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CHAPTER 3

A One-Sided Hydrogen Window and a Selectivity Runaway in an Acetylene Converter

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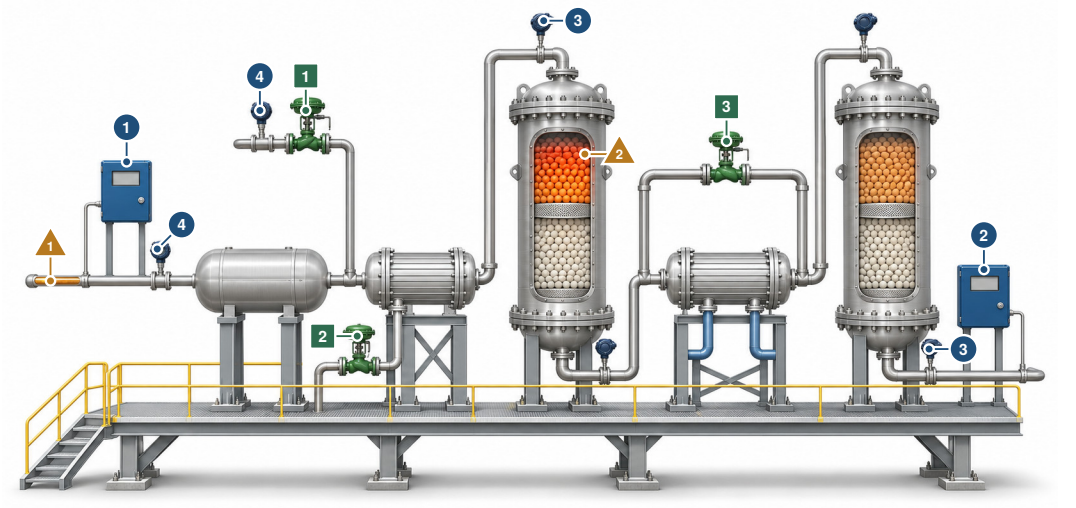
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CHAPTER 3

A One-Sided Hydrogen Window and a Selectivity Runaway in an Acetylene Converter



The controller moves 1 hydrogen valve, set in ratio to the acetylene fed
2 steam to the heater, which sets the first bed's inlet temperature
3 hot-gas bypass around the intercooler, which sets the second bed's inlet temperature

The controller reads 1 chromatograph on the feed, ahead of the drum
2 chromatograph on the product, which reports the acetylene left minutes late
3 temperature sensors at each bed's inlet and outlet 4 feed and hydrogen flowmeters

What disturbs it 1 acetylene and carbon monoxide in the feed, which the furnaces change
2 green oil that slowly fouls the catalyst, first at the front of the first bed ▲ a cut in the feed flow

Notice that the feed chromatograph samples ahead of the drum, so the hydrogen can follow a feed change before it reaches the beds, while the acetylene left is known only from the chromatograph at the far end. Illustration, not to scale.

IN PLAIN TERMS **Just Enough Hydrogen, and No More**

The main idea. Gas from a cracking furnace holds a trace of acetylene, which must go before the main gas, ethylene, is made into plastic. A converter adds hydrogen over beds of small pellets, which help it turn the trace into more of the main gas.

The challenge. Too little hydrogen leaves some of the trace and spoils all the product. Too much turns good ethylene into a gas worth less, and the heat it gives off can make a bed run hot before the thermometers know.

Why it matters. The best setting is the least hydrogen that clears the trace, and it moves when the feed changes.

THREE WAYS TO READ THIS CHAPTER

Explore	12 min	This page, the History boxes in Section 3.2, the Did you know? boxes in Sections 3.1 and 3.5, the Try it boxes in Section 3.5, and Key points in Section 3.8. No equations.
Study	45 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
Practice	15 min	This page, Section 3.5 with Figure 3.4, Section 3.6, and Section 3.7 with its two Open challenge boxes.

The control question Too little hydrogen puts the whole ethylene product off grade, and too much turns ethylene into ethane and can light off the bed. Where in this one-sided window should the hydrogen sit, and what keeps it there?

Learning objectives

- Price both failures of the one-sided hydrogen window in tonnes of ethylene a day.
- Compute the heats, the adiabatic rises and the temperature sensitivity of the two rates.
- Explain why a bed's rise falls while its selectivity collapses, and why an override on it cannot stop a light-off.
- Compare a fixed ratio, feedforwards with a trim and a predictive controller on a graded day.
- Judge what an inlet temperature schedule buys and costs over a catalyst run.

Prerequisites Sections 1.4.3 (selectivity and light-off), 1.4.6 (inferred quality), 1.4.8 (limits and guards), 1.6.2 and 1.6.4. Section 1.6.3 only for the predictive controller.

The app https://apmonitor.com/apps/acetylene-hydrogenation/

See also Volume 7, Chapter 2 for an ignition boundary. Volume 3, Chapter 6 and Volume 3, Chapter 4 for a ratio held by an analyzer trim. Volume 4, Chapter 2 for a protective override.

3.1 Introduction

At 1.3 mol of hydrogen per mol of acetylene the converter simulated here leaves 14.7 ppm of acetylene in its product, and at 1.9 it leaves 0.0002 ppm. The stream is 1400 mol/s (5040 kmol/h) of C_2 gas carrying 1.0 % acetylene, 79 % ethylene and 20 % ethane, and the same 0.6 mol/mol that clears five decades of acetylene raises the ethylene converted to ethane from 0.138 to 0.472 % of the ethylene fed. At the design ratio of 1.5 (75.6 kmol/h of hydrogen) the lined-out outlet holds 0.31 ppm and the loss is 0.200 %, which is 5.4 t of the 2680 t of ethylene the stream carries each day. Below a ratio of 1.43 the product fails the 1 ppm limit of this model and all of it is off grade.

The problem is old and general. Acetylene must be taken from cracked gas to a few ppm before ethylene can be polymerized, palladium catalysts do it selectively, a little carbon monoxide is added to hold the selectivity, and the adiabatic packed beds that carry the reaction are known for thermal runaway in industrial practice [1]. The catalytic literature has two reviews of its own [2, 3]. The runaway belongs to a class wider than this reactor, the parametric sensitivity of exothermic tubular reactors [4], and in particular of reactors carrying consecutive reactions in which the desired product is the intermediate [5]. The control problem has a familiar shape too. A reagent is dosed in ratio to a measured flow, a feedforward answers an upstream disturbance, a slow analyzer trims the dose, and a selector cuts it when a constraint is reached [6]. The shape recurs wherever a reagent is dosed to a parts-per-million specification against a costly side reaction. A water plant that doses coagulant from a raw-water turbidimeter and demotes its slow settled-water measurement to a ratio trim has the same structure (Volume 3, Chapter 6).

> **DID YOU KNOW? A Trace That Must Go**
>
> In the typical once-through yields of an ethane cracking furnace listed in a 2017 European reference document, ethylene makes up 56 % of the products and acetylene only 0.4 % [7]. The converter of this chapter takes a C_2 stream from 1.0 % acetylene to under 1 ppm.

The simulator corrects two beliefs. The first is that a margin on hydrogen is a margin on safety. The window is one-sided, so the operating point belongs just on the clean side of the breakthrough edge, and every mole beyond it buys ethylene loss and moves the plant toward the runaway. The second is that the runaway is a temperature problem that a temperature limit catches. In case 6 of this model, hydrogen raised by hand from 75.6 to 130 kmol/h empties bed 1 of acetylene in 14 s,

the loss reaches 0.79 % by 30 s after the change while bed 1's temperature rise falls from 30.2 to 26.9 K, and the rise reaches the 70 K trip only 3.95 min after the change. The selectivity is lost before a thermocouple can tell.

However, the published work treats these parts apart. Kinetic studies measure rates on commercial catalysts [8–10], reactor models are built to simulate and optimize an industrial train [10, 11], and catalysis research looks for more selective surfaces [12, 13]. This chapter works with a two-bed tail-end converter simulated in the browser, which records every cell temperature, the true outlet and the true loss beside the two chromatographs. It measures how a hydrogen ratio, its feedforwards, an analyzer trim, a temperature override and a predictive controller keep the plant inside its window through carbon monoxide swings, feed changes, an analyzer failure and catalyst aging. The rate law (the classical one-site form, given teaching constants), the heats of reaction and the controllers are all established methods. What the converter adds is numbers, and two of them matter most: an override on the bed rise cannot see a light-off coming, and the design point is not the point of least loss. The model has 110 states on the shared packed-bed module of the app framework, with carbon and hydrogen closing to round-off and a strict line between the simulator's truth and the instruments, and its nine graded cases give credit only when the plant has answered what the learner did. The general form of the one-sided reagent window and of the light-off is in Section 1.4.3.

Section 3.2 traces the process, its catalyst and its moderator. Section 3.3 builds the model: the rate law, the heats, the beds of cells, the green oil, the feed drum, the heater and intercooler, and the instruments. Section 3.4 describes the controllers, from the hydrogen ratio and its feedforwards to the balance inference and the predictive layer. Section 3.5 runs the cases, from the window and its two costs to the light-off, the end of a catalyst run and a graded day on the furnace cycle. Section 3.6 names the hardware and the practice behind the model, Section 3.7 states what the model cannot do, and Section 3.8 sums up.

3.2 Acetylene in Ethylene: Catalyst, Moderator and Runaway

Cracked gas carries about one percent of ethyne. It reaches the converter either inside a gas that still holds 10 to 20 % hydrogen (the front-end arrangement) or as a stream of ethene and ethane alone, after the light ends have gone (the tail-end arrangement, which needs hydrogen added) [1]. The cracking furnace that makes this stream is the subject of Chapter 2. In either case the ethyne has to fall below about 5 ppm while a larger loss of ethene is economically intolerable [1]. Supported palladium met these demands, on low-area alumina with only 0.01 to 0.1 % of the metal by weight and often as an egg-shell layer [1], and industrial catalysts are commonly modified with silver [13].

> ⧖ HISTORY **A Picture of Palladium Revised, 1993 to 2008**
>
> The first explanation of palladium's selectivity was thermodynamic. Ethyne adsorbs on the metal much more strongly than ethene, so the surface stays covered with ethyne until it is nearly gone. Carbon monoxide, which also adsorbs more strongly than ethene, was thought to help in the same way. A review of 1993 called this classical view an over-simplification. Ethene is hydrogenated even at high ethyne concentrations, a direct route from ethyne to ethane exists, at least two kinds of active site were by then generally assumed, and the effect of carbon monoxide was put down to competition with hydrogen rather than with ethene [1]. In 2008, measurements made during the reaction traced the selective state to carbon from broken-up feed molecules held just under the palladium surface, with unselective total hydrogenation on the hydrogen-saturated β hydride [12].

The classical picture of the selectivity, told in the History box above, is the one-site Langmuir–Hinshelwood law this simulator uses. The changes the catalyst undergoes in use, its steady-state kinetics and the effects of carbon monoxide and promoters have been reviewed at length [2, 3]. Ethyne also oligomerizes on the catalyst to a heavy liquid called green oil, which is a serious problem in practice [1].

Table 3.1 Variables, Roles and Design Values (Case 2, Lined Out)

Variable	Role	Design	Range
A_{out}	CV, outlet acetylene (analyzer)	0.31 ppm	SP 0.1–2
R	MV of the ratio logic, mol/mol	1.50	0.8–2.5
F_{H_2}	MV, hydrogen (kmol/h)	75.6	0–201.6
$T_{in,1}$, Q	CV, MV: bed 1 inlet, steam	41.0 °C, 35.7 %	SP 25–85
$T_{in,2}$, v_2	CV, MV: bed 2 inlet, bypass	58.0 °C, 69.5 %	SP 35–90
ΔT_1, ΔT_2	constraint, bed rises	30.2, 9.8 K	override 55
y_A	DV, feed acetylene	1.00 mol%	0.3–1.8
p_{CO}	DV, carbon monoxide	2.0 ppm	0–10
—	DV, C_2 flow, cooling water (%)	100, 100	50–120, 0–100
—	DV, either analyzer in or out	in service	—
L	output, ethylene lost	0.200 %	budget 0.33
T_i, g_i	states, 48 cells each	Fig. 3.1	—

Plant conditions entered the laboratory as micropilot and kinetic studies, which the History box below follows from 1982 to 1993.

> ⧖ HISTORY **1982 to 1993: Plant Conditions in the Laboratory**
>
> A micropilot-plant study of catalyst performance and aging was reported in 1982 [14]. A review of its results notes that the overall selectivity rose with the carbon monoxide content and that the best carbon monoxide level, hydrogen ratio and temperature depended on the catalyst [1]. In 1993 a kinetic study ran a commercial Pd/Al_2O_3 catalyst in a Berty reactor, which has internal recycle, at tail-end conditions: 0.3 to 1.3 % ethyne, 0.4 to 4 % hydrogen, 0 to 60 ppm carbon monoxide, 0.3 to 2.1 MPa and 299 to 330 K. It tested eight rate expressions and found the selectivity 0.3 to 0.6 without carbon monoxide and 0.7 to 0.9 with it, found the rates in ethyne-ethene mixtures typically two orders of magnitude below that of ethene alone, and showed that the classical model 1 cannot follow the effect of carbon monoxide on the differential selectivity [8].

Front-end kinetics with carbon monoxide followed [9], as did a fixed-bed study with catalyst deactivation and an industrial reactor simulated in plug and dispersed flow [10] and the modeling and optimization of a front-end train [11]. Catalyst design moved to calculation, which proposed nickel–zinc alloys as a cheaper selective catalyst [13]. The sources consulted here do not describe a commercial converter's control system, so the loops below are built from the general methods of ratio, feedforward, selective and inferential control [6, 15] and of industrial model predictive control [16] and describe no licensor's practice. The same contest between a wanted and an unwanted reaction on a hot catalyst returns in the ethylene oxide reactor of Chapter 6, where the unwanted one makes most of the heat.

3.3 The Converter Model

The converter is generic and sized without plant data (Figure 3.1). The C_2 stream from the deethanizer passes a feed drum, hydrogen is added in ratio to its acetylene, a steam heater sets bed 1's inlet, a cooling-water intercooler with a hot-gas bypass sets bed 2's inlet, and a chromatograph samples the gas ahead of the drum and another the product. Time in the engine runs in minutes, with flows in mol/s and heat in watts.

The variables are listed in Table 3.1. The integrated state holds the 48 cell temperatures, 48 green-oil loadings, the heater duty, the intercooler metal, the bypass position, the hydrogen flow and the acetylene and carbon monoxide leaving the feed drum, 102 physical states, and eight ledgers that integrate each of four species into and out of the converter, 110 states in all.

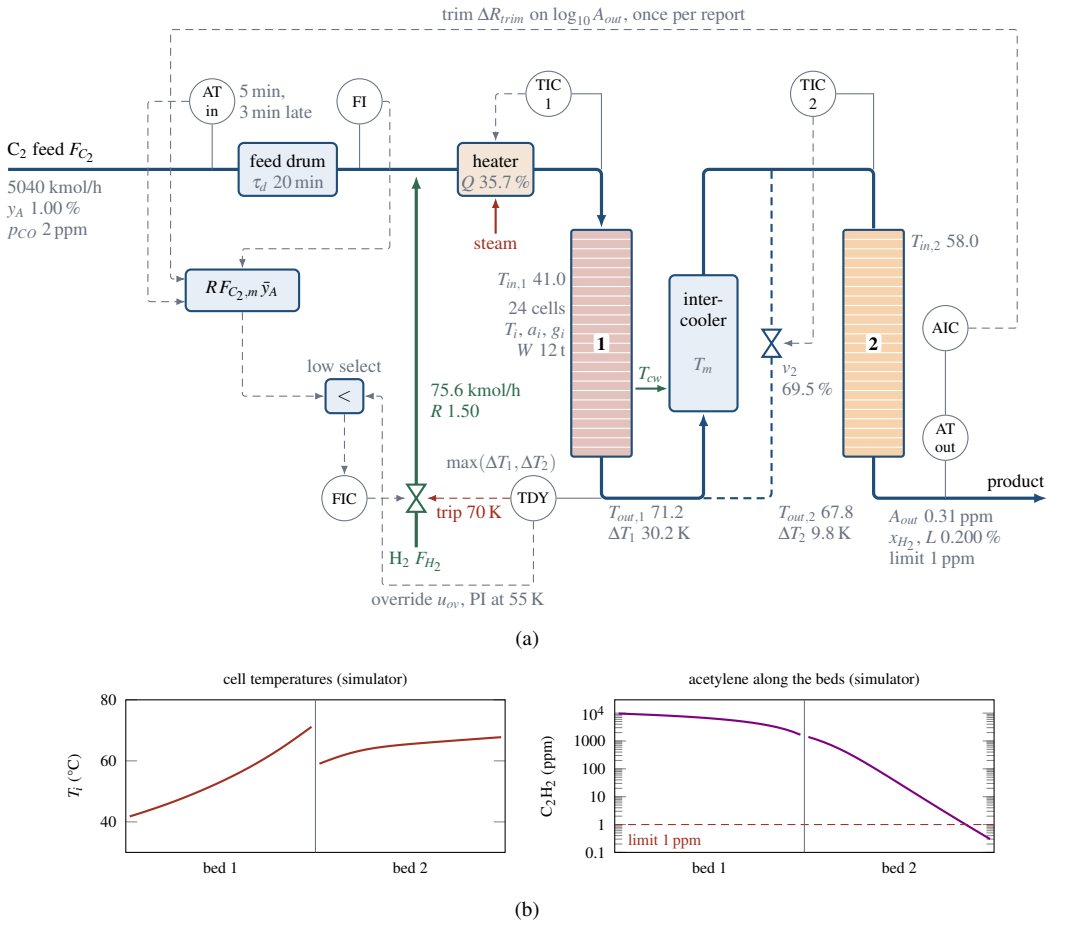


Figure 3.1 The tail-end converter as modeled, case 2 at $t = 1$ min, the design point. (a) After the app's Reactor view. The C_2 feed F_{C_2} with acetylene y_A and carbon monoxide p_{CO} passes the feed drum (lag τ_d), the inlet analyzer (AT in) sampling ahead of it. Hydrogen F_{H_2} follows the ratio logic $R F_{C_2,m} \bar{y}_A$ through a low select against the override u_{ov} from the larger bed rise. The heater duty Q (TIC 1) sets $T_{in,1}$, the bypass v_2 around the intercooler (metal T_m, water T_{cw}) sets $T_{in,2}$, each bed is 24 cells of temperature T_i, activity a_i and green oil g_i, and the outlet analyzer reports A_{out}, x_{H_2} and the loss L to the trim ΔR_{trim}. Printed values are the lined-out design: 75.6 kmol/h and rises of 30.2 and 9.8 K, where the app's panel prints the instruments, 75.5 kmol/h and 30.2 and 10.0 K. A model drawing, not piping. Not to scale. (b) The simulator's cell temperatures and acetylene along the 48 cells at the same instant. The Window view at this instant is Figure 3.3.

3.3.1 Two Hydrogenations on One Kind of Site

The rates per kilogram of catalyst have the classical Langmuir–Hinshelwood form, as shown in Equation (3.1).

$$\begin{aligned} &C_2H_2 + H_2 \rightarrow C_2H_4, \qquad C_2H_4 + H_2 \rightarrow C_2H_6 \\ &r_A = \frac{a k_A p_A p_H}{D^2}, \qquad r_E = \frac{a k_E p_E p_H}{D^2} \\ &D = 1 + K_A p_A + K_E p_E + K_{CO} p_{CO} \end{aligned} \tag{3.1}$$

where $p_i = P F_i / F_t$ is in bar at $P = 20\,\text{bar}$ absolute, a is the cell's activity, and the constants depend on temperature as shown in Equation (3.2).

$$\begin{aligned} k_j &= k_{j,r}\, \mathrm{e}^{-\frac{E_j}{R_g}\left(\frac{1}{T}-\frac{1}{T_r}\right)}, \qquad j = A, E \\ K_{CO} &= K_{CO,r}\, \mathrm{e}^{\frac{Q_{CO}}{R_g}\left(\frac{1}{T}-\frac{1}{T_r}\right)} \end{aligned} \tag{3.2}$$

with $T_r = 60\,^\circ\text{C}$, $k_{A,r} = 3$ and $k_{E,r} = 4 \times 10^{-4}$ mol/(s kg bar^2), $E_A = 25$ and $E_E = 60\,\text{kJ/mol}$, $K_A = 50$, $K_E = 0.01$ and $K_{CO,r} = 2.5 \times 10^4$ bar^{-1}, $Q_{CO} = 30\,\text{kJ/mol}$ and no temperature dependence of K_A or K_E. This is model 1 of Bos et al. [8] without its hydrogen adsorption term, and every constant is a teaching value. At the inlet at 60 °C, $K_A p_A = 9.85$, $K_E p_E = 0.156$ and $K_{CO} p_{CO} = 1.000$ at 2 ppm.

Three behaviors follow from the squared denominator, and one does not. The first is self-inhibition. The ethylene rate at the inlet is 31.0 times lower than with the acetylene gone, as shown in Figure 3.2a, against the two orders of magnitude measured on a commercial catalyst [8]. Without carbon monoxide the factor is 90.7, because carbon monoxide caps the ethylene rate that is released when the acetylene runs out (at 5 ppm the factor is 13.7). The apparent order in acetylene is −0.64 at the inlet and 0.98 at 100 ppm, where the review gives orders around zero or slightly negative and first order at low ethyne [1]. The ethylene rate rises faster with temperature, by 17.3 times from 40 to 80 °C against 3.8 for the acetylene, so a hotter bed is a less selective one, an ordering the published fits share [8]. What the law cannot do is the measured selectivity rise with carbon monoxide. Both rates share D^2, so carbon monoxide divides them by one factor, and the local selectivity $r_A/(r_A + r_E)$ at 1 % acetylene is 0.9896 at 0, 2, 6 and 20 ppm of carbon monoxide. Carbon monoxide is a brake on the catalyst in this model and nothing more.

Pause. Try Exercise 3.2 before reading on.

3.3.2 Heats From Standard Data

The heats of reaction are $\Delta H_1 = -174.26\,\text{kJ/mol}$ and $\Delta H_2 = -136.47\,\text{kJ/mol}$, from the standard heats of formation of acetylene, ethylene and ethane at 298 K in the NIST Chemistry WebBook [17] (226.73, 52.47 and −84.0 kJ/mol). The review gives −172 and −137 MJ/kmol [1]. Heat capacities are held at their values near 60 °C from the same source, 46.66, 29.02, 46.40, 57.40 and 29.13 J/(mol K) for acetylene, hydrogen, ethylene, ethane and carbon monoxide, which makes the feed's heat-capacity flow $\dot{F} C_p = 68.65\,\text{kW/K}$ at design. Hydrogenating the whole 1 % of acetylene therefore heats the gas 35.54 K, and each mol/s of hydrogen that finds ethylene instead adds 1.99 K.

3.3.3 Beds of Cells on the Shared Module

Each bed holds 12 t of catalyst in 24 cells of 0.5 t on the framework's packed-bed module, `core/beds.js`. A cell's composition is algebraic, because the gas crosses it in well under a second, and its temperature is a state on the catalyst's heat capacity, as shown in Equation (3.3).

$$\begin{aligned} \mathbf{F}_{out} &= \mathbf{F}_{in} + \boldsymbol{\nu}^{\mathsf{T}} \boldsymbol{\xi}, \qquad \xi_j = W_c\, r_j(T, \mathbf{F}_{out}) \\ W_c\, c_{cat} \frac{\mathrm{d}T}{\mathrm{d}t} &= \dot{F} C_p\,(T_{prev} - T) - \textstyle\sum_j \xi_j \Delta H_j \end{aligned} \tag{3.3}$$

where $\boldsymbol{\nu}$ holds the two reactions over acetylene, hydrogen, ethylene, ethane and carbon monoxide, $W_c = 500\,\text{kg}$, $c_{cat} = 900\,\text{J/(kg K)}$, T_{prev} is the cell upstream or the bed's inlet, and $\dot{F} C_p$ is evaluated at the converter feed and kept constant through both beds. A cell holds 450 kJ/K, 6.55 s of the gas's heat flow, and a bed 10.8 MJ/K, 2.62 min. The extents are found by Newton's method from zero with a fixed number of iterations and no convergence test, which keeps the derivative a pure function of the state. This app sets the count to seven through the module's option. The app's development record shows that six left a residual of 4.5×10^{-10} of the cell's acetylene and hydrogen at 1.8 % acetylene, 2.5 mol/mol and inlets of 85 and 90 °C, and with seven the residual is at most 1.3×10^{-15} over 729

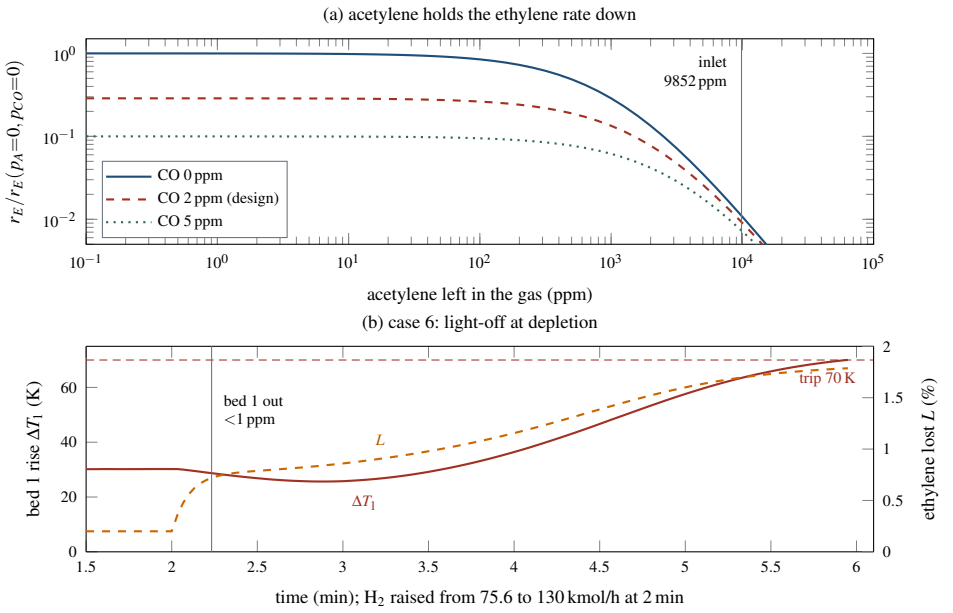


Figure 3.2 Self-inhibition and the light-off it hides. (a) The ethylene rate of Equation (3.1) at 60 °C and 20 bar against the acetylene left, relative to its value with neither acetylene nor carbon monoxide. At the inlet's 9852 ppm it is 31.0 times below its value at zero acetylene for 2 ppm of carbon monoxide. (b) Case 6 with the hydrogen raised by hand from 75.6 to 130 kmol/h at 2 min: bed 1's outlet falls under 1 ppm 14 s later, the loss L (dashed) climbs while the rise ΔT_1 first falls, and the trip comes at 5.95 min.

lined-out points of the Window view and 8.2×10^{-17} at every step of case 6 to its trip. Each of the 48 cells is a one-cell bed of the train, so that it carries its own activity, and the same record shows that a train of two 24-cell beds at uniform activity gives the same flows, heats and derivatives to the last bit.

The cell count is an axial dispersion, and the last ppm depends on it. At design the outlet is 1.01, 0.31 and 0.13 ppm with 12, 24 and 48 cells per bed, while the 1 ppm edge moves only from 1.501 to 1.433 to 1.401 mol/mol and the loss from 0.197 to 0.200 to 0.202 %. The difference reaches a verdict. The challenge's suggested settings, described in Section 3.5, pass at 24 and 48 cells (worst sample 0.53 and 0.49 ppm) and miss at 12, where two of 288 samples exceed 1 ppm (worst 1.39 ppm) and the loss averages 0.394 %. A verdict resting on tenths of a ppm belongs to the 24-cell model.

3.3.4 Green Oil and Activity

Each cell carries a green-oil loading g in weight percent of its catalyst, which grows with the acetylene there and sets the activity, as shown in Equation (3.4).

$$\frac{\mathrm{d}g}{\mathrm{d}t} = c_t\, k_g\, \mathrm{e}^{-\frac{E_g}{R_g}\left(\frac{1}{T}-\frac{1}{T_r}\right)} p_A, \qquad a = \mathrm{e}^{-g/g_0} \tag{3.4}$$

where p_A is the cell's outlet acetylene, $k_g = 0.4\,\mathrm{wt\%/(bar\,d)}$, $E_g = 40\,\mathrm{kJ/mol}$, $g_0 = 6\,\mathrm{wt\%}$, and c_t is a declared time compression, 1 except in case 7, where 1440 makes a minute a day. All three are teaching values.

3.3.5 Feed, Heater and Intercooler

The C_2 flow is $F_{C_2} = 1400\,\mathrm{mol/s}$ times the flow disturbance, and its acetylene and carbon monoxide reach the converter through the feed drum, as shown in Equation (3.5).

$$\begin{aligned} \tau_d \frac{\mathrm{d}y_A}{\mathrm{d}t} &= y_{A,up} - y_A \\ \tau_d \frac{\mathrm{d}p_{CO}}{\mathrm{d}t} &= p_{CO,up} + \Delta_c\, s(t/\Theta) - p_{CO} \end{aligned} \tag{3.5}$$

where $\tau_d = 20\,\mathrm{min}$, $y_{A,up}$ and $p_{CO,up}$ are the slider values, and in the challenge the furnace cycle adds $\Delta_c = 1.5\,\mathrm{ppm}$ times a trapezoid s of period $\Theta = 240\,\mathrm{min}$, low for the first half and high for the second with ramps over an eighth of the period. The bed 1 inlet is $T_{in,1} = T_{feed} + Q/\dot{F}C_p$ with $T_{feed} = 15\,^{\circ}\mathrm{C}$ and the duty Q following its command through a 0.5 min lag up to 5 MW. The intercooler passes a share $\beta = 0.9\,v_2$ of the gas past the exchanger, as shown in Equation (3.6).

$$\begin{aligned} G &= (1-\beta)\dot{F}C_p, \qquad \varepsilon = 1 - \mathrm{e}^{-UA_g/G} \\ T_x &= T_{out,1} - \varepsilon(T_{out,1} - T_m) \\ T_{in,2} &= \beta T_{out,1} + (1-\beta)T_x \\ C_m \frac{\mathrm{d}T_m}{\mathrm{d}t} &= G\varepsilon(T_{out,1} - T_m) - \phi\, UA_s(T_m - T_{cw}) \end{aligned} \tag{3.6}$$

with $UA_g = 60\,\mathrm{kW/K}$, $UA_s = 400\,\mathrm{kW/K}$, $C_m = 10\,\mathrm{MJ/K}$, $T_{cw} = 30\,^{\circ}\mathrm{C}$ and ϕ the cooling-water disturbance. The bypass follows its command with a 0.15 min lag and the hydrogen flow loop with 0.1 min, up to 56 mol/s. At design the bypass stands at 69.5 %, which passes 62.5 % of the gas.

3.3.6 Outputs and Instruments

The outlet acetylene is $10^6 F_{A,o}/F_{t,o}$ in ppm, and the ethylene loss is the ethane made as a share of the ethylene fed, $L = 100\,(F_{EA,o} - F_{EA,0})/F_{E,0}$. Thermocouples at each bed's inlet and outlet have a 6 s lag and 0.1 K of noise, and the C_2 and hydrogen meters 0.1 %. Both chromatographs run on the framework's analyzer module, draw a sample every 5 min and report it 3 min later, so a held reading is 3 to 8 min old. The inlet one reads acetylene (0.002 mol% noise) and carbon monoxide (0.03 ppm) ahead of the drum. The outlet one reads acetylene (0.02 ppm), hydrogen (0.005 mol%) and the loss (0.005 %). A chromatograph that has not reported for two periods reads STALE. The trip acts on either bed's true rise above 70 K, latches, closes the hydrogen and stops the run.

The exported file (Section 1.6.4) marks its simulator columns with a `truth_` prefix, out of reach of any controller replayed on it. In that file a column ending `_pct` is a percent of one of five things: the feed acetylene columns of the C_2 feed with hydrogen excluded, the hydrogen columns of the product gas, the loss columns of the ethylene fed, `heater_pct` of the full 5 MW and `bypass_pct` of valve travel, with the flow and cooling-water sliders in percent of design. The Instructions page lists each column's denominator.

3.3.7 Parameters, Initialization and Numerics

Table 3.2 lists the parameters. Every case starts lined out at its controllers' operating point, with the heater and bypass found for the inlet setpoints and the beds settled by the module's steady-state solver. With the hydrogen in Auto, a ratio that would line a bed out above the override's limit starts the plant where the override would hold it, which keeps a setting made before Run from starting an Auto plant past the trip. Classical fourth-order Runge–Kutta advances the state in 1 s steps, control runs every 2 s and a row is logged every 15 s, on the engine's three clocks of Section 1.6.1. The fastest speed runs 60 min of plant per second, and the engine needs 12.7 ms of computation per simulated minute headless in Node on the build host. Lined out, carbon and hydrogen close to 1.5×10^{-15} and 1.2×10^{-15}, and the engine's bed rises match the hand calculation from the conversions, 30.160 and 9.765 K, to the printed digits. Halving the step leaves every challenge verdict and every printed figure unchanged.

Table 3.2 Parameters. A: Adjustable in the Model Dialog. H: Hidden

Symbol	Meaning	Value	
$k_{A,r}$, $k_{E,r}$	rate constants at 60 °C	3, 4×10^{-4} mol/(s kg bar^2)	H, A
E_A, E_E	activation energies	25, 60 kJ/mol	H
K_A, K_E	adsorption constants	50, 0.01 bar^{-1}	H
$K_{CO,r}$, Q_{CO}	CO adsorption, its heat	2.5×10^4 bar^{-1}, 30 kJ/mol	A, H
P	reactor pressure	20 bar	H
W, c_{cat}	catalyst per bed, heat capacity	12 t, 900 J/(kg K)	H
k_g, E_g, g_0	green oil	0.4, 40 kJ/mol, 6 wt%	H
c_t	green-oil time compression	1	A
T_{feed}, Q_{max}	feed temperature, heater duty	15 °C, 5 MW	H
UA_g, UA_s	intercooler gas, water side	60, 400 kW/K	H
C_m, T_{cw}	intercooler metal, water	10 MJ/K, 30 °C	H
b_{max}	largest bypassed share	0.9	H
$F_{H_2,max}$	hydrogen valve capacity	56 mol/s	H
τ_Q, τ_v, τ_H	heater, bypass, hydrogen lags	0.5, 0.15, 0.1 min	H
τ_d	feed drum	20 min	H
Δ_c, Θ	furnace cycle	1.5 ppm, 240 min	H
—	ΔT trip	70 K	A
—	product acetylene limit	1 ppm	A

Table 3.3 Loops, Pairings and Default Tunings

Loop	PV → MV	K_c	τ_I	Output, period
TIC 1	$T_{in,1} \to Q$	1.5 %/K	0.6 min	0–100 %, 2 s
TIC 2	$T_{in,2} \to v_2$	3 %/K	1 min	0–100 %, 2 s
AIC trim	$\log_{10} A_{out} \to \Delta R_{trim}$, rev.	0.05/decade	5 min	±0.6, each report
override	$\max \Delta T \to u_{ov}$	0.3 mol/(s K)	3 min	0–56 mol/s, 2 s

3.3.8 Assumptions

The plant has two reactions on one kind of site with teaching constants, so carbon monoxide brakes the catalyst without raising its selectivity, which a real palladium catalyst does [8]. The direct route from acetylene to ethane, the oligomers other than the green oil and the hydrogenation of the green oil are left out, so carbon and hydrogen close on the two reactions exactly. The gas is ideal at 20 bar with constant heat capacities, there is no pressure drop, heat loss or internal diffusion, and the gas holds neither heat nor composition. Each bed is 24 well-mixed cells, an axial dispersion much larger than a real bed's, and the feed drum is one first-order lag. The hydrogen is pure and its flow loop ideal, and the analyzers carry noise but no drift. The 1 ppm limit, the 55 K override, the 70 K trip and the challenge's 0.33 % loss budget are teaching values. A real limit comes from the ethylene buyer's specification, which the review puts below 5 ppm [1], and a real trip from the catalyst supplier's and the vessel designer's temperature limits, implemented in the plant's safety instrumented system.

3.4 Ratio, Trim, Override and a Predictive Layer

The instrument code hands the controllers one packet of readings, and a test holds them to its keys. The hydrogen loop and the two inlet loops each carry their own Auto and Manual switch, the header's switch throws all three, and each idle controller follows the one in charge, so a switch of mode or of structure causes no bump.

3.4.1 The Shared PI Law

Every PI loop here is the framework's velocity-form law of Section 1.6.2, Equations (1.14) to (1.17), used without derivative action. Only the emitted output is clamped, and the integral is corrected toward the clamped output with a tracking time equal to τ_I. An integral time set to its slider's maximum removes the integral action. The loops are listed in Table 3.3.

3.4.2 Hydrogen in Ratio, With Two Feedforwards

The hydrogen flow is the lower of the ratio logic's request and the override's output, as shown in Equation (3.7).

$$\begin{aligned} F_{H_2} &= \min\bigl(R\,F_{C_2,m}\,\bar{y}_A,\; u_{ov}\bigr) \\ R &= \mathrm{clip}_{[0.8,\,2.5]}\bigl(R_{SP} + \Delta R_{trim} + K_{CO}(\bar{p}_{CO} - 2)\bigr) \end{aligned} \tag{3.7}$$

where $F_{C_2,m}$ is the C_2 meter. On Fixed ratio $\bar{y}_A$ is the design 1 % and there is no carbon monoxide term. On Feedforwards $\bar{y}_A$ and $\bar{p}_{CO}$ are the inlet chromatograph's readings passed through a first-order lag $\tau_{ff} = 20\,\mathrm{min}$, the drum's, and $K_{CO} = 0.15\,\mathrm{mol/mol}$ per ppm. The analyzer samples ahead of the drum, so the feedforward sees a change about 20 min before the converter does, while the outlet analyzer sees its effect only after the drum, the beds and its own delay. The app's development record shows that without the drum, with both analyzers at 5 and 3 min, the feedforward saw an upstream change no sooner than the trim and every structure that passed the challenge with one passed with the other, so the drum is what gives the feedforward its lead.

The trim is reverse acting on $\log_{10}\max(0.05, A_{out})$ against $\log_{10} A_{SP}$ and acts once per outlet report with the analyzer's 5 min period as its step. The logarithm suits a plant whose outlet moves a decade for a tenth of a mol/mol near the edge. The floor of 0.05 ppm is the analyzer's noise floor (its noise is 0.02 ppm), and the development record shows that without it a zero reading drove a limit cycle with a 10 min period between 0 and 8.7 ppm in the challenge. The override is a PI on the larger measured bed rise whose output is a hydrogen flow. While the ratio's request is lower it tracks that request, so it takes over at its limit and hands back without a bump. During development the tuning was settled at a gain of 0.3 mol/(s K) with 3 min after a gain of 0.5 with 1 min formed a growing cycle with the bed's thermal lag that tripped, and the limit at 55 K after a 65 K limit let an Auto run with 2 % acetylene reach the trip. A protective override of the same kind, a PI loop that acts only near its limit, guards the compressor of Volume 4, Chapter 2.

3.4.3 A Balance Inference for a Failed Analyzer

When the inlet chromatograph fails, the feedforward can take the feed acetylene from a hydrogen balance on each outlet report, as shown in Equation (3.8).

$$\begin{aligned} \xi_H &= \frac{F_{H_2,m} - x_{H_2}(F_{C_2,m} + F_{H_2,m})}{1 - x_{H_2}} \\ \xi_E &= \frac{L}{100}\,0.79\,F_{C_2,m} \\ \hat{y}_A &= \frac{\xi_H - \xi_E + 10^{-6} A_{out}(F_{C_2,m} + F_{H_2,m} - \xi_H)}{F_{C_2,m}} \end{aligned} \tag{3.8}$$

where the meters are taken at the instant the report's sample was drawn and x_{H_2} is the outlet hydrogen fraction. Every mole of hydrogen used made ethylene from acetylene or ethane from ethylene, so the hydrogen used less the ethane made, plus the acetylene left, is the acetylene fed. A bias against the inlet chromatograph is updated while that one reports and frozen when it fails, and lined out at 1.0, 1.3 and 1.5 % the inference is within 9.0×10^{-7} percentage points of the truth. A bed-temperature inference would be simpler, but it counts the heat of ethylene burned as acetylene converted. The development record shows its feedforward running away into the trip in case 5 at 33.2 min, which is why the balance replaced it. This is inferential control in the sense of secondary measurements standing in for an unmeasured quality [15].

3.4.4 The MPC on the Ratio and Both Inlets

With the architecture set to MPC, every 2 min a receding-horizon controller [16] of the kind set out in Section 1.6.3 moves R_{SP}, $T_{1,SP}$ and $T_{2,SP}$ for the least ethylene loss. It lines out its own 24-cell copy of the beds, built from the declared parameter defaults with fresh catalyst, for the feed the instruments

Table 3.4 The Nine Cases

#	Case and events	Teaching point
1	Fixed ratio from 1.3, learner steps it to 1.9	the window
2	Design point, learner raises $T_{2,SP}$ to 62 °C	the window map
3	Ratio 1.3, trim on, learner raises its gain	analyzer trim
4	Fixed ratio 2.0, CO 2 → 0.5 ppm at 10 min	override, CO feedforward
5	Acetylene 1.0 → 1.5 % at 10 min	feedforward
6	Hydrogen on Man, learner raises it to 130 kmol/h	runaway, trip
7	Trim on, green oil 1440 times faster	aging, schedule
8	Feedforwards, inlet analyzer fails at 10, acetylene 1.3 % at 20 min	balance inference
9	Challenge, 24 h, fixed ratio, no trim	the whole converter

report, fits the gains of four outputs (log ppm, loss and both rises) by central differences of ±0.05 mol/mol and ±1 K, and plans ten decisions ahead, as shown in Equation (3.9).

$$\begin{aligned} x_{j,k+1} &= a_j x_{j,k} + (1-a_j)u_{j,k}, \qquad a_j = \mathrm{e}^{-T_s/\tau_j} \\ \min\ & \textstyle\sum_k w_L L_k + \sum_k \Delta\mathbf{u}_k^{\mathsf{T}} S\,\Delta\mathbf{u}_k + \text{soft penalties} \\ \text{s.t. } & \log_{10} A_k \le \log_{10} A_{SP}, \quad \Delta T_{b,k} \le \Delta T_{lim} - 5 \end{aligned} \tag{3.9}$$

where both output limits are soft, $T_s = 2$ min, τ_j is the hydrogen loop's lag for the ratio and the bed's $C_{bed}/\dot{F}C_p$ for the inlets, $w_L = 1$ per percent, S is $100\,w_{\Delta u}$ for the ratio and $w_{\Delta u} = 0.5$ for each inlet, the inputs are bounded to 0.8–2.5, 25–85 and 35 °C–90 with moves of at most 0.1, 2 and 2 K, with the moves held over blocks of one, one and eight decisions. The outlet chromatograph corrects the model's log ppm and loss by half the mismatch at each report, the thermocouples its rises at each decision. Each program is solved by the dual algorithm of Goldfarb and Idnani [18] as coded in the framework's quadratic programming module, and a failed plan leaves the setpoints where they were.

3.4.5 Three Models Kept Apart

The simulated plant is the 48-cell model above. Any model a learner identifies from the logged data, the edge against carbon monoxide for one, is a second and separate model. The controllers' models are the ratio, the trim gains, the balance and the MPC's fresh-catalyst copy. Not one of them can read the activity, the true outlet between reports or the true carbon monoxide. A parameter changed in the app reaches the plant and not the MPC's copy, which meets it as mismatch through the chromatograph and thermocouple corrections. The status strip, the window map and the challenge's judge read the truth and act on nothing.

3.5 Measured on the Running Converter

The cases are listed in Table 3.4 and their outcomes in Table 3.5. Every number was measured with the engine run headless at its 1 s step on the default seed, with every case in its shipped form and every learner action made after Run at the instant the text gives. Rerun when these results were written up, the script of the app's technical review reproduced its recorded output exactly, and the challenge was run at four further seeds and at half the step.

3.5.1 The Window and Its Two Costs

Case 1 steps the fixed ratio from 1.3 to 1.9. About 14 min after each step the outlet held 14.7, 1.89, 0.30, 0.010 and 0.0002 ppm while the loss read 0.138, 0.177, 0.201, 0.275 and 0.472 %. The acetylene fell 4.97 decades and the loss rose 3.43 times, and not evenly. The last 0.2 mol/mol cost 0.198 points of ethylene, 3.14 times what the step from 1.3 to 1.5 cost, and lined out the loss climbs 0.40 % per mol/mol between 1.3 and 1.4 and 1.34 between 1.9 and 2.1. The two failures are priced very differently. Breakthrough puts all 2680 t/d of ethylene off grade, while each 0.1 % of loss is 2.68 t/d, so the window is one-sided and the right place is just clean of the edge, as shown in Figure 3.3.

Table 3.5 Case Outcomes Measured on the Engine

Case and condition	Result
1, ratio 1.3/1.4/1.5/1.7/1.9	14.7/1.89/0.30/0.010/0.0002 ppm; loss 0.138/0.177/0.201/0.275/0.472 %
2, $T_{2,SP}$ 58 → 62 °C	edge 1.433 → 1.375; at 1.5: 0.31 → 0.073 ppm, 0.200 → 0.275 %
3, trim gain 0.05	under 1 ppm at 13.3 min (analyzer 18.3); 0.30–0.37 ppm
3, gain 0.3 at 60 min	0.001–6.7 ppm, ratio 1.37–1.76 in the next hour
4, fixed ratio 2.0	loss 0.594 → 1.052 %; override at 40.0 min
4, Feedforwards at 40.8 min	ratio 1.78; override off 1.7 min later; loss 0.76 %
5, fixed ratio	over 1 ppm 2.0 min after; peak 2476 ppm; over 108 of 110 min
5, Feedforwards	peak 1.57 ppm, 2.5 min over; H_2 75.7 → 113.3 kmol/h; loss 0.39 %
6, 130 kmol/h at 2 min	bed 1 out <1 ppm +14 s; loss >1 % +1.58 min; trip +3.95 min at 70.05 K, 111.0 °C, 1.79 %
7, no schedule	over 1 ppm day 137.5; trim at its reach day 193.3; 3830 ppm day 300
7, 5 K per 100 days	over 1 ppm day 177.8; loss 0.446 against 0.334 % on day 150
8, left alone	STALE 18.25 min; over 1 ppm from 23.75; 212 ppm at 2 h
8, inference at 30 min	under 1 ppm 8 s later; loss 0.300 % at 2 h

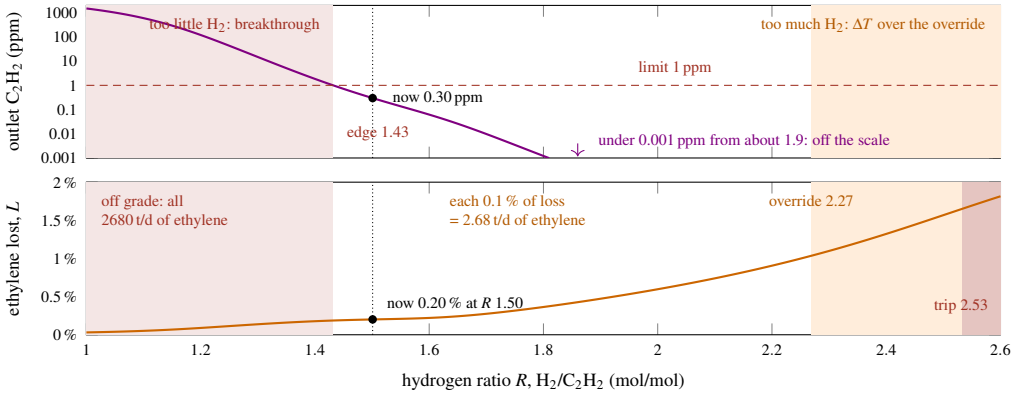


Figure 3.3 The Window view of case 2 at $t = 1$ min, the instant of Figure 3.1: the plant lined out at every ratio with these inlets, carbon monoxide and catalyst. The breakthrough edge is at 1.43, the override is reached at 2.27 and the trip at 2.53, with the two costs.

Further right the lined-out bed 1 reaches the 55 K override at a ratio of 2.27 and the 70 K trip at 2.53. The app's 17-point map places the three crossings at 1.434, 2.268 and 2.534 against 1.432, 2.269 and 2.533 by direct bisection.

🕮 **Pause.** Try Exercise 3.1 before reading on.

The window moves. In case 2, warming bed 2's inlet from 58 to 62 °C moves the edge from 1.433 to 1.375, but at the plant's own 1.5 the outlet falls only from 0.31 to 0.073 ppm while the loss rises from 0.200 to 0.275 %. Carbon monoxide moves the edge more, from 1.253 at 0.5 ppm to 1.433 at 2 and 1.981 mol/mol at 5 ppm, while the loss at the edge stays within 0.176 to 0.189 %, which is the one-site law's signature. The design point is also not the cheapest point in the window. Colder inlets favor the acetylene's smaller activation energy, and at 27.5 and 40 °C the edge is at 2.079 with a loss there of 0.112 %, against 0.186 % at the design inlets. A 2.5 K grid over the setpoint ranges finds 0.108 % at 27.5 and 35 °C. The app says the design point is one choice in the window and poses the colder, fatter point as a question on its Instructions page.

> **TRY IT IN THE APP** **2 · The window map and the operating point**
>
> Load the case and press Run. On the Window view, find where the outlet acetylene curve crosses the red 1 ppm line, near a ratio of 1.43. The black dots of the plant sit just to its right, at 1.5. Then raise the Bed 2 inlet setpoint to 62 °C and watch the crossing move left, to 1.375, while the loss at the plant's ratio rises from 0.200 to 0.275 %.

3.5.2 A Trim That Waits on Its Analyzer

Case 3 starts at a ratio of 1.3 with the trim on. The default trim took the outlet from 15.0 to under 1 ppm in 13.3 min, which the chromatograph showed at 18.3 min, and held it at 0.30 to 0.37 ppm with the ratio near 1.50. Raised six times to 0.3 at 60 min, the trim hunted, the outlet swinging between 0.001 and 6.7 ppm and the ratio between 1.37 and 1.76 over the next hour, because each report corrects a sample drawn before the last correction took effect. At a gain of 0.2 the outlet stays at 0.25 to 0.36 ppm.

3.5.3 Carbon Monoxide, Feed and the Override

Case 4 runs fat at 2.0 on a fixed ratio, and at 10 min the carbon monoxide falls from 2 to 0.5 ppm. The outlet acetylene never matters (below 0.000 03 ppm in the run with the switch), but the catalyst burns more of the spare hydrogen on ethylene, the loss rises from 0.594 to 1.052 % and bed 1's rise from 44.7 to 55 K, where the override takes over at 40.0 min and begins to cut the hydrogen from 100.9 kmol/h. Switched to Feedforwards at 40.8 min, the carbon monoxide term takes the ratio to 1.78, the override stands by 1.7 min later, and the loss settles at 0.76 %. The override keeps the beds safe and leaves the loss high. In case 5 the feed acetylene rises half again at 10 min. On a fixed ratio the true ratio falls to 1.00, the outlet crosses 1 ppm 2.0 min after the change, which the chromatograph reports at 8.25 min, and peaks at 2476 ppm. With the feedforward the hydrogen follows from 75.7 to 113.3 kmol/h, the outlet peaks at 1.57 ppm for 2.5 min and the chromatograph never reads above 0.82 ppm, at a loss of 0.39 % because the same ratio on more acetylene is more spare hydrogen.

3.5.4 Light-Off at Depletion and Where the Trip Is Reached

Case 6 puts the hydrogen in the operator's hands, where the override does not act, as shown in Figure 3.2b. Raised from 75.6 to 130 kmol/h (2.58 mol/mol) at 2 min, the hydrogen empties bed 1 of acetylene in 14 s, and the sites the acetylene held go to ethylene. The loss reaches 0.79 % at 2.5 min and passes 1 % 1.58 min after the change. Bed 1's rise first falls, to 25.65 K at 2.87 min, because the reaction has moved to the front cells, whose heat reaches the outlet only after a thermal wave crosses the bed in about 2.6 min. It then climbs to 70.05 K 3.95 min after the change, with the outlet at 111.0 °C, 1.79 % of the ethylene going to ethane and more ethylene burned than made. The jacketed reactor of Volume 7, Chapter 2 shows the same contest between heat that grows exponentially with temperature and removal that grows only linearly, at an ignition boundary. Lined out by hand, 110, 120, 125 and 130 kmol/h give bed 1 rises of 51.1, 60.9, 66.8 and 72.8 K. A plant started at 130 kmol/h, set before Run or kept through Reset, is already past the trip and trips in its first second, which the case's texts say. The lowest flow that completes case 6 is 128 kmol/h, which trips 4.57 min after it is set, while 125, 126 and 127 kmol/h peak at 67.0, 68.2 and 69.4 K in 40 min and never trip.

Pause. Try Exercise 3.3 before reading on.

> **TRY IT IN THE APP** **6 · The runaway: acetylene runs out in bed 1**
>
> Press Run, then raise the Hydrogen flow on the FIC card from 75.6 to 130 kmol/h. Watch the Bed temperature rise trend. Bed 1's rise first falls, to 25.65 K, while the ethylene loss passes 1 % 1.58 min after the change. The rise reaches the 70 K trip only 3.95 min after it, and the trip closes the hydrogen.

At the design C_2 feed no Auto setting reaches the trip. Over sixteen settings and disturbances held 90 min (ratio 2.5, the override at its 60 K top, 1.8 % acetylene, no carbon monoxide, a lost intercooler,

Table 3.6 The Challenge Over 24 h, Default Seed and Seeds 1–4

Configuration	Worst (ppm)	Over /288	Loss (%)	
fixed ratio 1.5, no trim (shipped)	1079	185	0.192	fail
fixed ratio 2.0	0.29	0	0.566	fail
trim alone at 0.07 ppm, gain 0.1	0.70	0	0.374	fail
trim alone at 0.085 ppm, gain 0.1	1.08	1	0.317	fail
Feedforwards at 1.6, no trim	0.28	0	0.455	fail
Feedforwards, trim at 0.3 ppm	1.36	12	0.242	fail
Feedforwards, trim at 0.1 ppm (sugg.)	0.53	0	0.297	pass
seeds 1–4	0.52–0.57	0	0.297–0.306	pass
same, 12 cells per bed	1.39	2	0.394	fail
same, feed acetylene from inference	0.78	0	0.276	pass[a]
MPC, A_{SP} 0.1 ppm	0.64	0	0.354	fail
seeds 1–4	0.48–0.67	0	0.352–0.356	fail

[a] Fails at seed 1 (1.10 ppm, two samples over) and passes at seeds 2 to 4 (0.94 to 0.99 ppm).

inlets at 85 and 90 °C), the largest true rise was 66.2 K. A smaller or richer feed moves the trip line left, to 2.379 at 85 % of the design flow, 2.281 at 70, 2.250 at 50 and 1.581 mol/mol at 1.8 % acetylene, and a ratio past it is held only by the override, which reads the bed outlets and a light-off can outrun. In Auto a ratio setpoint of 2.5 with the C_2 feed cut to 85 % at 20 min trips at 23.57 min, 2.2 with a cut to 70 % at 24.57 min, and Feedforwards at the shipped 1.5 with 1.8 % acetylene and a cut to 50 % at 64.98 min, while 2.2 at 85 % peaks at 64.5 K and 2.0 at 50 % at 67.4 K. A mistuned override can let a fat ratio through too. With a ratio setpoint of 2.5 and the carbon monoxide gone, a gain of 3 with 0.2 min trips at 68.93 min and a proportional gain of 0.05 at the 60 K limit at 42.10 min. The app's technical review tried an override scaled by the C_2 meter, a rate-limited hand-back and a ratio ceiling of 2.0, and none removed the feed-cut trips, so the trip is reachable in Auto by design of the physics, and the trip exists for exactly this.

3.5.5 Green Oil, the Analyzer Failure and an Honest Infeasibility

Case 7 compresses the run, a minute for a day. Bed 1's mean activity falls to 0.54 by day 100 and 0.30 by day 200 (bed 2's 0.86 and 0.64), the trim raises the ratio to 1.65 by day 100 and 1.86 by day 150, the outlet first passes 1 ppm on day 137.5, and the trim reaches its 0.6 mol/mol limit on day 193.3. A schedule of 5 K per 100 days on both inlets holds the outlet under 1 ppm to day 177.8 at a loss of 0.446 % on day 150 against 0.334 without it. On the catalyst left at day 480 (bed activities 0.061 and 0.143) no point meets the limit. A search over the full setpoint ranges with both rises under 55 K, refined to 0.5 K and 0.01 mol/mol, finds at best 9.31 ppm at 85.0 and 88.5 °C and a ratio of 2.49, and allowing the override's 60 K top gives 6.44 ppm. The catalyst must be regenerated. In case 8 the inlet chromatograph fails at 10 min and reads STALE at 18.25 min, the acetylene rises to 1.3 % at 20 min, and the outlet passes 1 ppm at 23.75 min and reaches 212 ppm at 2 h if left. Switched to the inference at 30 min, the outlet is under 1 ppm 8 s later, because the balance had followed the rise all along (1.159 percent at 40 min, 1.295 at 2 h).

3.5.6 A Day on the Furnace Cycle

The challenge runs 24 h. The carbon monoxide swings between 0.5 and 3.5 ppm every 4 h, the acetylene rises to 1.3 % at 6 h, the inlet chromatograph fails at 14 h and the acetylene returns to 1.0 % at 16 h. It is met when every one of the 288 outlet samples carries at most 1 ppm of true acetylene, the true loss averages at most 0.33 % (8.8 t/d) and nothing trips. The budget was set at 0.33 rather than the development plan's 0.5 % because at 0.5 the trim alone passed by aiming deep inside the limit, so the feedforward was not needed. The configurations are compared in Table 3.6, and Figure 3.4 draws the nine run at the default seed against the limit and the budget.

As shipped, the first rise of carbon monoxide breaks through, and the day ends with 185 of 288 samples over and a worst sample of 1079 ppm. A higher fixed ratio fails the other way, and the trim

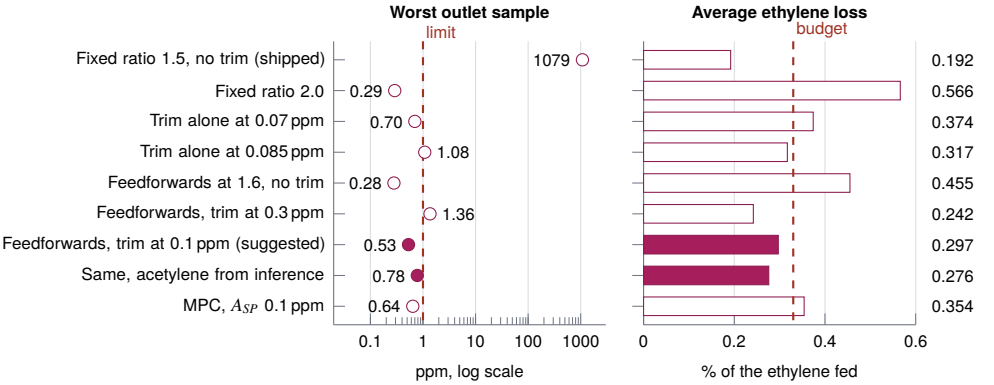


Figure 3.4 The challenge of Table 3.6 at the default seed. Filled marks and bars pass, open ones fail. The dashed lines are the 1 ppm limit on every sample and the 0.33 % budget on the average loss. Notice that only the two configurations with the feedforwards and a trim aimed at 0.1 ppm sit left of both lines, and that the MPC holds every sample but spends more than the budget.

alone holds the samples only aimed at 0.07 ppm, spending 0.374 %. With the feedforwards, the trim on and its setpoint at 0.1 ppm, the worst sample is 0.53 ppm and the loss averages 0.297 %, and the shipped and suggested verdicts hold at seeds 1 to 4 and at half the step. The MPC holds every sample but spends 0.352 to 0.356 %. It made 719 decisions with one failed plan in the day and, after the first hour, kept the inlet setpoints at a mean of 36.4 and 44.7 °C with the ratio setpoint at 1.71, the colder and fatter direction, but its loss enters as a linear cost on a fresh-catalyst copy and the plan does not find the suggested loop's economy.

> ✦ **DID YOU KNOW? Aiming Far Inside the Limit Is Not Enough**
>
> From the simulator (Table 3.6). On the day of the challenge, an outlet trim working alone and aimed at 0.085 ppm, far inside the 1 ppm limit, still let one of the 288 samples through, at 1.08 ppm. With the feedforwards added, a trim aimed at 0.1 ppm kept the worst sample at 0.53 ppm.

The outage leaves a lesson of its own, as shown in Figure 3.5. At 1000 min the suggested configuration still reads the inlet chromatograph's last report, 1.299 % acetylene and 3.0 ppm of carbon monoxide, while the true feed carries 1.041 % and 0.71 ppm. The ratio in force is 1.44, made of the setpoint 1.50, 0.15 mol/mol from the held carbon monoxide and a trim of −0.208, but on the true acetylene the ratio is 1.80, 0.54 mol/mol above the edge of 1.26 that the low carbon monoxide has set and only 0.09 below the override's 1.89. The outlet is at 0.000 007 ppm, the loss at 0.81 %, bed 1's rise at 51.1 K, and the trim is walking the ratio back one report at a time. The day still ends with the average under budget, 0.276 % at that instant.

3.6 Technology in Practice

Figure 3.6 draws the hydrogen ratio, its trim and override, the two inlet loops and the trip of Section 3.4 with the hardware of a converter in place of the schematic's symbols.

What Measures It

The controlled quality is the acetylene left in the product, a few parts per million read by a chromatograph on the outlet. A second chromatograph reads the acetylene and the carbon monoxide of the feed ahead of the drum, and thermocouples read each bed's inlet and outlet. The chapter's two chromatographs draw a sample every 5 min and report it 3 min later, with 0.02 ppm of noise on the

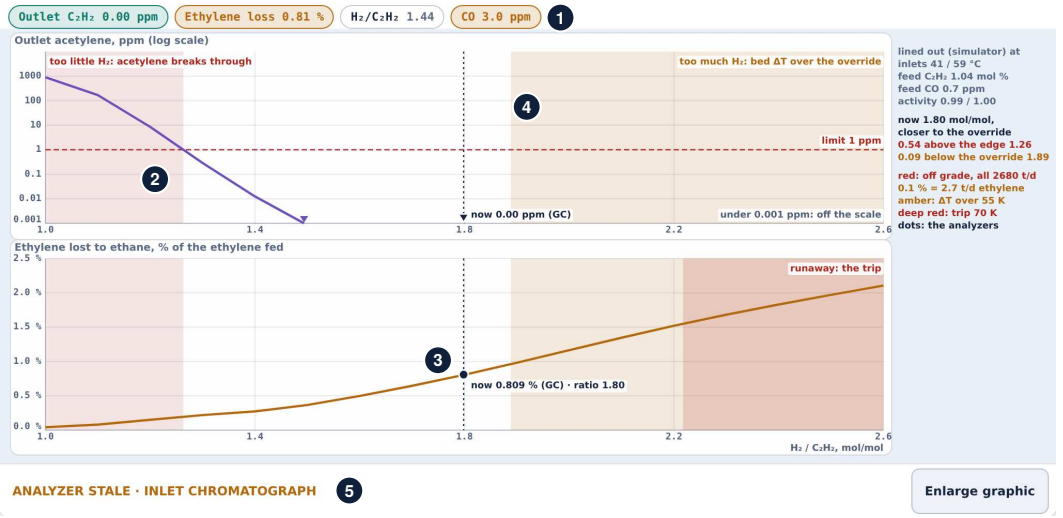


Figure 3.5 The challenge on its suggested settings (Feedforwards, trim on at 0.1 ppm) at $t = 1000$ min, on the Window view, 2.7 h after the inlet chromatograph failed. (1) The badges read the outlet chromatograph at 0.00 ppm, a loss of 0.81 %, a measured ratio of 1.44 and the held 3.0 ppm of carbon monoxide, and (5) the status strip reads ANALYZER STALE. The window, lined out at inlets of 41 and 59 °C, 1.04 % acetylene and 0.7 ppm of carbon monoxide, puts the plant at (3) a true ratio of 1.80, 0.54 above (2) the edge of 1.26, where the outlet curve crosses the 1 ppm line, and 0.09 below (4) the override at 1.89, where the shaded band begins, with the trip at 2.22 and the loss 0.809 % by the chromatograph.

outlet acetylene, and its thermocouples lag by 6 s. Figure 3.7 shows how a chromatograph separates its sample.

> **TECHNOLOGY** **Sensor: Process Gas Chromatograph**
>
> A process gas chromatograph injects a precise quantity of sample at the head of a long, narrow column, and a steady flow of carrier gas washes it through. Each compound leaves at its own time, so a detector that only tells carrier gas from anything else can measure many species. Hydrocarbons ionize easily in a flame, which suits a flame ionization detector, while carbon monoxide does not ionize and needs another kind. The area under each peak, scaled by a factor found with a calibration gas, gives the concentration. The weakness is time: cycles of minutes are not unusual, and that dead time can make a loop oscillate. Many faults start at the sample valve, where a leak can shift the baseline or corrupt the analysis [19]. A failed chromatograph in the chapter holds its last report, a flat trend line.

What Moves It

Three valves carry the handles. The hydrogen valve sets the ratio, the steam valve of the heater sets bed 1's inlet, and the bypass valve around the intercooler sets bed 2's. The chapter gives the hydrogen loop a lag of 0.1 min up to 56 mol/s, the heater a lag of 0.5 min up to 5 MW and the bypass a lag of 0.15 min. A fourth final element belongs to the protection rather than to control.

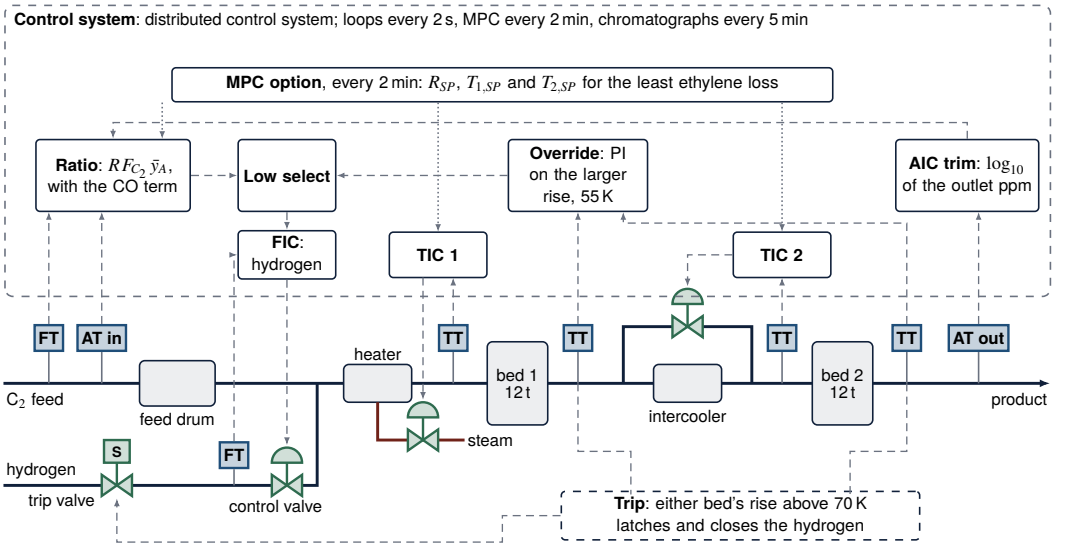
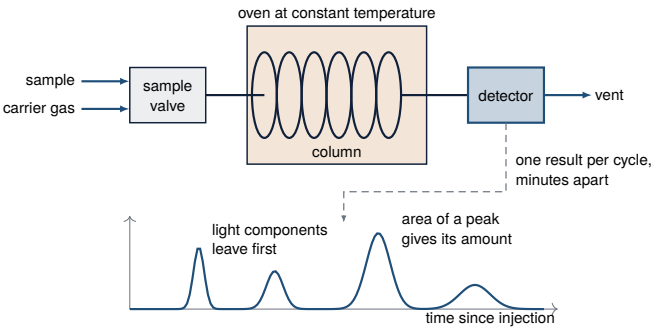


Figure 3.6 The converter's loops with their hardware. Blue boxes are sensing devices: FT on the C_2 feed and on the hydrogen, AT in and AT out, the two chromatographs, and TT at each bed's inlet and outlet. Green symbols are final elements: the hydrogen control valve, the hydrogen trip valve, the steam valve of the heater and the intercooler's bypass valve. Dashed arrows are signals, dotted arrows the setpoints that the MPC option writes. Notice that the override and the trip both read the bed outlets, and that the only reading of the outlet acetylene arrives every 5 min, 3 min late. Not to scale, and not a piping diagram.



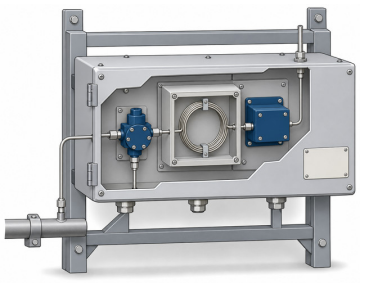


Figure 3.7 Principle of a process gas chromatograph, the instrument behind AT in and AT out. A valve injects a sample into the carrier gas, the column holds back each species for its own time, and the detector sees them leave one by one. Notice that a result exists only at the end of each cycle, which is why the chapter's chromatographs report each sample 3 min after it is drawn and only every 5 min.

TECHNOLOGY **Final Element: The Hydrogen Valve and Its Trip**

The hydrogen flow controller moves a modulating control valve. A trip that closes the hydrogen belongs to a safety instrumented system, built of its own sensors, a logic solver kept apart from the regulating controls so that one hardware fault cannot disable both, and final elements: on/off valves, or solenoids that force the control valve shut. The valves are generally the least reliable part. A full stroke would shut the unit down, so plants prove them with a partial stroke: a valve that moves well part of the way will very probably move all of it [19]. The chapter's trip reads the true bed rise, latches and closes the hydrogen.

Where the Controller Runs

A distributed control system has a supervisory level that sends set points to the field controllers, its loops are sometimes nested or cascaded, and their cycle times range from milliseconds to minutes [20]. The app's loops execute every 2 s, its MPC every 2 min, and each chromatograph reports every 5 min. The structure maps onto standard blocks: a ratio station with two feedforwards, a PI trim on the logarithm of the outlet acetylene that acts once per report, and a low selector between the ratio's request and the override. An override strategy selects among controller outputs so that only one at a time acts on the process [19]. In a plant the trip runs on hardware of its own.

What Is Modernizing It

Three developments touch this chapter. The first is the analyzer itself. Modern process chromatographs are smart instruments that compute their own results, can calibrate themselves from bottles of calibration gas on a schedule, and send many species over a digital bus [19]. The second is the soft sensor. Analyzers such as gas chromatographs suffer from long measurement delays and high investment and maintenance costs, and one purpose of a soft sensor is to validate an online analyzer against its estimate [21]. The balance inference of Section 3.4 is such an estimate, built from a hydrogen balance. The third is the layer above the loops. Crackers use multivariable control with online analyzers and constraint controls, often with online optimization [7], and a 2003 survey found predictive control well founded in refining and petrochemicals [16]. The predictive controller of Section 3.4 is a small example, and Table 3.6 shows it spending more ethylene than the suggested loops.

> **IN PRACTICE** **Regenerating the Catalyst**
>
> The alkynes in cracked gas are hydrogenated in the majority of European plants, and only two reported not doing it. The catalyst, which may hold palladium and silver among other metals, has a finite life. Most plants regenerate it on site, by thermal oxidation, by purging with steam and air, or by treating it with hydrogen, and send the gas from the regeneration to an abatement system. How often depends on the catalyst, the design and operation and the cracker's feed. A spent catalyst normally goes back to its supplier, who recovers the metal. The European reference document under Directive 2010/75/EU sets out these practices [7]. Case 7 of this chapter ends where only a regeneration helps.

3.7 Limitations

The converter is generic and its sizes, constants and limits serve teaching. The rate law is the classical one-site form, which a commercial palladium catalyst does not follow. Carbon monoxide here slows both reactions by one factor and leaves the loss at the edge between 0.171 and 0.189 % from 0 to 5 ppm, where measurement shows the selectivity rising from 0.3 to 0.6 to 0.7 to 0.9 [8]. A second kind of site would be needed, and it would move every number in the app. The self-inhibition at the inlet is 31 times where measurement gives about a hundred. The 24 cells set the last ppm, so a sub-ppm figure and the challenge's margin belong to this discretization. The green oil, the feed drum and the furnace cycle are teaching closures.

OPEN CHALLENGE A Catalyst That Stays Selective

Supported palladium remains the industrial catalyst of choice. Yet on it acetylene is also hydrogenated past ethylene to ethane, and its molecules couple and grow into green oil, which costs selectivity and activity. A 2023 review calls weakening the adsorption of ethylene and suppressing that coupling, to reach high selectivity with little green oil, the first and foremost challenge for palladium catalysts in industry and academia. Progress means such catalysts made by methods simple and efficient enough for industrial scale [22]. The green oil law of Equation (3.4) is a teaching closure for that chemistry.

On the control side the override reads the bed outlets and acts after the selectivity is gone, the trip is reachable in Auto after a feed cut at a fat ratio, and the MPC plans on a fresh-catalyst copy with a linear loss cost and spends more than the suggested loops. No case models a hydrogen supply upset, a regeneration or a front-end converter.

OPEN CHALLENGE Models That Age With the Catalyst

A 2003 survey of industrial predictive control found no method to verify whether a model had deteriorated after the controller was commissioned, and only two adaptive products on the market, which the authors read as the difficulty of adaptive control in the real world [16]. A 2013 review of soft sensors in the process industries names model maintenance as the most critical issue in their industrial use [21]. Progress means models that follow the plant as it changes and need no maintenance. The predictive controller of this chapter plans on a fresh-catalyst copy and meets the aging catalyst only as mismatch.

3.8 Conclusion

An acetylene converter dresses a parts-per-million specification in a selectivity problem, and this chapter's simulator measures both on two beds of 24 cells whose carbon and hydrogen close to round-off. The window is one-sided. At the design inlets the edge sits at 1.43 mol/mol, breakthrough costs 2680 t/d of product, and each tenth of a percent of loss costs 2.68 t/d. The one-site rate law reproduces self-inhibition, 31 times at the inlet, and a light-off at depletion in which, once the hydrogen is raised by hand, the loss passes 1 % in 1.58 min, well before the bed's rise reaches the trip, while it cannot reproduce carbon monoxide's measured gain in selectivity. Feedforwards from an analyzer ahead of a 20 min drum, with a log-ppm trim, pass a graded day at 0.297 %, where a fixed ratio either breaks through or spends 0.566 % and the predictive controller spends 0.354 %. A balance inference carries the feedforward through an analyzer failure, and at day 480 no setting meets the limit. A fuller model would add a second site so that carbon monoxide raises the selectivity, a predictive override on the outlet chromatograph rather than the bed outlets, and a front-end variant with hydrogen in the feed. The simulator shows that on a one-sided window the cheapest safe hydrogen is the least that clears the edge.

KEY POINTS

- Too little hydrogen puts the whole product off grade, and too much burns ethylene and moves the beds toward a runaway, so the cheapest safe hydrogen is the least that clears the edge.
- At the design inlets the edge sits at 1.43 mol/mol, breakthrough costs 2680 t/d of product, and each tenth of a percent of loss costs 2.68 t/d.
- With the hydrogen raised by hand, the loss passes 1 % in 1.58 min, well before the bed's rise reaches the trip.
- Feedforwards from an analyzer ahead of a 20 min drum, with a log-ppm trim, pass a graded day at 0.297 %.

Where else this applies. A ratio held by an analyzer trim returns in Volume 3, Chapter 6 and Volume 3, Chapter 4, and a protective override in Volume 4, Chapter 2.

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3.9 Exercises

3.1 Concept check · 2 min

The converter's lined-out window runs from a breakthrough edge near 1.43 mol/mol to the override near 2.27 mol/mol. Why does the operating point belong just on the clean side of the edge rather than in the middle of the window?

(a) The middle of the window is where the override acts, so a ratio there would fight the override

(b) The outlet chromatograph is most accurate near 1 ppm, so the trim works best close to the edge

(c) Breakthrough puts all the product off grade, while each extra mole of hydrogen costs only a little ethylene

(d) The window is symmetric, so crossing either side costs the same and any point inside it will do

3.2 Concept check · 2 min

At the design inlets the carbon monoxide in the feed rises from 2 to 5 ppm. What does the one-site rate law of this model predict?

(a) The local selectivity rises, so the loss at the 1 ppm edge falls by about half

(b) The edge moves to a lower ratio, because carbon monoxide frees sites for the acetylene

(c) Only the ethylene rate is braked, so the loss falls at every ratio while the edge stays put

(d) Both rates fall by one factor, so the edge moves to a higher ratio and its loss barely changes

3.3 Concept check · 2 min

In case 6 the hydrogen is raised by hand from 75.6 to 130 kmol/h. In the next minute bed 1's temperature rise falls from about 30 to about 26 K while the ethylene loss climbs. Why does the rise fall?

(a) The reaction moves to the front cells, and their heat reaches the outlet only after a thermal wave crosses the bed

(b) The ethylene hydrogenation absorbs heat, so the bed cools while ethylene is turned into ethane

(c) The temperature override cuts the hydrogen as soon as it is raised, which cools the bed for a minute

(d) The bed thermocouples lag by about two minutes, so the reading shown is from before the change

3.4 Theory and calculation · 8 min

Use the standard heats of formation (226.73, 52.47 and −84.0 kJ/mol for acetylene, ethylene and ethane) and the heat capacities of Section 3.3 (46.66, 29.02, 46.40 and 57.40 J/(mol K) for acetylene, hydrogen, ethylene and ethane). The design feed is 1400 mol/s of C_2 gas with 1.0 % acetylene, 79 % ethylene and 20 % ethane, plus 75.6 kmol/h of hydrogen. Neglect the carbon monoxide.

(a) Compute the heats of reaction ΔH_1 and ΔH_2. *Checkpoint:* $\Delta H_1 = -174.26\,\mathrm{kJ/mol}$, $\Delta H_2 = -136.47\,\mathrm{kJ/mol}$

(b) Compute the heat-capacity flow $\dot{F}C_p$ of the feed with its hydrogen. *Checkpoint:* 68.65 kW/K

(c) Compute the adiabatic rise from hydrogenating all the acetylene, and the extra rise from each mol/s of hydrogen that finds ethylene instead. *Checkpoint:* 35.54 K and 1.99 K

(d) At design the loss is 0.200 % of the ethylene fed and the outlet holds almost no acetylene. Estimate the total rise over both beds and compare it with the measured rises of 30.2 and 9.8 K. *Checkpoint:* 39.9 K against 40.0 K

3.5 Theory and calculation · 6 min

Case 5 raises the feed acetylene from 1.0 to 1.5 % at 10 min on a fixed ratio of 1.5 to the C_2 flow at the design 1 %. The change reaches the converter through the feed drum, a first-order lag of 20 min. At design the lined-out 1 ppm edge is at 1.433 mol/mol.

(a) What true ratio of hydrogen to acetylene does the converter see once the change has arrived in full? *Checkpoint:* 1.00

(b) Treating the beds as lined out at every instant, how long after the change does the outlet pass 1 ppm? *Checkpoint:* 1.96 min

(c) What hydrogen flow must the acetylene feedforward deliver at 1.5 % to hold the ratio at 1.5, and why does the loss rise even though the ratio is held? *Checkpoint:* 113.4 kmol/h

3.6 Theory and calculation · 7 min

Use Equations (3.1) and (3.2) with $E_A = 25$ and $E_E = 60\,\mathrm{kJ/mol}$, $Q_{CO} = 30\,\mathrm{kJ/mol}$, no temperature dependence of K_A or K_E, and the inlet values at 60 °C: $K_A p_A = 9.85$, $K_E p_E = 0.156$ and $K_{CO} p_{CO} = 1.000$. Hold the gas composition fixed and compare a catalyst at 40 °C with one at 80 °C.

(a) Compute $k_A(80\,^\circ\mathrm{C})/k_A(40\,^\circ\mathrm{C})$ and the same ratio for k_E. *Checkpoint:* 2.97 and 13.6

(b) Compute the denominator D at both temperatures and the factor $D^2(40\,^\circ\mathrm{C})/D^2(80\,^\circ\mathrm{C})$ that both rates share. *Checkpoint:* 13.00 and 11.55, factor 1.27

(c) Give the rise of each rate from 40 to 80 °C and the change in r_E/r_A. What does it say about a hotter bed? *Checkpoint:* 3.76 and 17.2, ratio up 4.58 times

3.7 App challenge · 8 min

Load case 1, The hydrogen ratio in steps, at the default seed. Before pressing Run, set the Hydrogen ratio setpoint on the FIC card to 1.30 (its shipped value), run to 10 min at speed 5 (5 min of plant per wall second) and export the CSV. Reload the case and repeat with the setpoint at 1.50, then at 1.90. Read `truth_ace_out_ppm` and `truth_loss_pct` in the 10.00 min row of each file.

(a) Give the outlet acetylene and the loss at each ratio. Use a tolerance of 0.5 ppm at 1.30 and 0.003 % on the losses. *Checkpoint:* 14.9, 0.30, 0.00016 ppm and 0.137, 0.200, 0.470 %

(b) By how many decades does the acetylene fall from 1.30 to 1.90, by what factor does the loss rise, and which step costs more ethylene per mol/mol of hydrogen: 1.30 to 1.50, or 1.50 to 1.90? *Checkpoint:* 4.97 decades, 3.43 times, the second step

(c) Price the step from 1.50 to 1.90 in tonnes of ethylene a day, with the 2680 t/d of ethylene the stream carries, and compare it with running at 1.30. *Checkpoint:* 7.2 t/d

3.8 App challenge · 8 min

Load case 6, The runaway: acetylene runs out in bed 1, at the default seed. The Hydrogen loop is on Man. Press Run at speed 1 (1 min of plant per wall second), pause near $t = 2$ min and note the clock, raise the Hydrogen flow on the FIC card from 75.6 to 130.0 kmol/h, and Run until RUNAWAY appears and the run stops. Export the CSV. To repeat the run, reload the case: Reset keeps the 130 kmol/h, and a plant started there trips in its first second.

(a) How long after your change does the trip come? Give it within 0.05 min. *Checkpoint:* 3.95 min

(b) In the CSV, what is `bed1_dT_K` in the last row before the change, and what is its lowest value after it? *Checkpoint:* 30.1 to 30.4 K, then 25.7 to 25.8 K

(c) In the first row after the change where `truth_loss_pct` exceeds 1, what does `bed1_dT_K` read, and what does that say about protecting the plant with the bed rise? *Checkpoint:* 29 to 32 K

3.9 App challenge · 9 min

Load case 9, the challenge (A day on the furnace cycle), at the default seed, and run each configuration below to 24 h at speed 60 (60 min of plant per wall second). The run stops by itself at 24 h. Read the Worst outlet sample and Average ethylene loss tiles, and hover over the So far tile for the number of samples over 1 ppm. Reload the case before each configuration and make every setting before Run.

(a) As shipped: fixed ratio 1.50, Outlet trim off. *Checkpoint:* 1079 ppm, 185 of 288, 0.192 %

(b) Hydrogen from set to Feedforwards and Outlet trim to On, with the Outlet acetylene setpoint left at 0.30 ppm. *Checkpoint:* 1.36 ppm, 12 of 288, 0.242 %

(c) As in (b), with the Outlet acetylene setpoint at 0.10 ppm. Which of the three runs pass, and why does (c) succeed where (b) fails? *Checkpoint:* 0.53 ppm, none over, 0.297 %

3.10 Application area · 4 min

Each 0.1 % of loss is 2.68 t/d of ethylene at the design feed. Over the graded day the suggested loops (feedforwards, trim at 0.1 ppm) average 0.297 % and the predictive controller 0.354 %, and both hold every sample.

(a) Convert both losses to tonnes of ethylene a day and the difference to tonnes a year. *Checkpoint:* 7.96 and 9.49 t/d, about 560 t a year

(b) Give the two reasons the chapter gives for the predictive controller spending more, and one change you would test before trusting it on a plant. *Checkpoint:* model and cost

3.11 Application area · 3 min

Case 7 compresses a catalyst run so that a minute is a day. Without a schedule the outlet first passes 1 ppm on day 137.5. With 5 K per 100 days on both inlets it holds to day 177.8, at a loss of 0.446 % on day 150 against 0.334 without it.

(a) What does the schedule buy, and what does it cost in tonnes of ethylene a day on day 150? *Checkpoint:* 40.3 days for 3.0 t/d

(b) What ends the run even with the schedule, and what does a plant do then? *Checkpoint:* regeneration

3.12 Review the agent · 5 min

An AI assistant asked to make the converter robust against breakthrough writes: “Set the hydrogen ratio setpoint to 2.2 on a fixed ratio. The window puts the override at 2.27 and the trip at 2.53, so 2.2 leaves a wide margin on the breakthrough side, and the temperature override at 55 K guarantees that no Auto setting can reach the 70 K trip.” Find the flaw in the claim and say how you would check it in the app.