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CHAPTER 4

Four Catalyst Beds, an Ignition Floor and Double Absorption in a Contact Plant

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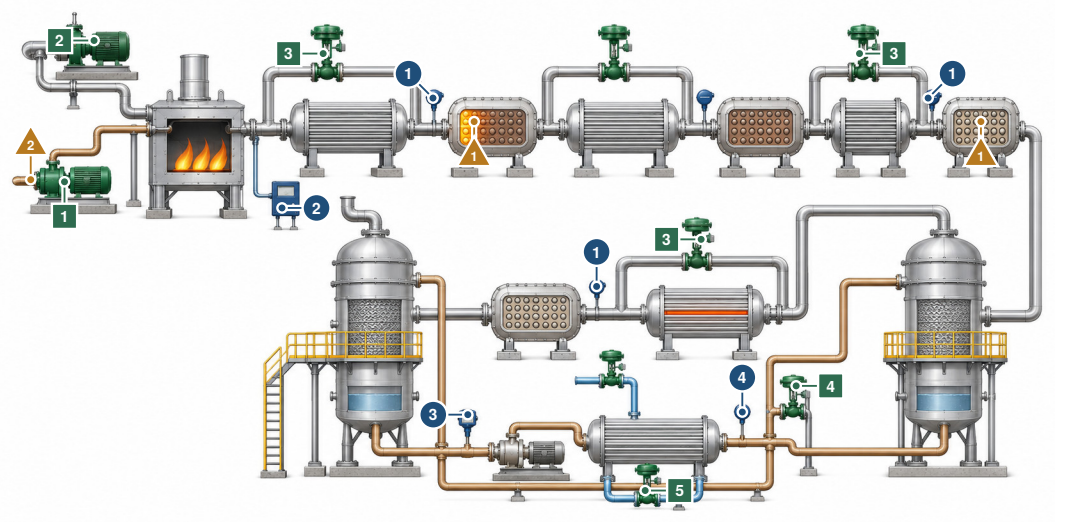
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CHAPTER 4

Four Catalyst Beds, an Ignition Floor and Double Absorption in a Contact Plant



The controller moves 1 sulfur pump, which sets the rate 2 air blower, in ratio to the sulfur 3 gas bypass valves around the coolers, one per bed 4 dilution water valve 5 acid cooler water valve

The controller reads 1 temperature at each bed inlet 2 sulfur dioxide analyzer on the gas to the beds 3 acid strength analyzer 4 acid temperature

What disturbs it 1 catalyst that ages 2 sulfur richer than its meter counts

Notice that each catalyst bed has a cooler with a bypass and a temperature head ahead of it, and that the absorber after the third bed lets the fourth start on fresh gas. Illustration, not to scale.

IN PLAIN TERMS The Coolest Gas That Still Lights

The main idea. A sulfuric acid plant burns sulfur and passes the gas through four layers of catalyst, with coolers in between. Each layer heats the gas as it reacts, and hot gas reacts less fully, so each layer stops short.

The challenge. The coolest gas the catalyst can still light makes the most acid, but a few degrees colder the layer goes out. When the plant slows down, its coolers chill the gas more, and layers go out one by one unless hot gas skips the coolers.

Why it matters. Gas that does not react leaves by the stack, and the law limits how much may leave.

THREE WAYS TO READ THIS CHAPTER

⊘	**Explore**	12 min	the first page; the fact box of Section 4.1; the history box of Section 4.2; the try-it boxes of Sections 4.4 and 4.6; the fact box of Section 4.6; the key points
🕮	**Study**	45 min	the whole chapter with its pause points and the exercises
⛰	**Practice**	10 min	the first page; Section 4.6 with its result chart; Section 4.7; Section 4.8 with its open challenge

The control question Each adiabatic bed of a contact plant climbs a straight line until it meets the equilibrium curve, so the coolest inlet that still lights the catalyst converts the most. How close to that ignition floor can inlet loops, an air ratio, an analyzer trim and a predictive layer hold four beds through a turndown, a richer sulfur and an aged catalyst?

Learning objectives

- Compute the adiabatic line of a bed from its feed and heat-capacity flow, and read where it meets the equilibrium curve.
- Explain how an ignition floor emerges from a two-regime rate law and the bed's heat balance, and why the break of the rate law is not the floor.
- Predict the wrong-way rise and the creeping front from the heat stored in the catalyst, and estimate how fast a front crosses a bed.
- Configure the inlet loops and the strength trim to pass a turndown day, and say what each loop protects.
- Relate a stack reading in ppmv to a limit per tonne of acid.

Prerequisites Sections 1.4.2 (adiabatic lines, interbed cooling, removing the product), 1.4.6 (ratio with a trim), 1.6.2 (velocity form) and 1.6.4 (scenarios and data). Section 1.6.3 is needed only for the predictive layer, and Chapter 2 shows a converter of quench beds.

The app https://apmonitor.com/apps/sulfuric-acid-plant/

See also Volume 7, Chapter 2 for ignition and extinction in a cooled stirred tank. Volume 9, Chapter 8 for a supervisory layer that chooses the setpoints PI loops hold. Volume 6, Chapter 8 for a plant whose loops must be closed before production can be set, with sampled analyzers.

4.1 Introduction

Every point of conversion in the first bed of a contact plant heats its gas by 3.20 K. In the generic plant simulated here, 13.66 t/h of sulfur burned with 1076 mol/s of dry air gives a gas of 11 % sulfur dioxide that enters bed 1 at 420 °C and leaves it at 630.6 °C with 65.77 % of its SO_2 oxidized, which is where that straight line meets the equilibrium curve. Three more beds, with cooling between them and an absorber that removes the trioxide after the third, raise the conversion to 99.837 % and leave 214.5 ppmv of SO_2 in the stack. Without the interpass absorber the same four beds stop at 97.910 %.

The process matters because of its size and its stack. More sulfuric acid is produced than any other chemical, about 150 million tonnes worldwide in 1997 by one estimate, and the European Union had 95 producing plants in 2004 [1]. Anthropogenic SO_2 emissions peaked worldwide in the early 1970s and then fell until 2000 [2], the same years in which the United States began to regulate acid plants built after August 17, 1971 [3]. The converter is analyzed on a diagram of conversion against temperature, on which equilibrium is a curve and each adiabatic bed a heatup path that climbs toward it [4, 5]. That diagram is the reason a converter has several beds, and the reason its inlet temperatures are its most watched variables. Section 1.4.2 draws it for the running example of Chapter 1, and the ammonia converter of Chapter 2 climbs the same kind of lines with quench gas between its beds.

DID YOU KNOW? World Sulfur, 2024

World sulfur production was an estimated 85 million metric tons in 2024, most of it a result of processing fossil fuels, as in the refinery unit of Volume 11, Chapter 13. In the United States about 90 percent of the sulfur consumed that year was in the form of sulfuric acid [6].

The simulator corrects the belief that a hotter catalyst always converts more. On an exothermic equilibrium the coolest inlet that still lights the catalyst converts the most, so the operating point sits near a floor below which the bed goes out, and the floor is not a number printed on the catalyst. In this model bed 1 lined out at the design gas converts 62.8 % with a 395 °C inlet and 3.7 % at 392.5 °C, while halving its catalyst raises that edge to about 400 °C. A second belief is that cooling a bed's

inlet cools the bed. Cooled to 385 °C, bed 1's outlet first rises to 653.4 °C, the wrong-way behavior of packed beds [7], and the bed goes out 32 minutes later. The class is wider than sulfuric acid. Any adiabatic packed bed that carries a reversible exothermic reaction shares the lines, the steps and the extinction, the transient rise after a cut in feed temperature is a property of packed beds in general [7], and a fixed bed whose inlet falls below ignition can keep converting on the heat stored in its catalyst while a reaction zone creeps toward the outlet [8].

🕮 **Pause.** Try Exercise 4.1 before reading on.

However, the sulfuric acid literature treats these parts apart. Plant models are built to optimize operation, dynamically or under uncertainty [9, 10], kinetic studies measure rates on an industrial vanadium catalyst [11], and the creeping and wrong-way transients are analyzed on idealized single beds [7, 8]. This chapter puts the parts together on a browser simulator of a four-bed double-absorption plant, which logs its cell temperatures, conversions and stack beside every instrument. It measures how inlet temperature loops, an air ratio, a strength analyzer trim and a predictive controller hold conversion and emissions through a turndown, a richer sulfur, an aged catalyst and a warm start-up. The rate law is a teaching law of the published shape, and the thermochemistry and the controllers are standard. What the chapter adds is measurement on one synthetic plant, among it the finding that an ignition floor near 395 °C and a creeping front at a 289 °C inlet both follow from the same heat balance. The model has 117 states, its sulfur and oxygen balances close to 2×10^{-15}, it is built on a packed-bed module that other applications share, and no controller sees anything but the instruments. Nine graded cases credit a learner's actions only when the plant responds to them.

Section 4.2 traces the process, its catalyst and its stack limit. Section 4.3 builds the plant: the rate law, the equilibrium, the beds as cells, the burner, exchangers and absorbers, and the instruments. Section 4.4 explores it uncontrolled, from what double absorption buys to the ignition floor, a creeping front and the wrong-way rise. Section 4.5 adds the seven loops and the predictive layer, and Section 4.6 runs the cases, ending with the graded turndown day. Section 4.7 names the hardware and the practice behind the model. Section 4.8 states the limitations and Section 4.9 concludes. The exercises at the end of the chapter run the same cases.

4.2 Contact Process, Melt Catalyst and the Stack Limit

The history box at the end of this section traces the contact process from 1901 to the catalyst used today, vanadium pentoxide in a melt at operating temperature. Cesium sulfate lowers the melting point so that the catalyst can be used cooler, and the lower range of industrial practice is 410 to 440 °C for conventional catalysts and 380 to 410 °C for cesium-promoted ones, against an upper range of 600 to 650 °C above which activity can be lost for good [1].

Design moved from one absorption to two, and the change from single to double absorption is one of the techniques the European reference document lists [1]. In a double contact plant the first catalysis stage converts 85 to 95 % of the SO_2 before an intermediate absorber, the SO_3 formed so far is absorbed in 98.5 to 99.5 % acid, and the removal shifts the equilibrium so that one or two further beds convert most of the rest [1]. The four-bed arrangement with three beds before the intermediate absorber is the 3+1 configuration of the European reference document, and five beds in 3+2 is described there as the normal one [1]. The equilibrium curves and the heatup paths of the stages are the subject of whole chapters of a modern text on the manufacture [4, 5].

The stack limit came with the regulation of new sources. The United States standard of performance applies to every sulfuric acid production unit that commenced construction or modification after August 17, 1971, and limits the SO_2 discharged to 2 kg per metric ton of acid produced as 100 % H_2SO_4 [3]. The rule converts a stack monitor's reading to that unit with a factor computed from the SO_2 entering the converter, $CF = k(1-0.015r)/(r-s)$ with $k = 0.0653$ and r and s the inlet and stack percentages [3], which puts 2 kg/t at 402.0 ppmv for an 11 % gas. The European reference document of 2007 associates best available techniques for an existing sulfur-burning double-absorption plant

with 99.8 to 99.92 % conversion and 30 to 680 mg/Nm^3 of SO_2 as daily averages, and new plants with 99.9 to 99.92 % and 30 to 340 mg/Nm^3 [1].

Models followed the plant into dynamics and optimization. A dynamic model of an industrial plant has been used to optimize its operation [9], and an industrial-scale plant has been optimized under uncertainty [10]. The transients of the beds themselves belong to the theory of fixed-bed reactors, which has represented a bed by a computational model extended to reacting systems since 1960 [12], has analyzed a creeping reaction zone with a model of cells [8], and has explained the transient temperature rise that follows a sudden reduction in feed temperature [7]. None of the sources read for this chapter documents a commercial converter's control configuration, so the simulator's loops are built on the structure above and claim to describe no plant's practice.

> ⧖ HISTORY **A Contact Process and Its Vanadium Melt, 1901 to the 1970s**
>
> In 1901 the contact process received a 47-page account by Knietsch in the *Berichte* of the German Chemical Society, on sulfuric acid and its manufacture by the contact method [13]. Of the catalysts tested for the oxidation of sulfur dioxide, only vanadium compounds, platinum and iron oxide proved technically satisfactory, and vanadium pentoxide is now used almost exclusively. A commercial catalyst carries 4 to 9 weight percent of it with alkali sulfate promoters on silica, and at operating temperature these form a liquid melt in which the reaction is thought to take place [1]. In the 1970s the catalyst was studied as a supported liquid phase: its kinetics and effectiveness factor were measured on an industrial vanadium catalyst, and its liquid dispersion and mass transport in their own right [11, 14]. The steep fall of the model's rate below its 420 °C break stands for that melt solidifying.

4.3 The Plant as Modeled

The plant is a generic sulfur-burning double-absorption unit of 1000 t/d, sized without any licensor's data (Figure 4.1). Liquid sulfur burns with dried air, a waste-heat boiler (WHB) cools the gas, and beds 1, 2 and 3 follow with an exchanger ahead of each of the last two. The reformer of Volume 11, Chapter 9 divides an endothermic reaction among beds in the same way, with a fired heater ahead of each. Each of these three coolers has a hot-gas bypass, so opening it warms the next bed's inlet. An economizer cools the gas leaving bed 3 to the interpass absorber, a reheater warms the returning gas for bed 4, and its bypass on the cold side cools bed 4's inlet when opened. A final absorber precedes the stack, and both absorbers drain into one acid loop held at 98.5 wt% by dilution water. The X–T diagram of the same instant is Figure 4.2. The engine's clock is the minute, flows in the converter are in mol/s, heat in watts and acid in kg/s.

Table 4.1 lists each variable's role and its design value. The integrated state holds the temperatures of the 96 bed cells, four exchanger metals, four bypass positions, the sulfur and air flows behind their pump and blower, the acid strength and temperature, the dilution water and the cooling water openings, 110 physical states in all, and seven ledgers that integrate the sulfur burned, the SO_2 and SO_3 leaving, the SO_3 absorbed, the water added, the acid made and its SO_3.

4.3.1 The Reaction and a Rate Law With a Break

Sulfur dioxide and oxygen react reversibly on the catalyst at a rate per kilogram that falls with the SO_3 it adsorbs, as shown in Equation (4.1).

$$\begin{aligned} &\mathrm{SO_2} + \tfrac{1}{2}\mathrm{O_2} \rightleftharpoons \mathrm{SO_3} \\ &r = a\,k(T)\,\frac{p_{SO_2}\sqrt{p_{O_2}} - p_{SO_3}/K_p(T)}{1 + K_s(T)\,p_{SO_3}} \\ &K_s = K_{s,0}\exp\!\left[\frac{Q_s}{R}\left(\frac{1}{T} - \frac{1}{T_{500}}\right)\right] \end{aligned} \tag{4.1}$$

where r is in mol/(s kg), the partial pressures $p_i = P_b F_i / F_t$ are in bar at the bed pressure P_b, a is the catalyst activity, $K_{s,0} = 2\,\mathrm{bar}^{-1}$ at $T_{500} = 773.15\,\mathrm{K}$ and $Q_s = 60\,\mathrm{kJ/mol}$. The rate constant is two

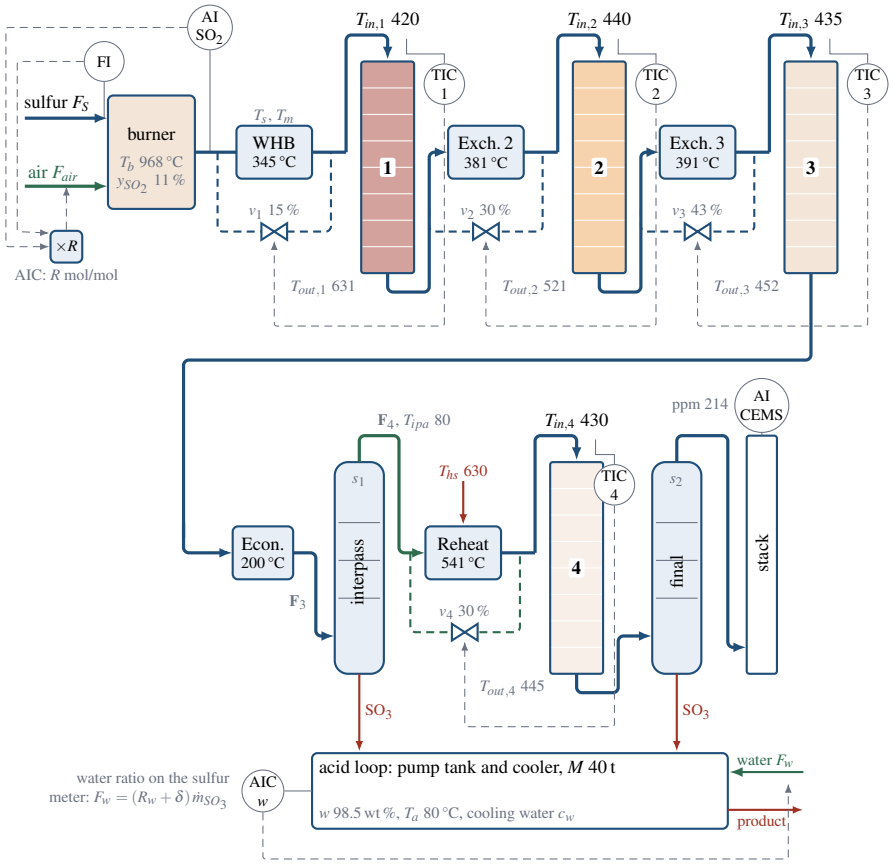


Figure 4.1 The double-absorption contact plant as modeled, case 1 at $t = 0$, after the app's Plant view, with the gas leaving each cooler and the bypass openings v_1 to v_4. The upper row runs from the burner to bed 3, and bed 3's outlet continues on the lower row. Sulfur F_S burns with air $F_{air} = R F_{S,m}$ to 11 % SO_2 at T_b, the WHB and exchangers 2 and 3 (sink T_s, metal T_m) set the inlets $T_{in,b}$ of beds 1 to 3, the interpass absorber passes a share s_1 of the SO_3 in $\mathbf{F}_3$, and the reheater, held on a stream at T_{hs}, heats $\mathbf{F}_4$ for bed 4 with its bypass on the cold side. TIC 1 to 4 move the bypasses, the AIC on the SO_2 analyzer sets the air ratio, and dilution water F_w follows the metered sulfur with a trim from the strength analyzer on the acid loop (w, T_a). A model drawing, not piping and not a safety layout. Not to scale.

Arrhenius terms in series, as shown in Equation (4.2).

$$\frac{1}{k} = \frac{1}{k_{hi}} + \frac{1}{k_{lo}}, \qquad k_{hi} = k_{500}\,\mathrm{e}^{-\frac{E_{hi}}{R}\left(\frac{1}{T}-\frac{1}{T_{500}}\right)}$$
$$\frac{k_{lo}}{k_{hi}} = \mathrm{e}^{-\frac{E_{lo}-E_{hi}}{R}\left(\frac{1}{T}-\frac{1}{T_{br}}\right)} \tag{4.2}$$

where $k_{500} = 0.5\,\mathrm{mol/(s\,kg\,bar^{1.5})}$, $E_{hi} = 80\,\mathrm{kJ/mol}$, $E_{lo} = 600\,\mathrm{kJ/mol}$ and the break $T_{br} = 420\,^\circ\mathrm{C}$. Above the break k follows k_{hi}, below it the steep k_{lo}, and at the break $k = k_{hi}/2$. The constant is 5.94×10^{-2} at 420 °C, 5.05×10^{-3} at 400 °C and 2.02×10^{-4} at 380 °C, the shape of a melt catalyst solidifying [1]. The law is a teaching law, not a vendor's kinetics. It was given a break because, while the model was built, a single Arrhenius term could not place the floor and keep the late beds active at once. With $E_{lo} = E_{hi} = 80\,\mathrm{kJ/mol}$ bed 1 lights at 380 °C, the bottom of the range searched (Section 4.4).

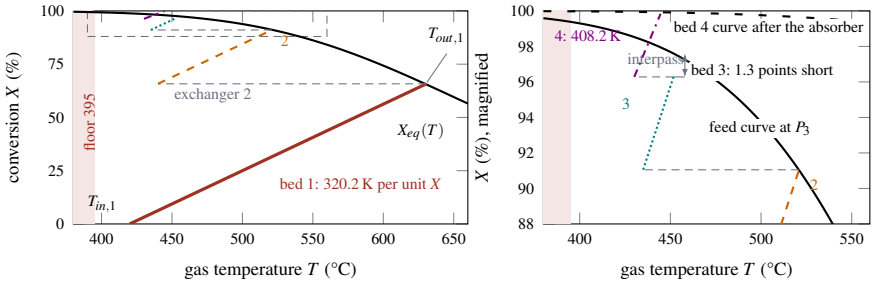


Figure 4.2 The X–T diagram of case 1 at $t = 0$, drawn from the engine's 96 cells: the feed's equilibrium $X_{eq}(T)$ at bed 2's pressure (solid), the floor shaded below 395 °C, the beds as adiabatic lines (bed 1 thick solid, bed 2 dashed, bed 3 dotted, bed 4 dash-dotted) and the exchangers as steps (thin dashed). The right panel magnifies the dashed box, with the feed's curve at bed 3's pressure (solid), which bed 3 ends 1.3 points short of, and bed 4's own curve after the interpass absorber (loosely dashed).

Table 4.1 Variables, Their Roles and Design Values (Case 2 at $t = 0$)

Variable	Role	Design	Range
$T_{in,b}$	CV, bed inlets	420, 440, 435, 430 °C	SP 370–480
v_b	MV, bypasses	15.0, 29.6, 42.6, 30.0 %	0–100
y_{SO_2}	CV, SO_2 to the converter	11.0 vol%	SP 7.5–12.5
R	MV, air-to-sulfur ratio	9.091 mol/mol	7–14
w	CV, acid strength (analyzer)	98.50 wt%	SP 97.5–99.5
F_w	MV, dilution water	2.305 kg/s	0–5
T_a, φ	CV, MV: acid, cooling water	80 °C, 63.0 %	SP 60–100
—	MV, production rate	100 % of 1000 t/d	30–110
π	DV, sulfur against its meter	100 %	90–110
a_b	DV, catalyst activity	100 %	20–120
—	DV, bypass 2 stuck, water supply	free, 100 %	0–100
$T_{out,b}$	outputs, bed outlets	630.6, 520.9, 451.7, 444.5 °C	—
X_b	outputs, after each bed	65.77, 91.05, 96.28, 99.837 %	—
—	output, stack SO_2, SO_3	214.5, 2.4 ppmv	limit 400
T_b	output, burner gas	967.9 °C	—
$T_{i,b}$	states, 96 cells	see Fig. 4.2	—

4.3.2 Equilibrium From NIST-JANAF

The equilibrium constant is a two-constant fit, as shown in Equation (4.3).

$$\ln K_p = -11.2583 + \frac{11839.8}{T}$$
$$\Delta H = -R \cdot 11\,839.8\,\mathrm{K} = -98.44\,\mathrm{kJ/mol} \tag{4.3}$$

with K_p in $\mathrm{bar}^{-1/2}$. It was fitted over 400 to 650 °C to the constant computed from the Shomate parameters of the NIST-JANAF tables [15] for SO_2, O_2 and SO_3. Recomputed by an independent route, $\Delta_r G^\circ = \Delta_r H^\circ - T\Delta_r S^\circ$, the fit gives 166.37 against 166.29 $\mathrm{bar}^{-1/2}$ at 450 °C (+0.05 %) and 9.990 against 9.991 at 600 °C, and its worst error from 350 to 700 °C is −0.91 %, at 350 °C. The tables' heat of reaction runs from −98.93 to −97.75 kJ/mol over that range against the constant −98.44. The same ΔH is the heat released in the energy balance, so the equilibrium curve and the adiabatic lines are consistent by construction. The heat capacities at 500 °C from the same tables are 52.1, 33.6, 72.2 and 31.3 J/(mol K) for SO_2, O_2, SO_3 and N_2.

4.3.3 Beds as Cells on the Catalyst's Heat Capacity

Each bed is 24 cells of equal catalyst mass on a bed module that several applications share. Gas spends a fraction of a second in a cell, so its composition is solved algebraically as a stirred tank at

the cell's temperature, and only that temperature, carried by the catalyst, is integrated, as shown in Equation (4.4).

$$\begin{aligned} \mathbf{F}_{out} &= \mathbf{F}_{in} + \nu\,\xi, \qquad \xi = W_c\, r(T, \mathbf{F}_{out}) \\ W_c\, c_{cat}\, \frac{\mathrm{d}T}{\mathrm{d}t} &= \dot{F}C_p\,(T_{prev} - T) + \xi\,(-\Delta H) \end{aligned} \tag{4.4}$$

where $\nu = (-1, -\frac{1}{2}, 1, 0)$ over SO_2, O_2, SO_3 and N_2, W_c is a twenty-fourth of the bed's 22, 28, 38 or 70 t, $c_{cat} = 1000\,\mathrm{J/(kg\,K)}$, T_{prev} is the previous cell or the bed inlet, and $\dot{F}C_p = \sum_i F_i c_{p,i}$ is the stream's heat-capacity flow, taken at the converter feed and held along beds 1 to 3, with bed 4 a second train on the gas the interpass absorber returns. The extent ξ is found by six damped Newton iterations from zero, a fixed count with no convergence test, so the right-hand side is a pure function of the state and runs replay bit for bit. Building this plant carried one change to the shared module. A species at zero flow whose Newton step is negative is now clipped at zero rather than allowed to set the damping to zero, which had frozen cells with inhibited rates at zero extent. The three applications then on the module, and two column applications checked alongside, logged byte-identical runs before and after this one guard. A bed-1 cell holds 917 kJ/K against an $\dot{F}C_p$ of 36.39 kW/K, a time constant of 25.2 s, and the beds' time constants $C_{bed}/\dot{F}C_p$ are 10.1, 12.8, 17.4 and 40.9 min. Pressures are fixed at 1.40, 1.36, 1.32 and 1.22 bar absolute.

Holding $\dot{F}C_p$ makes every bed a straight line on the diagram, as shown in Equation (4.5), the adiabatic line of Equation (1.3) in this plant's symbols.

$$T_{out} - T_{in} = \frac{F_{SO_2,0}\,(-\Delta H)}{\dot{F}C_p}\,(X_{out} - X_{in}) \tag{4.5}$$

where $X = 1 - F_{SO_2}/F_{SO_2,0}$ is the conversion of the SO_2 fed to the converter. By hand, $118.363 \times 98\,442/36\,389 = 320.20$ K per unit conversion for beds 1 to 3, 3.202 K a point, and bed 4's gas after the interpass absorber, with an $\dot{F}C_p$ of 28.545 kW/K, climbs 408.19 K per unit. The engine's beds lie on these slopes to 2.4×10^{-11} relative and every cell of beds 1 to 3 on its line to 9.8×10^{-10} K.

4.3.4 Burner, Exchangers and Absorbers

Each mole of sulfur takes one mole of oxygen, so the burner gas and its temperature follow from the two flows, as shown in Equation (4.6).

$$\begin{aligned} S &= \min(\pi F_S,\ 0.21 F_{air}) \\ \mathbf{F}_0 &= (S,\ 0.21 F_{air} - S,\ 0,\ 0.79 F_{air}) \\ T_b &= T_{air} + q_c\, S/(\dot{F}C_p)_{hot} \end{aligned} \tag{4.6}$$

where π is the sulfur burned per kilogram the meter counts, $T_{air} = 80\,^{\circ}\mathrm{C}$, $q_c = 279\,\mathrm{kJ/mol}$ is the heat of formation of SO_2, 296.8 kJ/mol in the tables, less a teaching furnace loss, and $(\dot{F}C_p)_{hot}$ uses heat capacities near 600 °C. At design $T_b = 967.9\,^{\circ}\mathrm{C}$. Each cooler passes a share $\beta = 0.8\nu$ of the gas around itself, as shown in Equation (4.7).

$$\begin{aligned} G &= (1-\beta)\dot{F}C_p, \qquad \varepsilon = 1 - \mathrm{e}^{-UA_g/G} \\ T_x &= T_h - \varepsilon(T_h - T_m), \qquad T_{in} = \beta T_h + (1-\beta)T_x \\ C_m \frac{\mathrm{d}T_m}{\mathrm{d}t} &= G\varepsilon(T_h - T_m) - UA_s(T_m - T_s) \end{aligned} \tag{4.7}$$

where T_h is the burner gas or the previous bed's outlet. The reheater is the mirror image, with the cold gas at $T_{ipa} = 80\,^{\circ}\mathrm{C}$ heated by metal held near a stream at $T_{hs} = 630\,^{\circ}\mathrm{C}$, $T_x = T_{ipa} + \varepsilon(T_m - T_{ipa})$ and $C_m \dot{T}_m = UA_s(T_{hs} - T_m) - G\varepsilon(T_m - T_{ipa})$, so opening its bypass cools bed 4. At design the coolers' gas leaves at 345.2, 380.9, 390.5 and 540.6 °C before the bypassed gas rejoins it, and one point of bypass moves the four inlets by 4.21, 1.32, 0.39 and −2.76 K.

The absorbers pass a share of the SO_3 that is least at 98.5 wt% and cool acid, and the acid loop balances its strength and its temperature, as shown in Equation (4.8).

$$\begin{aligned} s &= \frac{s_0(1+g)}{1+s_0 g/s_{max}} \\ g &= k_w\left(\frac{w-98.5}{0.2}\right)^2 + k_T(T_a-85)^+ \\ M\frac{\mathrm{d}\sigma}{\mathrm{d}t} &= \dot{m}_{SO_3} - \sigma(\dot{m}_{SO_3}+F_w) \\ Mc_a\frac{\mathrm{d}T_a}{\mathrm{d}t} &= \dot{n}_{abs}q_{abs} + Q_{gas} + F_w c_w(25-T_a) \\ &\quad - UA_c\varphi(T_a-T_{cw}) \end{aligned} \tag{4.8}$$

where s_0 is 0.1 % for the interpass and 0.05 % for the final absorber, $k_w = 3$, $k_T = 0.5\,\mathrm{K}^{-1}$, $s_{max} = 10\,\%$, σ is the acid's SO_3-equivalent mass fraction (0.804 at 98.5 wt%), $M = 40\,\mathrm{t}$, $\dot{m}_{SO_3}$ the SO_3 absorbed, $q_{abs} = 130\,\mathrm{kJ/mol}$, Q_{gas} the heat of the gas cooled to 200 and 180 °C in the two absorbers, the dilution water enters at 25 °C with $c_w = 4.186\,\mathrm{kJ/(kg\,K)}$, and φ is the cooling water opening. The interpass absorber returns $F_{4,SO_3} = s_1 F_{3,SO_3}$, and the stack's SO_2 is $10^6 F_{o,SO_2}$ over the gas leaving the final absorber. At 98.5 % the acid takes 0.244 kg of water per kilogram of SO_3. The bypass valves follow their commands with a lag of 0.15 min, the sulfur pump and the blower 0.5 min, and the water and cooling-water valves 0.2 min.

4.3.5 Instruments and the Lit Flag

Thermocouples on every bed inlet and outlet have a lag of 0.2 min and 0.3 K of noise, the SO_2 analyzer on the converter feed and the stack monitor (CEMS) a lag of 1 min with noise of 0.02 vol% and 3 ppm, and the acid thermocouple 0.3 min and 0.1 K. The sulfur meter reads the flow the pump delivers, not the sulfur in it, and the flow meters carry 0.2 % noise. The strength analyzer reports a sample every 5 min after a 1 min sample line and 1 min of analysis, with 0.02 wt% of noise. A bed counts as lit while it covers at least a fifth of the way from its inlet conversion to the equilibrium at its inlet temperature, which sets the BED EXTINCT status.

4.3.6 Parameters, Initialization and Numerics

Table 4.2 lists the parameters. Every case begins from the plant lined out for the settings it ships with, each bypass found by bisection so that its inlet sits on its setpoint, the exchanger metals at their balance, the beds lined out by the module's steady solver, and the acid loop solved for the water and the cooling water. The largest derivative of a physical state at the design point is 8.6×10^{-10}. Classical fourth-order Runge–Kutta advances the state in 2 s steps, control acts each 6 s, and a row is logged each 20 s (the clocks of Section 1.6.1). Over a disturbed three-hour run the sulfur and oxygen balances close to 1.3×10^{-15} and 7.9×10^{-16} at every step, and the acid's SO_3 to 1.7×10^{-15}. Halving the step through the whole engine moves no logged conversion by more than 2.2×10^{-6} points.

4.3.7 Assumptions

The plant has one reaction on one catalyst, and the rate law of Equations (4.1) and (4.2) is a teaching law of the published shape. Cesium-promoted catalysts that light lower are not modeled, and the break temperature and activation energies are not fitted to any measured catalyst. The gas holds no heat and no composition, so a cell's composition lines out at every instant and its heat sits in the catalyst. Heat losses, the change of $\dot{F}C_p$ with conversion along a train and pressure drop that varies with rate are left out, and each pressure is fixed. Each exchanger is one metal temperature, and the reheater's hot side is held at 630 °C where a plant would take it from bed 1's outlet through a hot interpass exchanger, so the beds are not coupled through it. The two absorbers share one acid loop of one strength and one temperature, and their slip against strength and temperature is a teaching

Table 4.2 Parameters. A: Adjustable in the Model Dialog. H: Hidden and Fixed

Symbol	Meaning	Value	
k_{500}	rate constant at 500 °C	0.5 mol/(s kg bar$^{1.5}$)	A
E_{hi}, E_{lo}	activation above, below the break	80, 600 kJ/mol	A
T_{br}	break of the Arrhenius plot	420 °C	A
$K_{s,0}$, Q_s	SO_3 inhibition, its heat	2 bar^{-1}, 60 kJ/mol	H
W_b	catalyst in beds 1–4	22, 28, 38, 70 t	H
c_{cat}	catalyst heat capacity	1000 J/(kg K)	H
P_b	bed pressures	1.40, 1.36, 1.32, 1.22 bar	H
T_{air}, q_c	air, net combustion heat	80 °C, 279 kJ/mol	H
β_{max}	largest bypassed share	0.8	H
UA_g	gas side, WHB, X2, X3, reheater	96, 52, 21, 50 kW/K	H
UA_s	sink side, same order	319, 195, 66, 261 kW/K	H
T_s, T_{hs}	sinks; reheater's hot stream	250, 300, 250; 630 °C	H
C_m	exchanger metal	30, 20, 20, 20 MJ/K	H
T_{ipa}	gas from the interpass absorber	80 °C	H
$s_{0,1}$, $s_{0,2}$	SO_3 slip at best	0.10, 0.05 %	A
k_w, k_T, s_{max}	slip growth, largest slip	3, 0.5 K^{-1}, 10 %	H
M, c_a	acid holdup, heat capacity	40 t, 1.45 kJ/(kg K)	H
q_{abs}	heat per mol SO_3 absorbed	130 kJ/mol	H
UA_c, T_{cw}	acid cooler, cooling water	700 kW/K, 30 °C	H
$F_{w,max}$	dilution water at full valve	5 kg/s	H
—	stack SO_2 limit	400 ppmv	A
—	ACID HOT alarm	100 °C	H

law, not a design correlation. The sulfur pump's flow loop is ideal. The stack limit of 400 ppmv, the floor marked at 395 °C, the strength band of 98.3 to 98.7 % and the ACID HOT alarm at 100 °C are teaching values. A real stack limit comes from the plant's permit (the United States standard above gives 402.0 ppmv at 11 % SO_2 [3]), a real floor from the catalyst supplier, and the strength band and the acid temperature from the absorbers' design, for which the European reference document lists 98.5 to 99.5 % acid normally at 70 to 120 °C [1].

4.4 Lines, a Floor and Fronts

4.4.1 What Double Absorption Buys

Figure 4.2 shows the design point on the diagram. At the design inlets bed 1 climbs to its curve and stops on it, at 65.773 % and 630.6 °C, bed 2 stops 0.09 point short of its own outlet's equilibrium at 91.053 %, and bed 3 ends at 96.282 % and 451.7 °C, where the feed's curve at its pressure reads 97.599 %, 1.3 points away, because its catalyst is too cool and its gas too lean to go further. The interpass absorber then removes all but 0.1 % of the SO_3, bed 4 sees a gas of 4.40 mol/s SO_2, 50.6 mol/s O_2 and 0.114 mol/s SO_3, and it converts 95.62 % of what it receives to finish at 99.837 % overall. With the interpass absorber's SO_3 left in the gas, the same inlets give 97.910 %. Removing the product starts bed 4 on a new equilibrium curve, the effect Section 1.4.2 shows for the running example of Chapter 1.

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

4.4.2 An Ignition Floor From the Heat Balance

Nothing in the model clamps a temperature, a rate or a conversion. The floor appears because a bed lights only if the reaction near its inlet warms the gas fast enough to light the catalyst behind it before the gas leaves. Lined out at the design gas, bed 1 converts 62.80 % at a 395.0 °C inlet, 17.48 % at 394.0 °C and 3.04 % at 392.0 °C, as shown in Figure 4.3a. The inlet at which the bed passes 30 % is 395.12 °C in an independent plug-flow integration of the transcribed law, and 393.44, 394.33 and 394.74 °C at 12, 24 and 48 cells. Started lit at 420 °C and held ten hours at each inlet, the 24-cell bed ends where it does from cold to within 1×10^{-4} points between 384 and 404 °C, so the floor shows no hysteresis at this resolution. The rate constant at 395 °C is 3.93 % of its value at the 420 °C break,

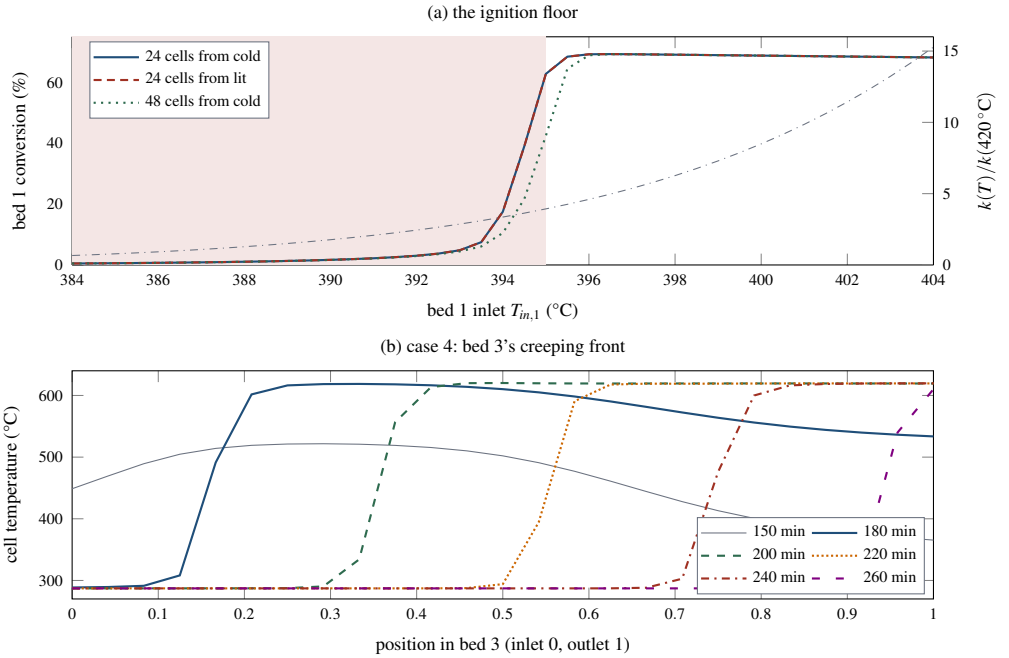


Figure 4.3 The floor and the front, from the engine's bed module. (a) Bed 1 lined out at the design gas against its inlet temperature, from cold (solid) and from a lit bed (dashed) at 24 cells and from cold at 48 (dotted), with the rate constant relative to its value at 420 °C (dash-dot, right axis). The shaded band is the 395 °C floor. (b) Case 4 as shipped, bed 3's 24 cell temperatures from inlet to outlet at six instants, each in its own line style as the legend shows. From 180 min the inlet is at 289 °C and the bed converts on the heat stored in its catalyst.

and the bed at 420 °C still converts 65.77 %, so the break is where the catalyst slows, not where it goes out. The floor belongs to the bed as well as the catalyst. It moves to 386.5 or 402.2 °C with the break at 410 or 430 °C, to 389.2 or 400.3 °C with k_{500} doubled or halved, and to 400.3 °C with half of bed 1's catalyst, while a single Arrhenius term at 80 kJ/mol lights the bed at 380 °C. Six cells per bed, the count first planned, kept a lit bed 1 burning down to a 370 °C inlet and lit it from cold only at 392 °C, a heat-smearing artifact that set the count at 24. The stirred-tank reactor of Volume 7, Chapter 2 ignites and goes out at folds of the same contest between heat released and heat carried away, there through a cooling jacket.

4.4.3 Turndown and a Front That Creeps Out

Half the gas through the same exchangers is cooled further, because each exchanger then has twice the transfer units. In case 4 the rate falls to 50 % at 20 min with the four bypasses held, and by 60 min the inlets are 367.7, 400.5, 393.7 and 477.3 °C. The stack first falls to 89 ppmv at 45 min, then bed 3, which has little conversion left and so little heat of its own, goes out at 1 h 9 min, the CEMS passes 400 ppmv at 1 h 22 min, bed 1 goes out at 1 h 53 min and bed 2 at 2 h 48 min. In between, bed 2, taking over bed 1's work on hot catalyst, relights bed 3 at 2 h 11 min. At 3 h the inlets are 367.8, 320.6, 288.6 and 476.7 °C, yet bed 3 adds 88.33 points of conversion with a 288.6 °C inlet, 106 K under the floor, and the stack reads 2128 ppmv.

Bed 3 is lit by the heat in its own catalyst. Its hottest cell is the 8th of 24 at 618.7 °C at 180 min, the 12th at 200 min, the 21st at 220 min and the last at 240 min, as shown in Figure 4.3b, and the bed is out at 4 h 26 min. This is the creeping reaction zone of fixed-bed theory [8]. At 50 % rate a thermal wave would cross bed 3 in 34.8 min (38 MJ/K of catalyst over 18.18 kW/K), and the reaction

heat behind the front slows it by $1 - \Delta T_{rx}/(T_{hot} - T_{in}) = 1 - 68.4 \times 3.20/(620 - 287) = 0.34$, about 102 min to cross, against the 80 to 90 min measured. Run with the four loops in Auto instead, the bypasses open to 25.2, 48.2, 79.6 and 42.0 %, every bed stays lit and the stack reads 74 ppmv at 3 h.

> **TRY IT IN THE APP** **4 · Turndown to 50 % on Fixed Bypasses**
>
> Load scenario 4 and press Run. At 20 min the rate falls to half with the four bypasses held. Watch the stack trend fall to 89 ppmv at 45 min, then climb past the 400 ppmv limit at 1 h 22 min, after bed 3 has gone out. Reload, switch the header to Auto and run again: every bed stays lit, and the stack reads 74 ppmv at 3 h.

4.4.4 Outlets Above Equilibrium and the Wrong-Way Rise

The same stored heat explains a transient that looks wrong on the diagram. A bed's outlet can sit above the equilibrium of its own temperature, by at most 2.60 points (bed 4 in the shipped challenge at 355.7 min) and 1.12 points (bed 4 in case 3). In every such instant the outlet cell is the bed's hottest, the conversion peaked in a cooler cell upstream, and the last cells run backward, five of them in the challenge, because gas converted in cooler cells meets catalyst still hot from before. Six and forty Newton iterations give the same outlet to 1×10^{-8} points, so the excess is physics of the model and not a solver artifact. Lined out, every outlet lies under its curve. In case 3 bed 1's inlet setpoint drops from 420 to 385 °C at 5 min, the cold gas cools the catalyst at the front first, the reaction zone moves down the bed into catalyst that is still hot, and the outlet rises to 653.4 °C at 15.2 min after the change before the bed goes out 31.8 min after it.

Pause. Try Exercise 4.2 before reading on.

4.4.5 How Many Cells

The cell count does not move the floor by more than 1.3 K from 12 to 48 cells, but it does set the speed of a front and the last ppm. At 48 cells bed 1 goes out 21.6 min after case 3's change instead of 31.8 min, with a peak of 677.8 °C instead of 653.4, case 4's bed 1 goes out at 1 h 14 min instead of 1 h 53 min, and the design stack is 198.6 ppmv instead of 214.5 ppmv (conversion 99.849 against 99.837 %). Twelve cells lose the wrong-way rise altogether. The lessons hold at 24 and 48 cells, and 24 were kept because 48 nearly double the cost, 14.66 against 7.76 ms per simulated minute headless in Node, on which the fastest speed of 60 min/s depends. Front times and the stack's last ppm are therefore this model's numbers.

4.5 Seven Loops and a Predictive Layer

The instrument code builds a single packet of readings for the controllers, and the application's tests whitelist its keys. Each loop carries a separate Auto/Manual switch on its card, and the header's Manual and Auto is the master of the four bed loops alone, so the header's Manual followed by its Auto throws all four while the SO_2, strength and acid temperature loops keep their own switches. Per-loop switches were chosen because the challenge ships with fixed bypasses that the suggested settings must undo, and because case 3 moves one loop while the others hold. Every controller not acting tracks what acts, so changes of mode and structure are bumpless (Section 1.6.2).

4.5.1 The Shared PI Law

The seven loops share the framework's velocity-form controller of Section 1.6.2, Equations (1.14) to (1.17), with the derivative term switched off in every loop here. Each loop executes every 6 s except the strength trim, only the emitted output is limited while the running sum runs free, and the integral is corrected toward the limited output with a tracking time equal to τ_I. Setting τ_I to the top of its slider turns integral action off. The integral reaches the output one execution after the error. The pairings and defaults are listed in Table 4.3. Bed 4's loop acts in the opposite sense to the other bed loops, direct acting in the convention of Section 1.6.2, because its bypass is on the reheater's cold

Table 4.3 Loops, Pairings and Default Tunings

Loop	PV → MV	K_c	τ_I	Output
TIC 1	$T_{in,1} \to v_1$	0.2 %/K	1 min	0–100 %
TIC 2	$T_{in,2} \to v_2$	0.5 %/K	1 min	0–100 %
TIC 3	$T_{in,3} \to v_3$	1.0 %/K	1 min	0–100 %
TIC 4	$T_{in,4} \to v_4$, direct	0.3 %/K	1 min	0–100 %
AIC	$y_{SO_2} \to R$, direct	0.4 per %	2 min	7–14 mol/mol
AIC	$w \to \delta$ (trim), direct	0.05 per wt %	15 min	±0.08 kg/kg
TIC	$T_a \to \varphi$, direct	8 %/K	4 min	0–100 %

side, and the production rate setpoint ramps at 2 % of design a minute, a teaching value in place of a step.

4.5.2 Air by Ratio, Water by Ratio and a Trim

The air is the ratio R times the metered sulfur, and the SO_2 loop moves R on the analyzer, so a sulfur richer than its meter shows first as a stronger gas. Both feeds follow the ratio station with a trim of Equation (1.10), and the Claus unit of Volume 11, Chapter 13 sets its air the same way, on a stoichiometric feedforward with a trim from a tail gas analyzer. The dilution water is a feedforward on the SO_3 the meters imply, as shown in Equation (4.9).

$$\begin{aligned} F_w &= \big(R_w(w_{SP}) + \delta\big)\, F_{S,m} X_m M_{SO_3}, \qquad R_w = \frac{1-\sigma_{SP}}{\sigma_{SP}} \\ X_m &= \frac{y_{in} - y_{out}}{y_{in}(1 - 1.5 y_{out})} \end{aligned} \tag{4.9}$$

where $F_{S,m}$ is the sulfur meter, y_{in} and y_{out} are the SO_2 analyzer and the CEMS as mole fractions, and δ is the trim. With Strength control on Ratio only, $\delta = 0$ and nothing looks at the acid. On Ratio + analyzer, the trim of Table 4.3 acts once per analyzer report with the analyzer's own 5 min period as its step and holds between reports. The ratio uses the conversion the analyzers report, so a change in conversion does not move the strength.

4.5.3 The MPC on the Inlet Setpoints

With Inlet setpoints from set to MPC, a receding-horizon controller moves the four inlet setpoints every 10 min for the least stack SO_2, and the four TICs hold what it sets. It is the framework's predictive option of Section 1.6.3 with an economic cost in place of a tracking error: the stack, as a steady copy of the beds predicts it. Its model is a coarser copy of the beds, 12 cells per bed with fresh catalyst, lined out at the inlets around the present setpoints u_0 and fed the gas the analyzers report (air meter times SO_2 analyzer). By central differences of ±2 K it fits $\text{ppm}(u_0 + \delta) \approx p_0 + \sum_b g_b \delta_b + \frac{1}{2}\sum_b H_b \delta_b^2$, and it plans over one hour as shown in Equation (4.10).

$$\begin{aligned} & x_{b,k+1} = a_b x_{b,k} + (1-a_b) u_{b,k}, \quad a_b = \mathrm{e}^{-T_s/\tau_b} \\ & \min \ \textstyle\sum_{k=1}^{6} \sum_b \left[\frac{1}{2} H_b (x_{b,k} - x_b^*)^2 \text{ or } g_b x_{b,k} \right] \\ & \qquad + w_{\Delta u} \textstyle\sum \Delta u^2 \\ & \text{s.t. } 395 + \Delta T_{fl} \le u_b \le 470\,^\circ\text{C}, \qquad |\Delta u_b| \le 3\,\text{K} \end{aligned} \tag{4.10}$$

where $T_s = 10\,\text{min}$, $\tau_b = C_{bed,b}/\dot{F}C_p$, a bed with curvature $H_b > 0.02\,\text{ppm}/\text{K}^2$ tracks its local optimum $x_b^* = u_{0,b} - g_b/H_b$, a bed without it, bed 1 on its equilibrium curve, gets its gradient as a linear cost, $w_{\Delta u} = 1$ per K^2, the margin ΔT_{fl} is 15 K, and the moves are blocked one, one and four steps. Goldfarb and Idnani's dual active-set algorithm [16] in the framework's shared module solves each program, and only the first move is implemented, as in industrial MPC [17]. If a plan is not optimal or not finite, the setpoints stay where they are and the loops keep holding them. Nine steady solves of the

Table 4.4 The Nine Cases

#	Case and events	Teaching point
1	Manual, learner opens bypass 2 from 29.6 to 39.5 %	reading the diagram
2	Auto, rate to 80 % at 15 min	the inlet loops
3	Auto, learner sets bed 1 to 385 then 420 °C	the ignition floor
4	Manual, rate to 50 % at 20 min	turndown, fronts
5	Auto, learner sets SO_2 to 9 %	gas strength
6	Ratio only, sulfur +5 % at 20 min	ratio and analyzer
7	Auto, activity 60 % at 15 min	aging, infeasibility
8	Warm beds 430/430/400/400 °C, rate 30 to 100 %	start-up emissions
9	Challenge, 8 h, bed loops Man, Ratio only	the whole plant

copy make a decision. Over the eight-hour challenge it made 48 decisions with no failure. The model knows nothing of an aged catalyst or a richer sulfur except through the analyzers, and its masses, heat capacity, rate law, pressures and interpass slip are the declared defaults, so a change to the plant's parameters is a mismatch it does not see. The supervisory layer of Volume 9, Chapter 8 also chooses the setpoints that PI loops hold, against an optimum that sits on a moving constraint.

4.5.4 Plant, Identified and Controller Models

The simulated plant is the 24-cell model of Section 4.3, an identified model is whatever a learner fits from a run, such as a bypass's inlet gain, and the controllers' models are the PI gains, the water ratio and the MPC's 12-cell fresh-catalyst copy on the declared parameters, none of which sees the activity, the sulfur's purity, the true acid or a change to the plant's parameters. The status strip and the verdict read the truth and act on nothing.

4.6 Nine Cases on the Running Plant

The cases are listed in Table 4.4 and their outcomes in Table 4.5. Every number was measured with the application's engine run headless at its 2 s step and default seed, each case loaded as it ships, with any setting a row names entered at the time it names. An independent measuring script, run again for this chapter, reproduced its earlier output line for line, and every verdict is unchanged for seeds 0, 1, 2 and 3 and with the step halved. The exported file logs each reading beside its true value, in columns marked as truth that no controller reads (Section 1.6.4).

> **DID YOU KNOW? A Weaker Gas Gives a Cleaner Stack**
>
> From the simulator: burning the same sulfur with more air, to 9 instead of 11 percent sulfur dioxide, raises the conversion from 99.837 to 99.867 % and lowers the stack from 215 to 138 ppmv. The price is 22.2 % more air and a burner at 815 instead of 968 °C (Table 4.5, case 5).

4.6.1 Inlet Loops Through a Rate Change

Opening exchanger 2's bypass by ten points in case 1 moves bed 2's line 12.4 K to the right, and because the line then meets the curve lower, the conversion after bed 2 falls from 91.05 to 89.85 %, while bed 3, whose bypass is held, sees a 5.8 K warmer inlet and the stack rises from 214 to 218 ppmv. In case 2 the rate cut opens every bypass, 15.1 to 20.4, 29.6 to 40.0, 42.5 to 66.0 and, through bed 4's direct-acting loop, 30.0 to 36.7 %, and less gas per kilogram of catalyst takes the stack from 214 to 133 ppmv.

4.6.2 The Gas, the Acid and an Aged Catalyst

Lowering the SO_2 setpoint from 11 to 9 % in case 5 takes 22.2 % more air, cools the burner from 968 to 815 °C, shortens the temperature rise to 2.650 K a point, and raises the conversion from 99.837 to 99.867 % while the stack falls from 215 to 138 ppmv. In case 6 a sulfur cargo 5 % richer than its

Table 4.5 Case Outcomes Measured on the Engine

Case and condition	Result
1, bypass 2 at 1 min	at 46 min bed 2 in 440.0 → 452.4, out 521.0 → 529.4 °C; after bed 2 91.05 → 89.85 %; bed 3 in +5.8 K; stack 214 → 218 ppmv
2, rate 80 %	inlet error at most 2.77 K, within 1.5 K 11.7 min after; bypasses 20.4/40.0/66.0/36.7 %; stack 214 → 133 ppmv
3, bed 1 at 385 °C	outlet 653.4 °C 15.2 min after; BED 1 EXTINCT 31.8 min after; bed 2 out at 74.6 min; 7242 ppmv at 125 min
3, back to 420 °C	relit 3.2 min after; stack under 220 ppmv 56.5 min after
4, Manual	bed 3 out 1 h 9 min, CEMS > 400 at 1 h 22 min, bed 1 out 1 h 53 min; 2128 ppmv at 3 h
4, Auto	every bed lit, 74 ppmv at 3 h
5, 9 % SO_2	conversion 99.837 → 99.867 %; stack 215 → 138 ppmv; burner 968 → 815 °C; air +22.2 %
6, Ratio only	analyzer past 98.7 % 21 min after; true 99.381 % at 4 h; stack 215 → 348 ppmv
6, trim at 41 min	analyzer back under 98.7 % 30 min after
7, nothing done	762 ppmv at 60 min
7, bed 4 at 460 °C	under 400 ppmv 23.4 min after; 388 ppmv at 3 h (342 with bed 3 at 453 °C)
8, as shipped	CEMS peak 3948 ppmv at 18.3 min; 44.5 min over 400
8, bed 4 at 460 °C	2288 ppmv at $t = 0$, then at most 1817; 37.1 min over 400

meter arrives at 20 min with the water on the ratio alone. The analyzer reads above 98.7 % 21 min later and the true strength reaches 99.381 % at 4 h. The stack rises too, from 215 to 348 ppmv of SO_2, because off-strength acid lets the interpass absorber pass 3.745 % of the SO_3 instead of 0.100 %, which lowers bed 4's conversion of its own feed from 95.62 to 93.10 %, and the stack's SO_3 climbs from 2.4 to 216.5 ppmv. Switched to Ratio + analyzer at 41 min, the trim brings the reading back inside 98.7 % 30 min later.

> **TRY IT IN THE APP** **6 · Acid Strength: The Ratio and the Analyzer**
>
> Load scenario 6 and press Run on the Acid view. At 20 min a sulfur 5 % richer than its meter arrives with the dilution water on the ratio alone, and the analyzer reads above 98.7 % 21 min later. Set Strength control on the AIC · acid strength card to Ratio + analyzer. Switched at 41 min, the trim brings the reading back inside 98.7 % 30 min later.

Case 7 ages every bed to 60 % activity at 15 min, and the stack reaches 762 ppmv by 60 min. At 3 h bed 2 stops 2.0 points short of its curve and bed 4 converts 89.37 of its own feed's 97.67 %. Bed 4 at 460 °C brings the stack under the limit 23.4 min later and to 388 ppmv at 3 h, and bed 3 at 453 °C as well gives 342 ppmv. Below some activity no inlet answers. A search over inlets from 400 to 480 °C on the lined-out plant finds a best stack of 150.2 ppmv fresh, 333.2 ppmv at 60 % activity and 443.3 ppmv at 50 %, at 404.5, 453.5, 457.5 and 466.0 °C and 99.663 %, and the dynamic plant held five hours at those setpoints reads 443 ppmv. At half activity the 400 ppmv limit cannot be met by any inlet, which is why the case ages the catalyst to 60 % and the aging button to 50.

4.6.3 A Warm Start-Up

Case 8 starts with beds preheated to 430, 430, 400 and 400 °C and the rate ramping from 30 to 100 % from 1 min. At $t = 0$ the gas reaches beds 2 and 3 at 358.9 and 374.4 °C and the CEMS reads 2288 ppmv. As the rate rises the stack peaks at 3948 ppmv at 18.3 min, bed 3 lights at 32.4 min, and the stack is over the limit for 44.5 min in all. The lever the case offers is bed 4's inlet. With bed 4 at 460 °C the later peak falls to 1817 ppmv and the time over the limit to 37.1 min, while the reading at $t = 0$, fixed by the start, stays at 2288 ppmv. Over seeds 0 to 3 that first reading lies between 2281 and 2288 ppmv, and bed 4's setpoint moves only the later peak.

4.6.4 A Turndown Day

The challenge runs eight hours. The rate falls to 60 % at 1 h and returns at 5 h, and a sulfur 5 % richer than its meter arrives at 4 h. It is met when the average true conversion is at least 99.7 %, the true

Table 4.6 The Challenge Over 8 h at the Default Seed

Configuration	$\bar{X}$ (%)	Stack (ppmv)	Coldest (°C)	Acid (wt %)	
loops Man, Ratio only (shipped)	95.969	48 468	292.4	98.47–99.38	fail
loops Auto, Ratio + analyzer (sugg.)	99.878	260	417.2	98.45–98.63	pass
MPC, Ratio + analyzer	99.904	215	409.4	98.45–98.63	pass
loops Auto, Ratio only	99.852	350	417.2	98.47–99.38	fail
loops Man, Ratio + analyzer	96.042	48 481	292.4	98.45–98.63	fail

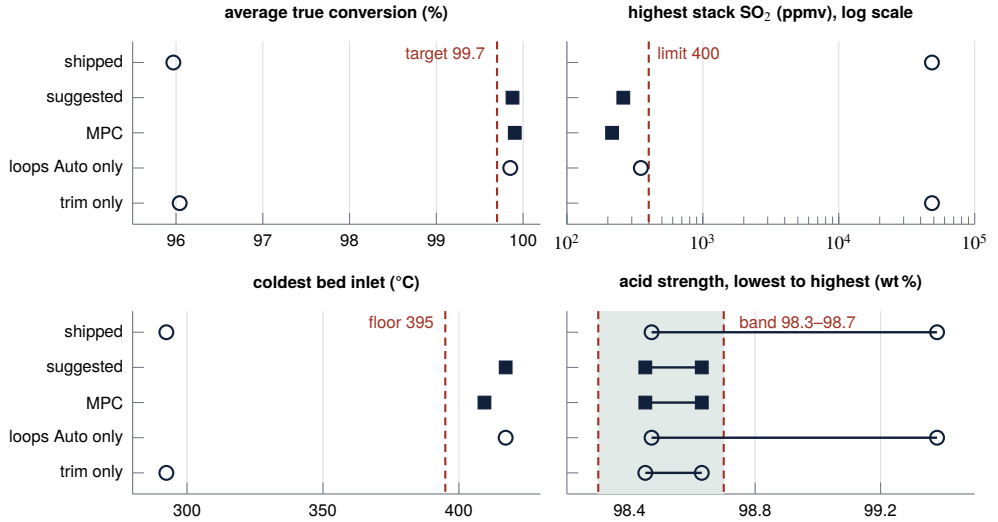


Figure 4.4 Table 4.6 as dots, digit for digit: the average true conversion against its target, the highest stack reading on a logarithmic axis against the limit, the coldest bed inlet against the floor, and the range of the acid strength against its band. The rows are the table's: shipped (loops Man, Ratio only), suggested (loops Auto, Ratio + analyzer), MPC (Ratio + analyzer), loops Auto only (Ratio only) and trim only (loops Man, Ratio + analyzer). Filled squares are the configurations that pass, open circles those that fail. Notice that each half of the fix fails on its own: the loops alone miss only the acid band, and the trim alone loses the converter.

stack SO_2 never exceeds 400 ppmv, no bed inlet falls below 395 °C and the acid stays within 98.3 to 98.7 wt%, scored every step against the simulator's truth. It ships with the four bed loops in Manual and the water on the ratio alone. The configurations are compared in Table 4.6, and Figure 4.4 draws its four measured columns against the target of each.

As shipped, the 60 % rate cools bed 1's inlet to 375.9 °C by 1 h 40 min, bed 1 goes out at 2 h 17 min, the stack passes the limit at 2 h 21 min and the beds go out one after another, while the richer sulfur takes the acid to 99.38 %. Each half of the fix fails alone. The loops without the trim pass on conversion, stack and inlets but not on the acid, and the trim without the loops keeps the acid but loses the converter. With both, the inlets never fall below 417.2 °C, the stack peaks at 260 ppmv and the conversion averages 99.878 %. The MPC with the same two changes averages 99.904 % with a stack of at most 215 ppmv, taking bed 1's inlet down to 409.4 °C, within a kelvin of its lower bound of 410 °C. Over four further seeds and a halved step the suggested settings and the MPC always pass and the shipped settings always fail. The turndown case at 3 h is shown in Figure 4.5.

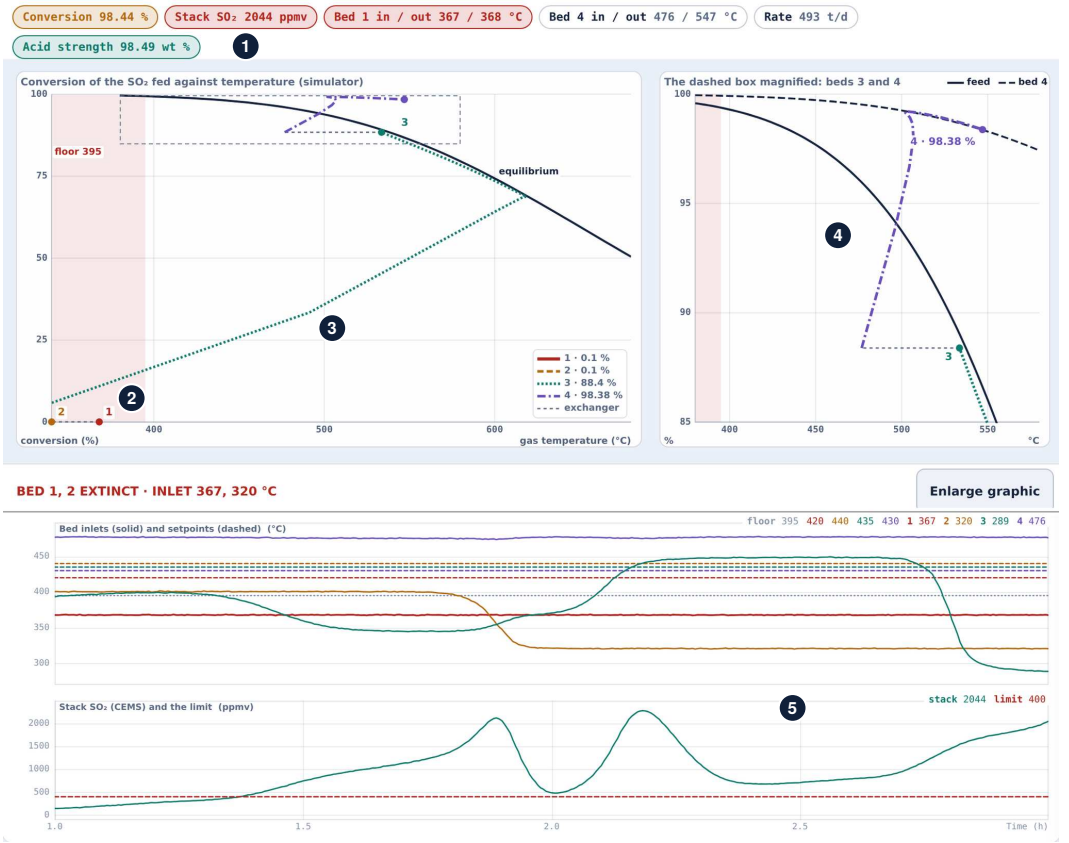


Figure 4.5 Case 4 at $t = 180$ min on the X–T diagram view, in Manual with the four bypasses held, more than two hours after the rate fell to 50 %, cropped to the plant view above the bed inlet and stack trends. Numbered callouts mark (1) the stack badge, (2) beds 1 and 2 on the floor, (3) bed 3's bent line, (4) bed 4 in the magnifier and (5) the CEMS trend above its limit. The badges read a conversion of 98.44 % from the analyzers, a stack of 2044 ppmv on the CEMS against 2128 ppmv true, bed 1 in and out at 367 and 368 °C, bed 4 at 476 and 547 °C, 493 t/d and acid at 98.49 wt%, and the status strip BED 1, 2 EXTINCT, INLET 367, 320 °C. On the diagram beds 1 and 2 lie flat on the shaded floor at 0.1 %, and bed 3 climbs a bent line from a 289 °C inlet to 88.4 % on its stored heat, while the magnifier, which has followed the plant down to bed 4's start, shows bed 4 reaching 98.38 %. The trends show bed 1's inlet flat at 367 °C below the 395 °C floor line, bed 3's inlet rising while bed 2 burned and falling once bed 2 went out, and the CEMS above its 400 ppmv limit since 1 h 22 min.

4.7 Technology in Practice

What Measures It

Figure 4.6 draws the loops of Section 4.5 with their devices. The variable the chapter turns on, each bed's inlet temperature, is a gas temperature read by an element in a well, and a few kelvin of it decide whether a bed stays lit. The gas itself is read twice, by the analyzer on the converter feed and by the stack monitor, and the acid by a strength analyzer that reports a sample every 5 min. No case of Table 4.4 breaks a thermocouple, so the model's trends show the gas, never a failed element. Figure 4.7 shows the element in its well.

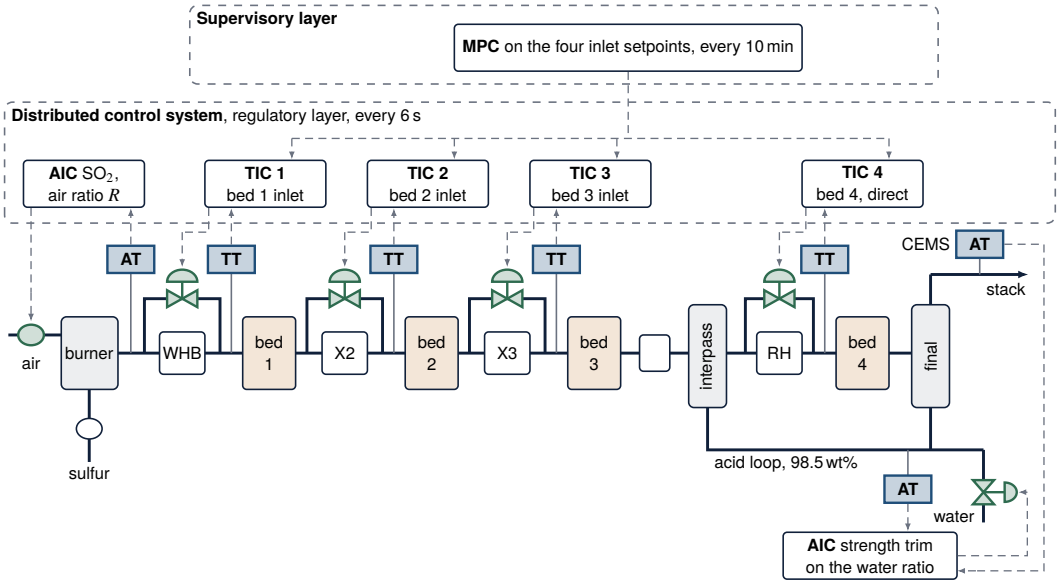


Figure 4.6 The loops of the contact plant with their hardware. Lettered boxes are sensing devices: a temperature element (TT) at each bed inlet, the SO_2 analyzer (AT) on the converter feed, the stack monitor (CEMS) and the strength analyzer (AT) on the acid loop. Valve symbols and the blower are final elements, dashed arrows are signals, and WHB, X2, X3 and RH are the waste-heat boiler, exchangers 2 and 3 and the reheater, and the small box after bed 3 is the economizer. Notice that each bed has its own loop on its own bypass, that bed 4's bypass sends cold gas around the reheater, which makes its loop direct acting, and that the predictive layer writes the four setpoints the same loops hold. The sulfur meter, the water ratio's other inputs and the acid temperature loop are left out. Not to scale, and not a piping diagram.

> **TECHNOLOGY** **Sensor: A Thermocouple in a Thermowell**
>
> Two wires of dissimilar metals joined at one end produce a voltage at the other that is roughly proportional to the junction's temperature. Thermocouples are less accurate than resistance thermometers but more rugged, with wider spans, and the pair of alloys is chosen for the gas: type K, for one, is attacked by sulfur and by reducing gases. A thermowell lets the element be replaced without opening the process, at the price of a slower first-order lag, and an air gap at its bottom adds a second lag. The most common failure is an open circuit. Without burnout detection the reading then wanders wildly with electrical noise, and with it the transmitter drives the reading high or low by design [18]. The model's 0.2 min lag and 0.3 K noise stand in for the element and its well.

What Moves It

Besides the sulfur pump, which sets the rate, seven handles move the plant: four gas bypasses, the air through the blower's ratio station, the dilution water and the acid cooler's water. A 2019 study of a smelter's acid plant describes the same structure in service, heat exchangers equipped with bypass valves to regulate the temperatures throughout the plant [19]. Three bypasses here send hot gas around a cooler and warm the next bed, and the fourth sends cold gas around the reheater.

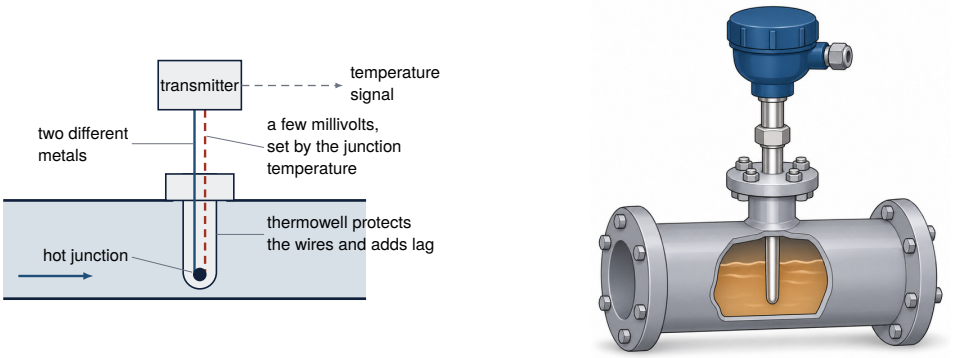


Figure 4.7 A thermocouple in a thermowell, the element behind TT 1 to TT 4. Notice the metal of the well between the gas and the junction: it is the 0.2 min lag of the model, and an air gap at the bottom of the well would add a second lag [18].

TECHNOLOGY **Final Element: A Rotary Valve on a Gas Bypass**

Large flows of air at low pressure are throttled by dampers, whose vanes turn together, as in furnace and boiler draft. A butterfly valve is a single disk turning across the pipe: edge-on it barely obstructs the flow, square to it it blocks the flow, and tight shutoff is hard to obtain unless its seat is lined with a soft material. It passes far more flow than a globe valve of the same pipe size. Installed, a valve sees less pressure drop as it opens, so its flow droops against its position, and a valve with excess friction ignores small reversals of the signal [18]. The model's bypass passes a share of the gas in proportion to its opening, none when shut, and follows its command with a 0.15 min lag.

Where the Controller Runs

A plant runs such loops in a distributed control system, in which a supervisory level oversees local controllers and sends them set points, loops are sometimes nested, and cycle times range from milliseconds to minutes [20]. The app executes its PI loops every 6 s, the strength trim once per analyzer report and the predictive layer every 10 min, all inside that range. The PI loops and the two ratio stations belong to the regulatory layer. The predictive controller is supervisory: it writes the four inlet setpoints the TICs hold, and when a plan fails the setpoints stay where they are.

IN PRACTICE **Two Analyzers and a Factor Three Times a Day**

A plant is judged by its conversion and its stack sulfur dioxide. A 2007 European reference document has both rest on sulfur dioxide measured at the converter inlet and after the final absorber, with the conversion determined daily and the levels monitored continuously [1]. The United States rule for new acid plants requires a continuous monitor with its span set at 1000 ppm, a conversion factor from the gas entering the converter at least three times a day, and it counts as excess emissions every three-hour period whose average exceeds the standard [21]. The chapter's feed analyzer and CEMS are those two instruments, and its challenge judges every step, a stricter test than a three-hour average.

What Is Modernizing It

Three developments bear on this converter. Cesium-promoted catalysts are active at 380 to 400 °C and can be run from 380 to 620 °C, in the first bed to lower its inlet or in the final bed at a low inlet, and at double-contact plants burning sulfur they reach 99.9 % conversion [1]. Heat recovery has made the plant an exporter of energy: up to 67 % of the waste heat of a double-contact plant burning sulfur is recovered as high-pressure steam, and a modern one can export about 6 GJ per tonne of acid [1]. And models identified from plant data now inform the temperature control: the 2019 study fitted dynamic models to industrial operating data and explored a feedforward and feedback scheme [19].

4.8 Limitations

The plant is generic, and its sizes, rates and limits serve teaching. The rate law has the published shape but its break, activation energies and inhibition are not fitted to a measured catalyst, so the floor of about 395 °C is this model's, below the 410 to 440 °C quoted for conventional catalysts and inside the 380 to 410 °C quoted for cesium-promoted ones [1]. The equilibrium constant is a two-constant fit within 0.91 % of NIST-JANAF from 350 to 700 °C, and holding $\dot{F}C_p$ and ΔH constant makes the lines exactly straight where real ones bend slightly. The gas carries no heat, so a front's speed is the catalyst's, and front times and the stack's last ppm depend on the 24 cells. The reheater's hot side is held, and the absorbers' slip law is a teaching closure that sets how strongly off-strength acid reaches the stack.

The MPC plans on a steady 12-cell copy with fresh catalyst, so after aging its model is wrong in a way only the analyzers report. The PI loops are not scheduled with the rate, and no case models a trip, a blower failure or the start-up preheat itself.

> **OPEN CHALLENGE** **A Converter Fed by a Smelter**
>
> Non-ferrous metal smelting accounts for 39 percent of sulfuric acid production, and its gas, unlike a sulfur burner's, varies in strength and flow. A 2007 European reference document puts 99.8 percent conversion within reach of four beds on gas of low variability and 99.7 percent on smelter gas, and tabulates a larger loss the more the sulfur dioxide varies in an hour [1]. A 2019 study of a smelter's acid plant found its feed typically between 5 and 15 percent sulfur dioxide and noted that most models assume a burner's steady feed, so continued research is required [19]. Progress would be loops that keep every bed lit through such swings, proven on plant data.

4.9 Conclusion

A sulfuric acid contact plant is a train of adiabatic beds on an exothermic equilibrium, and this simulator draws its beds live on the conversion–temperature diagram from balances that close to 2×10^{-15}. Each point of conversion heats the gas 3.20 K, and four beds with an interpass absorber reach 99.837 % where the same four beds without the absorber would leave 97.910 %. A floor near 395 °C emerges from a two-regime rate law and the heat balance with no clamp, while the 420 °C break of the rate law is not the floor. A turndown on fixed bypasses puts the beds out one by one, leaving bed 3 converting 88.33 points from a 289 °C inlet on stored heat. Four inlet loops and an analyzer trim together pass an eight-hour turndown day with 99.878 %, and an MPC on the inlet setpoints reaches 99.904 %, while at half activity no inlet meets the limit. A fuller model would fit the rate law to a measured catalyst, add a cesium-promoted bed 4 and couple the reheater to bed 1. The simulator shows that the best inlet temperature on an exothermic equilibrium is the coolest one the catalyst can still light.

KEY POINTS

- A contact plant converts sulfur dioxide in several catalyst beds with cooling between them, because each bed climbs only until it meets equilibrium.
- The interpass absorber starts bed 4 on a new curve: 99.837 % with it, 97.910 % without.
- The coolest inlet that still lights the catalyst converts the most, and the floor near 395 °C comes from the heat balance, not from the 420 °C break of the rate law.
- On fixed bypasses a turndown puts the beds out one by one. Inlet loops and the strength trim pass the turndown day at 99.878 %, and the MPC reaches 99.904 %.

Where else this applies. Chapter 2 climbs the same adiabatic lines with quench gas between its beds, and Volume 7, Chapter 2 ignites and goes out on the same heat balance.

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4.10 Exercises

4.1 Concept check · 2 min

In case 1 the Exchanger 2 bypass is opened from 29.6 to 39.5 % with the other bypasses held, and bed 2's inlet rises by 12.4 K. Bed 2 was already at its equilibrium curve. What happens to the conversion after bed 2?

(a) It rises, because a hotter catalyst reacts faster and climbs further along its line

(b) It falls, because a line that starts further right meets the falling curve lower

(c) It stays the same, because the bypass does not change the slope of bed 2's line

(d) It rises, because bed 3's warmer inlet is credited to the conversion after bed 2

4.2 Concept check · 1 min

In case 3 the bed 1 inlet setpoint is lowered from 420 to 385 °C, below the ignition floor. What does bed 1's outlet temperature do first?

(a) It falls at once by about the 35 K of the inlet change

(b) It holds steady until the bed goes out, and then it falls

(c) It rises for about a quarter of an hour, and then the bed goes out

(d) It falls at first, and then the inlet loop brings it back

4.3 Concept check · 2 min

With the same four inlets the plant converts 99.837 % with the interpass absorber and 97.910 % with its SO_3 left in the gas. Why does removing SO_3 after bed 3 help bed 4?

(a) The absorber cools the gas, so bed 4 runs further below its floor and converts more

(b) The absorber takes out part of the SO_2, so less is left for bed 4 to convert

(c) The absorber puts oxygen back into the gas, which bed 4's rate law needs

(d) Bed 4 starts on a new equilibrium curve, because less SO_3 slows the back reaction

4.4 Theory and calculation · 6 min

The converter is fed 118.363 mol/s of SO_2. The heat of reaction is −98.442 kJ/mol, and the heat-capacity flow is held at 36.389 kW/K along beds 1 to 3 and at 28.545 kW/K for bed 4 after the interpass absorber. Conversion X is counted on the SO_2 fed to the converter.

(a) Find the temperature rise of beds 1 to 3 per unit conversion and per point of conversion. *Checkpoint:* 320.20 K and 3.202 K.

(b) Bed 1 enters at 420.0 °C with no conversion and stops on its curve at 65.77 %. Find its outlet temperature. *Checkpoint:* 630.6 °C.

(c) Bed 4 enters at 430.0 °C with $X = 96.28$ % and leaves at 99.837 %. Find its rise per point and its outlet temperature, and say why its line is flatter on the diagram. *Checkpoint:* 4.082 K a point and 444.5 °C.

4.5 Theory and calculation · 6 min

Use the rate constant of Equation (4.2) with $k_{500} = 0.5\,\mathrm{mol/(s\,kg\,bar^{1.5})}$, $E_{hi} = 80\,\mathrm{kJ/mol}$, $E_{lo} = 600\,\mathrm{kJ/mol}$, $T_{500} = 773.15\,\mathrm{K}$, the break at 420 °C and $R = 8.314\,\mathrm{J/(mol\,K)}$.

(a) Find k_{hi} and k at the break. *Checkpoint:* 0.1189 and 0.0594.

(b) Find k at 400 °C. *Checkpoint:* 5.05×10^{-3}.

(c) Find k at 395 °C as a share of its value at 420 °C, and the same share for a single Arrhenius term at 80 kJ/mol. *Checkpoint:* 3.93 % against 59.5 %.

4.6 Theory and calculation · 7 min

A thermal front in a bed moves at the speed at which the gas can change the temperature of the catalyst. The catalyst holds 1000 J/(kg K), and beds 1 to 4 hold 22, 28, 38 and 70 t.

(a) Find the time constant $C_{bed}/\dot{F}C_p$ of bed 1 at an $\dot{F}C_p$ of 36.39 kW/K, and of bed 4 at 28.545 kW/K. *Checkpoint:* 10.1 min and 40.9 min.

(b) In case 4 the rate is 50 % and $\dot{F}C_p$ is 18.18 kW/K. Find the time a thermal wave takes to cross bed 3. *Checkpoint:* 34.8 min.

(c) Behind the front bed 3 converts 68.4 points at 3.20 K a point, from a 287 °C inlet to a 620 °C hot spot. The reaction slows the front by the factor $1 - \Delta T_{rx}/(T_{hot} - T_{in})$. Find the factor and the crossing time, and compare it with the 80 to 90 min measured. *Checkpoint:* 0.34 and about 102 min.

4.7 App challenge · 8 min

Load scenario 2, The inlet temperature loops, and change no setting. The production rate setpoint goes to 80 % at 15 min. Use the default seed and run at 20 min/s.

(a) Run to 135 min and read the four bypass openings on the TIC cards. Accept 0.3 % on each. *Checkpoint:* 20.4, 40.0, 66.0 and 36.7 %.

(b) Export the CSV file. Its time column is in hours. Read the true stack SO_2, column `truth_stack_so2_ppm`, in the rows at 0 and 2.25 h. Accept 1 ppmv. *Checkpoint:* 214.5 and 132.8 ppmv.

(c) Raise the Bed 4 inlet setpoint on TIC 4 to 440 °C and run 40 min more. Say which way the reheater bypass moves and read where it settles, within 0.4 %. *Checkpoint:* It closes, to about 33.7 %.

Explain why all four bypasses opened for the rate cut.

4.8 App challenge · 8 min

Load scenario 7, An aged catalyst: higher inlets. Every bed falls to 60 % activity at 15 min. Use the default seed, run each case to 180 min at 20 min/s, export the CSV file (time column in hours), and read the true stack SO_2, column `truth_stack_so2_ppm`. Accept 2 ppmv.

(a) Run the scenario as shipped and read the rows at 1 and 3 h. *Checkpoint:* 762 and 766 ppmv.

(b) Press the reload button, set the Bed 4 inlet setpoint on TIC 4 to 460 °C before Run, and read the row at 3 h. *Checkpoint:* 388 ppmv.

(c) Also set the Bed 3 inlet setpoint to 453 °C before Run, and read the row at 3 h. *Checkpoint:* 342 ppmv.

Explain why bed 4 is the inlet to raise first.

4.9 App challenge · 9 min

Load scenario 9, Challenge, a turndown day. The rate goes to 60 % at 1 h, a sulfur 5 % richer than its meter arrives at 4 h, and the rate returns at 5 h. Use the default seed and run at 60 min/s until the case

pauses at 8 h. For each run read the So far tile: average conversion, highest stack SO_2, coldest bed inlet and the acid strength range. Accept one unit in the last digit the tile shows.

(a) Run it as shipped. *Checkpoint:* 95.97 %, 48 468 ppm, 292 °C, 98.47 to 99.38 %.

(b) Press the reload button. Before Run, put the four bed loops in Auto (the header's Manual and then Auto throws all four), keep Strength control on Ratio only, and run again. *Checkpoint:* 99.85 %, 350 ppm, 417 °C, 98.47 to 99.38 %.

(c) Press the reload button, put the bed loops in Auto and set Strength control to Ratio + analyzer before Run, and run again. *Checkpoint:* 99.88 %, 260 ppm, 417 °C, 98.45 to 98.63 %.

Say which limit each run breaks and which loop protects it.

4.10 Application area · 4 min

The United States standard limits a sulfuric acid plant to 2 kg of SO_2 per metric ton of acid. A stack reading C in ppmv converts to that unit by multiplying it by $CF = k(1 - 0.015r)/(r - s)$, with $k = 0.0653$ and r and s the SO_2 percentages entering the converter and in the stack.

(a) Find the reading in ppmv that equals the limit for an 11 % gas. *Checkpoint:* 402.0 ppmv.

(b) Find the same for the 9 % gas of case 5, and the emission of the design point, 214.5 ppmv at 11 %, in kilograms per ton. *Checkpoint:* 317.5 ppmv and 1.07 kg/t.

4.11 Application area · 4 min

Industrial vanadium catalysts are quoted with a lower operating range of 410 to 440 °C for conventional and 380 to 410 °C for cesium-promoted grades, and an upper range of 600 to 650 °C, above which activity can be lost for good.

(a) Compare the design inlets and bed 1's design outlet with these ranges.

(b) In case 3 bed 1's outlet peaks at 653.4 °C after its inlet is cooled, and at 677.8 °C in the 48-cell model. What does this mean for an operator who tests the floor on a real converter?

(c) Where should a real plant take its floor, and what does the MPC's margin of 15 K above 395 °C give against the conventional range?

4.12 Review the agent · 5 min

After case 7 ages the catalyst to 60 % activity, an AI assistant advises: "On an exothermic equilibrium the coolest inlet that still lights the catalyst converts the most. Lower the four inlet setpoints to 410, 430, 425 and 420 °C, all above the 395 °C floor, and the extra conversion will bring the stack back under 400 ppmv." Find the flaw and say how you would check it.