	Over 28 (min)	Override (min)	Mean X	IAE_X (min)	Inlet IAE (°C min)	Heater (°C)	Outcome
11, 120 min feed cut	MPC (override On or Off)	27.50/27.50	0.0	0.0	0.5501	4.57	159.0	6.9	480 plans, 0 rejected
	loops and override	28.80/29.92	98.9	99.0	0.5427	3.68	6.7	4.9	—
	loops, override Off	34.05/34.05	98.9	0.0	0.5683	6.75	3.6	0.0	76.0 min over the alarm
	loops, bed 1 at 379.496 °C by hand	27.50/27.50	0.0	0.0	0.5501	4.57	158.2	6.0	—
	hindsight, none over 28[a]	27.72/28.48	0.0	102.3	0.5369	2.99	3.0	2.8	—
	highest X of the 48[b]	29.99/30.44	98.9	96.8	0.5503	4.59	2.5	1.7	—
10, 600 min conversion to 0.600	loops and override	29.28/29.80	512.3	514.3	0.5470	21.27	30.9	36.5	—
	MPC (override On or Off)	27.50/27.53	0.0	0.0	0.5659	9.90	1465.7	9.4	2400 plans, 0 rejected
	loops, MPC's bed 1 target	27.50/27.50	0.0	0.0	0.5659	9.92	—	6.5	—
	hindsight, least IAE_X[c]	31.13/31.33	496.9	415.1	0.5554	16.23	221.9	15.5	—
6, 180 min stuck valve	loops and override	28.37/28.88	149.6	149.8	0.5589	8.44	645.0	2.2	—
	MPC (override On or Off)	27.05/29.12	0.0	0.0	0.5415	5.32	316.7	40.2	720 plans, 0 rejected
	hindsight, least inlet IAE[d]	26.32/28.23	0.0	156.1	0.5374	4.57	359.4	16.0	—
	highest X, none over 28[e]	27.60/27.95	0.0	156.1	0.5463	6.18	524.6	1.2	—
4, 120 min activity 1.30	loops, override Off (shipped)	41.90/41.96	10.0	0.0	0.1362	47.92	4.9	81.0	trip, 27.25 min
	loops, override On	30.67/34.43	102.8	102.8	0.5486	4.39	18.4	17.1	—
	MPC (override On or Off)	27.52/31.30	0.0	0.0	0.5809	8.27	471.0	22.7	480 plans, 0 rejected
	loops, MPC's bed 1 target	29.11/30.65	19.3	0.0	0.5814	8.33	—	16.0	—
7, 300 min feed cut, X loop	loops and override	28.80/29.90	45.2	48.2	0.5244	5.48	78.4	48.4	—
	MPC (override On or Off)	27.32/27.97	0.0	0.0	0.5242	5.80	140.0	41.6	1200 plans, 0 rejected
12, 400 min challenge	loops, suggested	29.84/32.49	33.3	38.5	0.5284	7.09	196.4	414.6	passes, 0.61 °C
	MPC, rest as shipped	28.06/31.72	0.3	0.0	0.5741	24.83	1391.4	346.2	fails, 5.25 °C, 1600 plans
	MPC, suggested	27.55/29.54	0.0	0.0	0.5284	9.48	471.8	235.9	fails, 2.43 °C, 1600 plans

Rise is the largest compensated and raw bed rise before any trip, over 28 is the time the compensated rise spends above the shipped override threshold, IAE_X is the conversion against its setpoint, inlet IAE sums the four inlets against the common setpoint after the override, and heater is the travel of the heater command. The challenge outcome is the worst inlet error in the last third, and no MPC plan was rejected. The 48 hindsight settings are four tunings (cautious, with $K_c = 0.8$ and $\tau_I = 8$ min on the heater and 0.25 t/h per degree and 6 min with no derivative on the quench, shipped, shipped without the quench derivative, and fast, with 4 and 2 min on the heater and 1.5 t/h per degree and 1 min on the quench) by K_o of 1, 2.5, 5 and 8 by margins of 4, 5 and 7 °C. [a]Fast, $K_o = 1$, margin 7. [b]Fast, $K_o = 1$, margin 4. [c]Cautious, $K_o = 1$, margin 4. [d]Fast, $K_o = 8$, margin 7. [e]Cautious, $K_o = 1$, margin 7.

7.6.4 One Bed at Its Limit

Scenario 11 is the feed cut of scenario 5 with the shipped tuning and the override armed, loaded with the MPC on the inlets, and it is compared with the same run repeated after Reset under the inlet loops. Table 7.5 measures scenarios 11, 10, 6, 4 and 7 and the challenge under both structures, the MPC with the settings scenario 11 ships and no retuning, every row sharing one seed, one set of instruments and noise, and one duration. The rows that locate the gain are the override Off, the loops with bed 1's setpoint alone lowered by hand on a copy of the controller, which the shipped structure cannot do, the loops given the MPC's own bed 1 target as it moved, and the best of 48 fixed loop and override settings chosen in hindsight inside the application's ranges. Figure 7.4 draws three columns of the table for the two structures.

Under the MPC the largest compensated rise climbs to the 27.5 °C ceiling and holds there, and the override never acts. Only bed 1 gives up temperature. From 17.5 min its inlet sits at 379.5 °C while beds 2 to 4 return to 381 °C, and the conversion averages 0.5501 over the two hours, 245.9 t converted. Under the loops the override engages at 21.1 min, the compensated rise peaks at 28.80 °C at 24.1 min and settles at 28.49 °C, above the override's own threshold because the cut is proportional, all four inlets are pulled down together to 379.79 °C, and the conversion averages 0.5427 (242.6 t), as shown in Figure 7.3.

The gain is the per-bed target. The rise row is active in none of the 480 plans of scenario 11, because bed 1's target already places its predicted steady rise on the ceiling, and the loops with bed 1's setpoint alone lowered by hand to 379.496 °C at the cut give the MPC's result exactly, a largest rise of 27.50 °C, no override action, a mean conversion of 0.5501 and 245.9 t, with the override On or

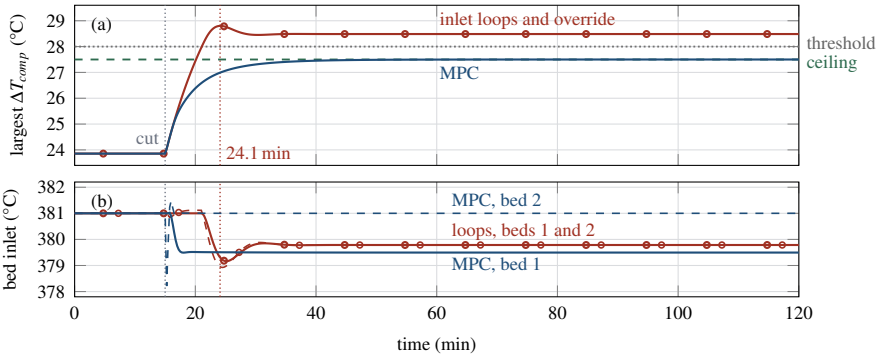


Figure 7.3 Scenario 11, the feed cut from 250 to 220 t/h at 15 min, under the MPC as loaded and, after Reset, under the four inlet loops, default seed. The loops' curves carry open circles and the MPC's carry no marker. (a) The largest compensated bed rise against the MPC's 27.5 °C ceiling and the override's 28 °C threshold. The loops' rise peaks at 28.80 °C at 24.1 min, with the override cutting all four inlets toward 379.0 °C. (b) The bed 1 inlets (solid) and bed 2 inlets (dashed). The MPC holds bed 1 alone at 379.5 °C from 17.5 min while bed 2 returns to 381 °C, and the loops hold all four inlets on the one cut setpoint.

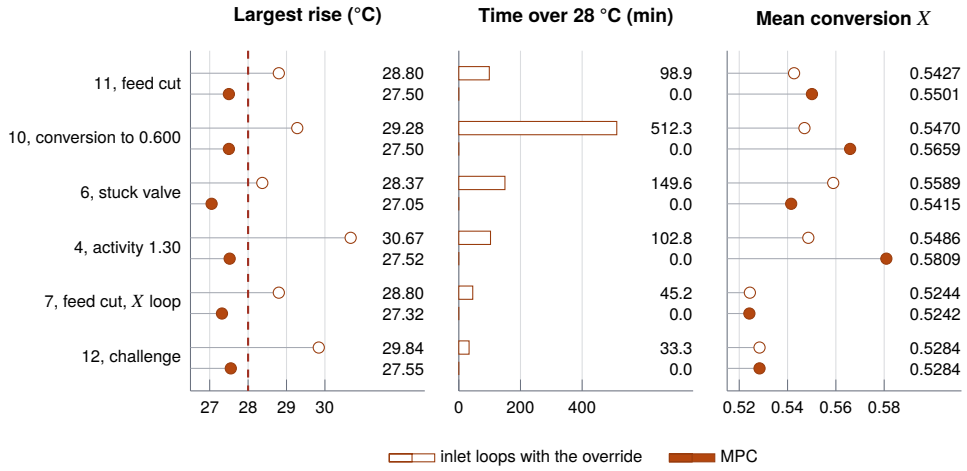


Figure 7.4 Three columns of Table 7.5 for its six cases, the inlet loops with the override as open circles and white bars and the MPC as filled circles and solid bars. For case 4 the loops' row is the one with the override On, and for case 12 both rows use the suggested settings. The dashed line is the override's 28 °C threshold. Notice that every MPC point lies left of that line and spends no time over it, while its conversion is the higher one in cases 11, 10 and 4 and the lower one in case 6.

Off. What the MPC contributes in this case is that it finds that target by itself, from the thermocouples and without the feed, while the shipped structure has one setpoint for four beds and no place to hold one of them lower. The override, with only that setpoint to move, cools all four beds to cool one. No fixed setting of the shipped structure closes the gap. The best of the 48 with no time over 28 °C converts 0.5369, and the one that matches the MPC's conversion, 0.5503, holds the rise above 28 °C for 98.9 min.

Scenario 10 gives the same attribution with the conversion loop above both structures. The MPC more than halves the conversion IAE, 9.90 against 21.27, with no time above 28 °C against 512.3 min, but the loops given the MPC's bed 1 target as it moved reach 9.92, and the best fixed setting reaches

16.23 with 496.9 min above 28 °C.

The plan itself counts on a fast event. Through the activity step of scenario 4 the rise row is active in 10.2 % of the plans, from 15.8 to 27.8 min, and the MPC holds the compensated rise at 27.52 °C with a peak index of 0.716, where the loops following the MPC's own bed 1 target avoid the trip but reach 29.11 °C with 19.3 min above 28 °C.

The losses each have a mechanism. Scenario 6 sticks quench valve 1 at 15 min and raises the activity to 1.10 at 20 min. The MPC is not told that the valve is stuck, so it raises that valve's request at every plan while its estimator reads each unanswered request as a larger offset, and when the request reaches its 30 t/h bound at 59.8 min the plan turns to the heater at once. One decision moves the heater command down 13.08 °C, bed 1's inlet falls to 377.59 °C, and the heater travels 40.2 °C against 2.2 °C under the loops. The MPC halves the inlet IAE, 316.7 against 645.0 °C min, and keeps the rise below 28 °C, but converts 0.5415 against 0.5589, and a fixed setting with no time over 28 °C converts 0.5463. No rise row binds in scenario 6, so the pulse is not the ceiling's doing. The likely cause is the move price of 0.1, chosen on a slow cut and applied with a one-step first block to a heater that has a 2.5 min lag and no rate limit in the model. In scenario 7, with the conversion loop's 25 min analyzer above both structures, the MPC's conversion IAE is 5.80 against 5.48, at a mean conversion of 0.5242 against 0.5244. Its inlet IAE against the common setpoint is larger in every case, 159.0 against 6.7 °C min in scenario 11, because bed 1 is held below that setpoint by design. The cheap move price shows again on a switch to the MPC in the middle of an upset, which with the noise off moves the heater command 11.10 °C on the next scan at 30 min of scenario 11 and 25.59 °C at 70 min of scenario 6.

The challenge's rule is the same under the MPC, and the MPC does not meet its target. With the suggested settings the reactor never trips, the compensated rise stays at or below 27.55 °C and the peak index is 0.669, but the worst inlet error in the last third is 2.43 °C against the ±1 °C band, because the MPC holds bed 1 where its rise meets the ceiling. With everything else as shipped, a 382 °C start with no override and no conversion loop, it again never trips, with a peak index of 0.685 and a worst inlet error of 5.25 °C, where the shipped loops trip at 150.0 min. Neither MPC run breaks an unscored limit, with no trip, no time over the 33 °C alarm and every index below one, and the verdicts hold at half the physics step and at seeds 1 and 777.

> **✦ DID YOU KNOW? The Predictive Controller Fails the Challenge**
>
> From the simulator (Table 7.5). With the suggested settings the four inlet loops pass the graded challenge with a worst inlet error of 0.61 °C. The predictive controller never trips and keeps the compensated rise at or below 27.55 °C, yet it fails at 2.43 °C, because it holds bed 1 below the common setpoint on purpose.

7.6.5 The Graded Challenge

The challenge runs 400 min with catalyst activity steps to 1.08 at 40 min and 1.13 at 260 min and a feed cut to 225 t/h at 140 min, starting a degree above the design inlet temperature with cautious tuning, no override, no conversion loop, 0.15 °C of thermocouple noise and 0.8 % of analyzer noise. It is met when every bed inlet is held within 1 °C of setpoint through the last third of the run, no runaway index reaches one, and the reactor does not trip. As shipped the reactor trips on bed temperature rise at 150.0 min, ten minutes after the feed cut. The suggested configuration arms the override with an index limit of 0.72, closes the conversion loop on the design target and applies the tuning of Section 7.5, and it passes with a worst inlet error of 0.61 °C, inside the band by 0.39 °C, and a peak index of 0.724, whether the settings are applied before Run or carried through a Reset. The override is what decides it, because the same settings with the override Off trip at 145.4 min, while armed it carries even the 382 °C start through with a peak index of 0.718. The heater tuning matters next. With the override armed and the cautious heater tuning left in place, bed 1's inlet is still 1.28 °C off in the last third, and the suggested heater tuning brings it to 0.33 °C. Over five other noise seeds the

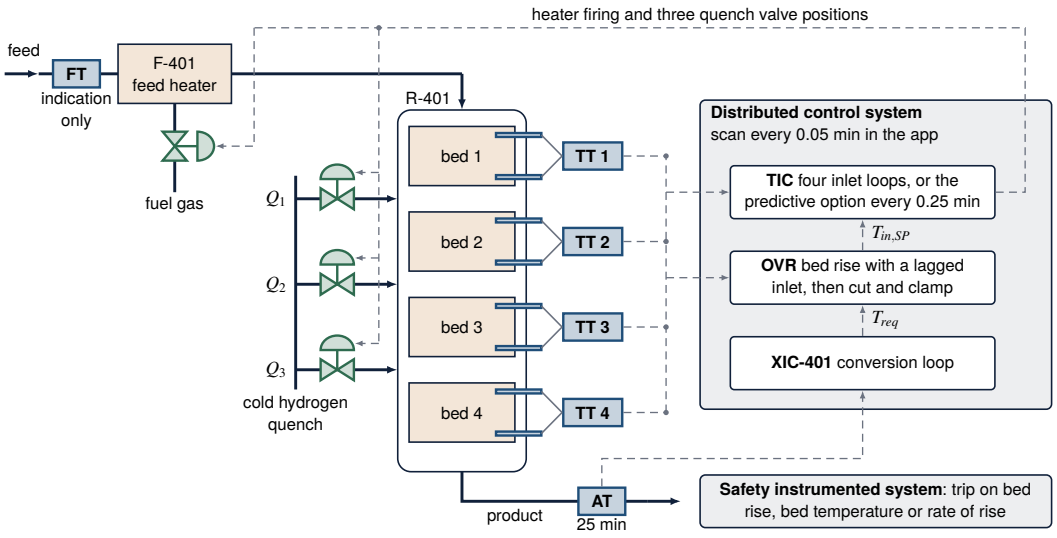


Figure 7.5 The loops of the hydrocracker reactor with their hardware. Lettered boxes are sensing devices: the thermocouples and transmitters at the inlet and outlet of each bed (TT), the conversion analyzer (AT) and the feed flow transmitter (FT). Valve symbols are final elements and dashed arrows are signals. Notice that every bed below the first has a valve of its own, while bed 1 is reached only through the feed heater, and that the override writes nothing but the common setpoint of the inlet loops. The trip sits outside the control system. Not to scale, and not a piping or safety diagram.

shipped case trips between 149.5 and 150.2 min and the suggested one passes with worst errors of 0.50 to 0.65 °C.

7.7 Technology in Practice

Figure 7.5 draws the loops of Section 7.5 with the hardware a refinery installs.

What Measures It

Every bed is read by thermocouples at its inlet and outlet. In the reactor of a 1997 investigation the center inlet thermocouple of each lower bed fed the controller of its quench flow, and the bed outlets were displayed but regulated by nothing [1]. The bed rise that the override reads is a difference of two such sensors, which Equation (7.12) puts on one clock. Conversion on a real unit is inferred from a distillation, for which the analyzer AI-401 stands. A soft sensor, a model that predicts from fast measurements a quality known only at a low sampling rate, is the usual supplement in refinery processes [15].

> **TECHNOLOGY** **Sensor: Thermocouple Array in the Catalyst Beds**
>
> Two wires of different metals joined at one end produce a voltage roughly proportional to temperature. Thermocouples are less accurate than resistance thermometers but more rugged and wider in span [16]. One hydrocracker reactor carried 96 flexible sheathed thermocouples inside its beds, at the inlet, middle and outlet of each, to show axial and radial gradients [1]. The most common failure is an open circuit, which can read as a wildly varying temperature, so the instrument is set to drive its reading high or low, whichever is safer [16]. In that reactor a failed or over-range point was sent as zero, and operators did not understand that zero could mean an extremely high temperature [1]. On a trend such a point drops to zero while its neighbors climb. The 0.15 min thermocouple filter of Table 7.2 is the model's account of this sensor.

What Moves It

Three quench valves and the firing of the feed heater are the handles. In the unit of the investigation the reactor inlet temperature controller set the outlet temperature of a trim furnace, whose controller set the fuel gas pressure [1]. The model folds that cascade into the single lag τ_h. A sudden opening of one quench valve there made the hydrogen flow to the furnaces fluctuate, and both streams came from the recycle gas [1]. The model's quench supply is fixed.

> **TECHNOLOGY** **Final Element: Quench Control Valve**
>
> In a pneumatic control valve the stem position follows the air pressure on a diaphragm or piston against a spring [16]. Friction in the stem packing and the force of the pressure drop on the plug disturb that balance, so a positioner compares the stem position with the control signal and adjusts the air until they agree. With excess friction the stem moves in jerks, or not at all for a small change of signal, which is called stiction. The failure position follows the hazard: a valve that must open on loss of air is built air-to-close [16]. In the hydrocracker of the 1997 report the quench valves leaked when shut, and an alarm warned when one stood more than half open [1]. The model's valve is a 0.30 min lag, tight and free of friction, until scenario 6 sticks one.

Where the Controller Runs

A refinery runs such loops in a distributed control system, in which a supervisor sends set points to distributed controllers that act through actuators from sensor feedback, with cycle times from milliseconds to minutes [17]. The app scans its loops every 0.05 min and plans its predictive controller every 0.25 min, inside that range. The four inlet loops and the conversion loop are PID blocks. The override is a calculation block, the lag of Equation (7.12) followed by the cut and the clamp of Equation (7.11). Conventional constraint control is built in this way from PID algorithms, lead-lag blocks and select logic, and a predictive controller replaces the combination [5]. The trip belongs to a safety instrumented system of sensors, logic solvers and final elements, designed to IEC 61511 and often independent of the control system [17].

> **IN PRACTICE** **A Limit Is a Shutdown, Not a Target**
>
> What the model's trip leaves out is the decision to use it. The reactor of the 1997 report had written limits, among them a maximum reactor temperature of 800 °F, and two depressuring systems, of 100 and 300 psi per minute [1]. In earlier excursions the operators had answered with more quench, a lower inlet temperature or a feed stop, and most could recall one depressuring. The investigators found that quench is typically sized for minor excursions. Past the point where it can hold a bed, only a lower hydrogen pressure slows the reaction. Their advice was limits that are not flexible, emergency systems that are tested, and emergency alarms that stand apart from operating alarms [1].

What Is Modernizing It

The first development is denser thermometry tied to the safety system. A 2019 account of a hydrotreating reactor revamp describes flexible thermocouples in place of two vertical probes near the wall, 20 to 50 sensors in a reactor for radial and axial coverage, and a trip that opens the emergency depressuring valve when a sensor reads too high. A faulty signal is recognized by its current range, so that it does not trip the unit [18]. The second is the valve. An electronic positioner measures stem position and actuator pressure, and the plot of one against the other, the valve signature, shows excessive packing friction [16]. In scenario 6 the valve sticks with no such warning. The third is control from the feed. A 2022 study sets the reactor temperatures of an industrial hydrocracker by a feedforward predictive controller, because feedback has a long response time [11]. The app's predictive controller is given no feed measurement.

7.8 Limitations

The beds are lumped stages, so there is no axial profile and no hot spot position. A real bed's peak temperature is above its outlet and the difference matters at the limits.

One lumped reaction with one activation energy represents a network whose lumping is a research subject in its own right [6, 7]. The application therefore gets the thermal behavior right and the product slate not at all.

Quench maldistribution is absent, which removes the mechanism most often responsible for real hot spots [8].

Catalyst deactivation over a twelve-month cycle is represented only by an activity slider, so the slow walk of the weighted average bed temperature that dominates real hydrocracker operation cannot be studied.

The trip is instantaneous and does not cut the feed. A real depressuring takes minutes at a controlled rate and the reaction continues while it happens, which is precisely the period a safety analysis is about.

The override is a proportional cut, so it holds the largest rise above its 28 °C threshold by the conversion loop's standing cut divided by K_o, 1.2 °C at the end of scenario 10.

The MPC's model is the simulator's own lumped beds on the declared values, exact on the declared plant, which no real reactor offers, and on a changed plant its accuracy rests on the estimator, with up to 1.63 °C of open-loop error at an E/R of 21 000 K. It is told neither the feed nor a valve's position, its heater has no rate limit, which lets one decision move the heater command by 13.08 °C, and the separate price on bed 1's inlet cap rests on four restart cases.

Finally, the application implements the regulatory, override and trip layers, with the optional MPC in place of the inlet loops, and not the multivariable controller that sits above them on a real unit [5, 10]. Scenario 10 shows the economics running into the override and does not show an optimizer resolving the trade.

> **OPEN CHALLENGE** **Seeing a Hot Spot Before It Spreads**
>
> Each bed of the model has one temperature, and a real runaway can start at one point. In the 1997 accident a single outlet point jumped while the other four points of the same bed stayed normal, and the cause of the poor flow distribution could not be determined [1]. A 2021 review of reactor runaway finds that most studies neglect the flow patterns of the vessel, although these can weigh heavily on how a runaway develops, and that uncertain kinetic parameters affect how early a criterion warns [4]. It states that nothing guarantees a developing runaway is seen in every case. Progress would be a warning that holds under such uncertainty and reads the whole thermocouple array.

7.9 Discussion

Three results generalize past hydrocrackers.

The first is that stability can be a property of the plant and a computable one. The index $r = \frac{1}{2} K \, \mathrm{d}x/\mathrm{d}T$ is available from a heat of reaction and an activation energy before any control system is designed, and it says both whether the plant needs a controller to stand up and how much it amplifies when it does not. Any exothermic reactor with an exponential rate law has such a number and it is worth computing early.

The second is that an override is only as good as the sign of its measurement in the transient. The measured failure here takes the setpoint down 35.5 °C in 2.5 min and trips the unit 8.25 min after a feed cut, on an override that is correctly designed for the steady state. Any difference of two measurements with different dynamics deserves the same check, and the fix is usually one lag rather than a retuning.

The third is structural. Bed 1's only actuator is upstream of it behind a 2.5 min lag, so no tuning makes the control system fast enough once that bed is past its boundary. Asking of any fast instability

where the nearest actuator is, and how long it takes to reach the place the heat is being made, is a question that belongs in the process design rather than in the control design.

7.10 Conclusion

A hydrocracker bed is one of the few plants a control course meets that can be unstable without a controller, and the property is a number rather than an opinion. In the simulated reactor of this chapter the first bed sits at a runaway index of 0.538 and amplifies its inlet by 3.3, the index rises to 0.763 at 384 °C of inlet and the cool steady state vanishes at 384.8 °C, and the same fold is reached at a catalyst activity of 1.180 or a feed rate of 212 t/h. Cutting the feed from 250 t/h to 220 t/h raises the steady first bed rise from 23.9 °C to 34.1 °C, which is the opposite of what a production trend suggests. The override installed to protect the reactor trips it 8.25 min after that feed cut when it reads a raw bed temperature rise, because the inlet answers a quench valve within 0.30 min while the outlet carries a 3.5 min catalyst time constant and the difference is therefore inverted during the correction. One lag on the inlet, matched to the bed, holds the largest rise at 29.9 °C instead. An optional model predictive controller holds the same feed cut at its 27.5 °C ceiling with a mean conversion of 0.5501 against 0.5427, a gain the loops reproduce when bed 1's setpoint alone is lowered to 379.5 °C, and on a stuck quench valve it converts 0.5415 against 0.5589. Further work would add an axial bed profile so that the hot spot position becomes visible, quench maldistribution, a catalyst deactivation model over a full cycle, and a depressuring that takes the minutes a real one takes. The simulator is a place to learn what an override reads.

KEY POINTS

- A catalyst bed that makes its own heat can be unstable with no controller, and one number, the runaway index, says how close it is.
- Below an index of one a bed amplifies its inlet, 3.33 times at design, and the quench loops break the chain of four beds.
- Less feed is hotter: a cut from 250 to 220 t/h raises the first bed rise from 23.9 to 34.1 °C.
- An override is only as good as the sign of its measurement in the transient, and one matched lag cures the raw bed rise.
- Bed 1 has no fast handle, so past its boundary the answer is a trip.

Where else this applies. The same ignition boundary stands in the stirred tank of Volume 7, Chapter 2, a protective override that rests at its clamp guards the machine of Volume 4, Chapter 2, and a safety override for each zone bounds the throughput of Volume 4, Chapter 6.

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7.11 Exercises

7.1 ⌕ Concept check · 2 min

The reactor runs at the design condition with every bed inlet held at 381 °C. A charge pump loses suction and the feed falls from 250 to 220 t/h, with the inlet setpoint left where it was. What happens to the steady rise and the runaway index of bed 1?

(a) Both fall, because less feed through the reactor releases less heat of reaction

(b) Both rise, because the feed spends longer on the catalyst and its heat warms less mass

(c) The rise is unchanged and the index falls, because the conversion per tonne is fixed

(d) The rise grows and the index falls, because the bed now reacts at a hotter mean temperature

7.2 ⌕ Concept check · 2 min

In scenario 8 the override reads the raw bed rise $T_{out} - T_{in}$, engages 5.8 min after a feed cut and then trips the reactor 2.45 min later on a bed rise it created. Which explanation is right?

(a) The override gain of 2.5 is too high, so the override oscillates and overshoots into the trip

(b) The override is wrongly signed for the steady state, so each cut raises the inlet temperature

(c) After a cut the inlet falls faster than the outlet, so for minutes each cut raises the rise it reads

(d) The 0.15 min thermocouple filter delays the rise, so the override acts too late to help

7.3 ⌕ Concept check · 1 min

In scenario 4 all four inlet loops are in Auto with the shipped tuning, the override is Off, and the catalyst activity steps to 1.30. Bed 1's index passes one and the reactor trips on its bed rise. Why can the loops not hold bed 1?

(a) The quench loops are tuned too slowly, with an integral time of 1.5 min
(b) The heater loop has the wrong action and drives bed 1's inlet up
(c) The conversion loop raises the common inlet setpoint as conversion falls
(d) Bed 1's only handle is the feed heater, upstream and behind a 2.5 min lag

7.4 Theory and calculation · 6 min

At the design condition bed 1 enters at 381.0 °C and rises 23.86 °C. Use $K = 90.0\,^{\circ}\mathrm{C}$ per unit of x, $E/R = 20\,000\,\mathrm{K}$, $\tau = 3.5\,\mathrm{min}$ and the Arrhenius form of the index, $r = KxE/(2RT^2)$ with T the mean bed temperature in kelvin.

(a) Compute the bed's conversion x, its mean temperature in kelvin and its runaway index r. *Checkpoint:* $x = 0.2651$, 666.08 K, $r = 0.538$.

(b) Compute the steady amplification from inlet to outlet, the time constant of the linearized bed and its pole. *Checkpoint:* 3.33, 7.6 min, $-0.132\,\mathrm{min}^{-1}$.

7.5 Theory and calculation · 8 min

Bed 1 leaves at 404.86 °C on 250 t/h of oil. Quench hydrogen enters at $T_q = 60\,^{\circ}\mathrm{C}$ with $c_{p,H_2}/c_{p,oil} = 5.5$, and bed 2's inlet is held at 381.0 °C. Use Equation (7.5).

(a) Compute the quench flow that holds bed 2's inlet at 381.0 °C. *Checkpoint:* 3.38 t/h.

(b) Differentiate Equation (7.5) with respect to $\dot{q}$ at that point. By how much does bed 2's inlet move per t/h of quench, and what extra quench lowers it by 2.0 °C? *Checkpoint:* −6.57 °C per t/h; 0.30 t/h.

(c) Treat that 2.0 °C cut as a step and hold the reaction rise of bed 2 constant. Using Equation (7.7), how far above the reaction rise does the raw rise read just after the cut and 3.5 min later? What does the compensated rise of Equation (7.12) read? *Checkpoint:* 2.0 °C, 0.74 °C; the reaction rise throughout.

7.6 Theory and calculation · 7 min

The MPC is not told the feed. After the cut of scenario 11 from 250 to 220 t/h it estimates an apparent activity $\hat{a}_1$ on bed 1 and sets the bed's inlet target by Equation (7.15), with $\Delta T_{ceil} = 27.5\,^{\circ}\mathrm{C}$, $K = 90.0\,^{\circ}\mathrm{C}$, $k_{ref} = 0.2600$, $R_1 = 1$, $E/R = 20\,000\,\mathrm{K}$ and $T_{ref} = 392.5\,^{\circ}\mathrm{C}$.

(a) Using Equation (7.2), explain why the cut looks to the estimator like a change of activity, and compute $\hat{a}_1$. *Checkpoint:* $250/220 = 1.136$.

(b) Compute the inlet target r_1 for bed 1. *Checkpoint:* 379.50 °C.

(c) Compute the runaway index of bed 1 at that target, where its rise is 27.5 °C, and the bed's amplification. *Checkpoint:* 0.619 and 4.25.

7.7 App challenge · 8 min

Load scenario 1, "A bed is an amplifier", at the default seed and the default speed of 5 (a 120 min run takes 24 s). The reactor is in Manual and lined out. Press Run, and at any time in the first 20 min raise Feed heater outlet from 381.0 to 382.0 °C. Run to 120 min after the step and export the CSV.

(a) In column `bed1_out_C`, read bed 1's outlet just before the step and 120 min after it. What gain per degree does the step give? *Checkpoint:* 404.86 and 408.45 °C (±0.02 °C); 3.59 per degree.

(b) Read the Bed 1 gain tile at the end and compare both numbers with the 3.33 of Equation (7.4) at the design point. Why do the three differ? *Checkpoint:* 3.9; the index rises from 0.538 to 0.592 across the step.

7.8 App challenge · 9 min

Load scenario 8, “The number the override reads”, at the default seed and speed 5. It loads with Bed rise compensation on Raw ΔT, the conversion loop in Auto and a feed cut to 220 t/h at 20 min.

(a) Run 120 min and export the CSV. Find the first rows with `override_active` $= 1$ and with `tripped` $= 1$, the inlet setpoint `tin_sp_C` on the last row before the trip, and `dt_max_C` on the trip row. *Checkpoint:* 25.80 min, 28.25 min, 346.1 °C, 42.2 °C.

(b) Press Reset, set Bed rise compensation to Compensated, run the same 120 min and export again. Find the first override row, the lowest inlet setpoint, the largest `dt_max_C` and the Trips tile. *Checkpoint:* 26.25 min, 377.45 °C, 29.9 °C, 0 trips.

7.9 App challenge · 8 min

Load scenario 11, “One bed at its limit, not four cut”, at the default seed and speed 5. It loads with Inlet control on MPC, the override armed and a feed cut to 220 t/h at 15 min.

(a) Run 120 min. Read the four bed inlets (`bed1_in_C` to `bed4_in_C`) at 120 min, the largest `dt_max_C`, whether `override_active` is ever 1, and the Converted tile. *Checkpoint:* 379.50, 381.00, 381.00, 381.00 °C; 27.50 °C; never; 246 t.

(b) Press Reset, set Inlet control to PID loops, run the same 120 min and read the same quantities and the first override row. *Checkpoint:* all four at 379.79 °C; 29.92 °C; from 21.10 min; 243 t.

(c) Where does the MPC’s extra conversion come from?

7.10 Application area · 4 min

A safety review of this reactor asks whether the rate-of-rise trip, set at 28 °C/min on a 0.8 min filter, is a protective layer. In scenario 9, with the reactor in Manual and the activity stepped to 1.45, the bed rise trip fires at 16.6 min with the hottest bed at 423.1 °C, while the filtered rate peaks at 2.7 °C/min.

(a) Is the rate trip a protective layer on this reactor? Explain from the bed equation.

(b) From what should its setting be derived, and what goes wrong if it is set far lower than 28 °C/min?

7.11 Application area · 4 min

A charge pump loses suction and the feed falls from 250 to 220 t/h while bed 1’s inlet is held at 381 °C.

(a) At 220 t/h the fold of bed 1 is at 381.87 °C. How much margin does the unit have, and what does the steady rise do?

(b) What should the console operator do at once, and what permanent change to the control system would you propose?

7.12 Review the agent · 5 min

An AI assistant reviewing the reactor writes: “Bed 1 amplifies its inlet 3.33 times, and the four beds are in series, so a 1 °C upset at the feed heater reaches the bed 4 outlet as $3.33^4 \approx 123$ °C. The inlet loops act only on the inlets, so they cannot change this chain.” Find the flaw and say how you would check it in scenario 2, “Four inlet loops”.