INTERACTIVE CONTROL ENGINEERING
Principles and Applications

Volume 12 Control in Petrochemicals and Polymers

CHAPTER 10

Peak Temperature Control Against Ethylene Decomposition in a Tubular LDPE Simulator

Pages 226–256

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How to cite this chapter. "Peak Temperature Control Against Ethylene Decomposition in a Tubular LDPE Simulator," in *Control in Petrochemicals and Polymers*, John D. Hedengren, Ed., vol. 12 of *Interactive Control Engineering: Principles and Applications*. Advanced Process Solutions, LLC, 2026, ch. 10, pp. 226–256.

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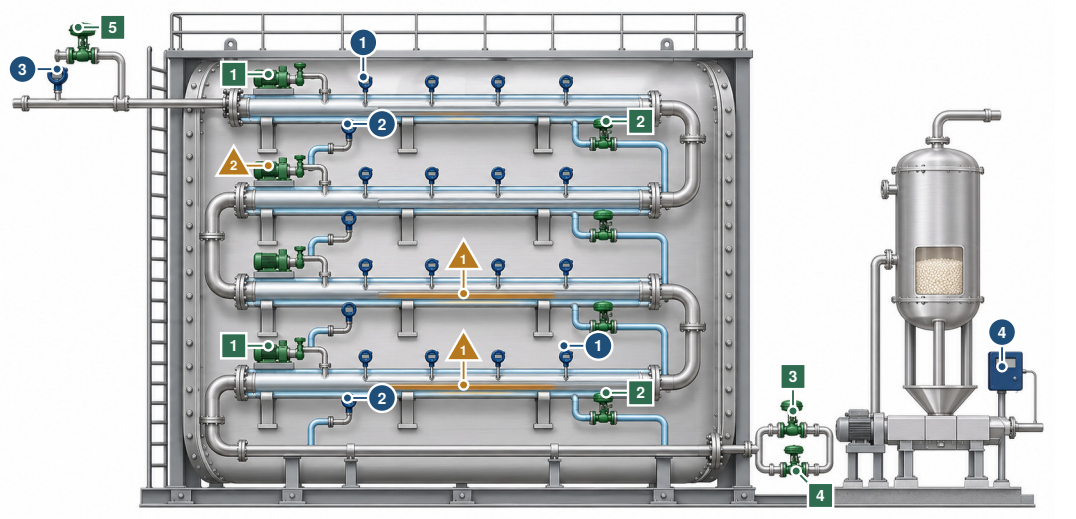
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CHAPTER 10

Peak Temperature Control Against Ethylene Decomposition in a Tubular LDPE Simulator



The controller moves 1 initiator pump at the start of each zone 2 cooler valve on each jacket's water 3 let-down valve that holds the pressure 4 pulse valve, opened on a timetable 5 chain-transfer agent feed

The controller reads 1 thermocouples along each zone, the hottest one read 2 jacket water inlet thermometers 3 reactor pressure 4 melt index of the pellets

What disturbs it 1 polymer layer on the wall 2 strength of the initiator lot

Notice the four injection points along one tube: each lights its own peak, the polymer layer on the later runs slows their cooling, and the pulse valve drops the pressure every three minutes to strip that layer. Illustration, not to scale.

IN PLAIN TERMS Four Hot Spots Kept Below a Danger Line

The main idea. Soft plastic for bags and film is made from a gas squeezed hard into a long, thin pipe. A chemical is pumped in at four places, and each one starts a short hot zone where some of the gas turns into plastic.

The challenge. Hotter zones make more plastic. Too hot, and the gas itself breaks apart. The thermometers see the heat a little late, and a planned drop in pressure every few minutes shakes every zone at once.

Why it matters. The gap kept below the danger line has to cover the worst swing the pipe ever makes, not only the steady temperature the controls aim for.

THREE WAYS TO READ THIS CHAPTER

⊘	**Explore**	12 min	This page, the two History boxes in Section 10.2, the Did you know? boxes in Sections 10.3 and 10.6, the two Try it boxes in Section 10.6, and Key points at the end of the Conclusion. No equations.
🕮	**Study**	60 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
⛰	**Practice**	20 min	This page, Section 10.6 with Figure 10.6, Section 10.7, and Section 10.8 with its Open challenge box.

The control question Four peroxide injections hold four temperature peaks a few tens of kelvin below the temperature at which ethylene decomposes, and the conversion rises with the peaks. How large must the margin to that line be when a scheduled pulse valve, late thermocouples and a changing initiator lot all make excursions that the setpoints do not show?

Learning objectives

- Compute the adiabatic rise per percent of conversion and explain why the tube converts in four separate peaks.
- Explain why a peak's gain falls as its pump strokes up, and why each zone is a disturbance to the zones after it.
- Use a feedforward keyed to the pulse schedule to stop the peak loops winding up, and measure the margin it buys.
- Size a peak setpoint from the largest excursion, the measurement error and a reserve, and explain why a trip below the line can still be too late.
- Tell a setpoint from a constraint by comparing the peak loops with a model predictive controller that carries a ceiling.

Prerequisites Sections 1.4.3 (runaway), 1.4.4 (heat removal), 1.4.8 (back-off from a limit), 1.6.1 and 1.6.2 (engine and velocity-form PID). Section 1.6.3 is needed only for the predictive controller.

The app https://apmonitor.com/apps/ldpe-tubular-reactor/

See also Volume 4, Chapter 10 and Volume 4, Chapter 9 for mid-ranging and valve-position control, and Volume 4, Chapter 2 for a protective override that guards a limit. Volume 3, Chapter 6 for a feedforward that acts before feedback sees the disturbance, and Volume 3, Chapter 2 for matching loop structure to where a disturbance enters.

10.1 Introduction

Low-density polyethylene (LDPE) is made from ethylene by free-radical polymerization at very high pressure, either in stirred autoclaves or in long jacketed tubes [1, 2]. The product matters in volume. Polyethylene is the largest group of nonfiber plastics produced, 36 % of the total, and about 42 % of all nonfiber plastics have gone into packaging [3]. The tube of this chapter is 1500 m of 55 mm bore, fed 64.8 t/h of ethylene at 2500 bar, which carries the gas through in 109 s. Peroxide is injected at four points, and each injection lights a reaction front that heats the gas by 12.8 K for every percent of ethylene it converts. Four peaks at 290 °C convert 27.51 % and make 17.8 t/h of polymer. A single front could not, because converting that much in one rise would heat the gas by 353 K, from 165 °C to about 518 °C.

Above the peaks lies the temperature at which ethylene itself decomposes, to carbon, hydrogen and methane [4]. The model draws that line at 335 °C, 45 K above the design peaks, as a teaching value. A tempting reading of that gap holds that a peak kept on its setpoint by a well-tuned loop is as safe as the distance from its setpoint to the line, and the simulator is built to show why that reading fails. With all four loops at 290 °C, the pulse valve that the plant opens every three minutes takes the hottest thermocouple to 299.7 °C once the pressure has recovered, because the loops wound their pumps up while the pulse held the peaks down. During that recovery the hottest gas runs 10.9 K ahead of every thermocouple. An initiator lot twice as strong as the one the loops have adapted to sets off a 320 °C trip 25 s after it arrives, and a high-high trip set 5 K below the line fires 1.5 s before a decomposition it does not prevent, since it stops the pumps and not the initiator already in the gas, while a trip one 1 s scan earlier leaves 1.4 K. Excursions set the margin, and the setpoint is what they leave.

This shape recurs well beyond polyethylene. A tubular reactor with a steeply temperature-dependent reaction can be parametrically sensitive, so that a small change in the wall heat-transfer coefficient or a small dilution of the feed produces a large change in what leaves it [5], as Section 1.4.3 sets out and as the ethylene oxide tube of Chapter 6 shows on a catalyst bed. In the LDPE tube the

wall changes on its own, because polymer deposited on it lowers the heat-transfer coefficient and, in rare cases, the lost heat removal leaves hot spots that trigger decomposition [6]. Excess initiator, a feed impurity, a feed temperature disturbance, a failed controller and a poorly tuned one each drive an LDPE autoclave toward runaway [7]. A slow actuator that keeps a fast one inside its range is the mid-ranging structure, used wherever a small fast valve works beside a large slow one [8], as on the power block of Volume 4, Chapter 10, and a disturbance that arrives on a timetable is a case for feedforward rather than for feedback [9]. A sensitive hot spot, a fine valve kept in range by a coarse one, a disturbance on a schedule and an interlock that must act inside the process's own dead time are each familiar from other plants, and in the LDPE tube all four meet.

The published models of the tubular process were written to predict, fit and optimize a plant [1, 10–12], and none of them hands a student four pumps, a pulse valve and a trip and counts the cost of each choice in kelvin of margin. This chapter makes the margin to decomposition a measured quantity, on a tubular LDPE reactor built to run in a browser, whose gas is carried as parcels that ride the flow, whose thermocouples see that gas late and in pieces, and whose decomposition is an event that ends the run rather than a soft penalty. The kinetics are illustrative, and PI peak control, pulse feedforward, mid-ranging and a high-high trip are established practice. The optional model predictive controller follows the industrial form, a receding-horizon quadratic program on a model identified from plant step tests with a soft constraint on each output [13], as Section 1.6.3 describes.

The chapter runs as follows. Section 10.2 traces the process from the high-pressure laboratory to the pulsed tube. Section 10.3 states the model, a 1021-state model whose energy balance closes parcel by parcel and whose mass balance is its pressure equation, on a Lagrangian grid that keeps plug-flow kinetics exact where fixed well-mixed cells cannot, with every constant given. Section 10.4 measures how a peak forms and what moves it, among them a peak gain that falls from 1.9 to 0.6 K per percent of pump stroke while the peak moves toward its injector. Section 10.5 describes the thirteen loops, the pulse feedforward, the trip and the supervisor, and a model predictive controller on the four pumps whose model was fitted to step tests of the simulator and is given with its residuals. Section 10.6 reports nine cases and a four-hour challenge, which separate a peak from its measurement, feedback from a scheduled disturbance, a slow handle from the pump it serves, a setpoint from a margin, and a request from a constraint, and which measure the margin a scheduled pulse costs with and without feedforward. Section 10.7 names the hardware and the practice behind the model, Section 10.8 states the limitations and Section 10.9 sums up.

10.2 From a High-Pressure Laboratory to the Pulsed Tube

The high-pressure route to polyethylene came out of a laboratory that was studying how pressure changes organic reactions [14], a discovery told as a case history [15] and in the first History box below. The process that grew from it still polymerizes ethylene by free radicals at pressures of that order, in stirred autoclaves or in long jacketed tubes [1, 7], with the reaction started by oxygen, by organic peroxides or by both [12].

> ⧖ HISTORY **Polythene Out of a High-Pressure Laboratory, 1930s**
>
> In 1935 three chemists reported how pressure changes reactions in solution, taking one reaction to 3000 kg/cm^2 and another to 8500 kg/cm^2 [14]. Polyethylene was invented in the same decade by a British chemical company, and its process needed extreme pressures of 20 to 30 thousand pounds per square inch [16]. When Karl Ziegler's group made polyethylene at normal pressure at the end of 1953, the British product had been known for some seventeen years and was made at 1000 to 2000 atmospheres and about 200 °C. In that process the chain grows with interruptions, so the molecule is strongly branched [17]. The branches make the polymer soft, tough and flexible, with a density between 915 and 935 kg/m^3. Its value was first established as insulation for electric cables, and film is its most popular use today [18].

Models of the tube arrived with the computer. A model published in 1976 assumed plug flow without axial mixing and computed the axial temperature profile, the conversion and the molecular weights and their distribution along the reaction coordinate [10], the plug-flow assumption this simulator keeps. The kinetics of olefin polymerization in high-pressure tubes were reviewed and updated in 1992 [2], and the modeling, optimization and quality control of these reactors were reviewed together in 1993 [1]. Models of industrial tubes then had to account for the wall. An improved model for industrial tubular reactors appeared in 1996 [11], and the same authors noted that the zones of such reactors exhibit different flow patterns and critical fouling behavior, so that neither a constant heat-transfer coefficient nor the usual Nusselt correlations predicts the temperature profiles accurately enough [19]. A reduced model built for the periodic parameter updates of a plant had to include the pressure pulse equations, and it treated each peroxide mixture as one fictitious initiator [12], which is the simplification the simulator makes zone by zone. Optimization followed the models, and a nonlinear model predictive control strategy for the operation of these tubular reactors was reported in 2009 [20].

The hazard was studied alongside, in a kinetic model of an autoclave that could run away [7] and in experiments on the decomposition boundary of ethylene and its comonomers [4], as the second History box tells. Models of a whole plant joined the reactor to the rest of the process [21], and the mechanisms by which polymer fouls the wall have been set out for a reactor that must remove about half of its heat of polymerization to the jacket water [6]. These studies describe the arrangement that the simulator implements, a tube divided into zones [19] with initiator injected along it and a pressure that is pulsed [12], though none of them can switch a piece off and read what it costs.

> ⧖ HISTORY **Mapping Where Ethylene Gives Way, 1996 and 1999**
>
> The hazard behind this chapter's line was mapped in the 1990s. A kinetic model of a stirred autoclave published in 1996 added free-radical reactions for the decomposition of ethylene to the usual initiation, propagation and termination steps, so that a simulated reactor could run away, and its stability analysis gave safe operating limits for typical conditions [7]. In 1999 an experimental study filled ethylene mixed with comonomers into a preheated autoclave at up to 450 °C and 150 MPa. Depending on the starting pressure and temperature, each mixture either polymerized stably or polymerized with decomposition. Vinyl acetate and methyl methacrylate lowered the boundary between the two outcomes, while acrylic acid, 1-butene and 1-hexene raised it [4].

10.3 The Tube as Modeled

One tube of length $L = 1500\,\text{m}$ and bore $D = 55\,\text{mm}$ is simulated, fed $F_{in} = 18.0\,\text{kg/s}$ of ethylene by a hyper-compressor through a preheater at $T_{in} = 165\,^\circ\text{C}$, and discharged through a let-down valve and a pulse valve to a high-pressure separator at $P_{sep} = 250\,\text{bar}$. Its four zones begin at 0, 380, 750 and 1120 m, their injectors sit 15 m into each zone, and every symbol in the equations below appears in Figure 10.1.

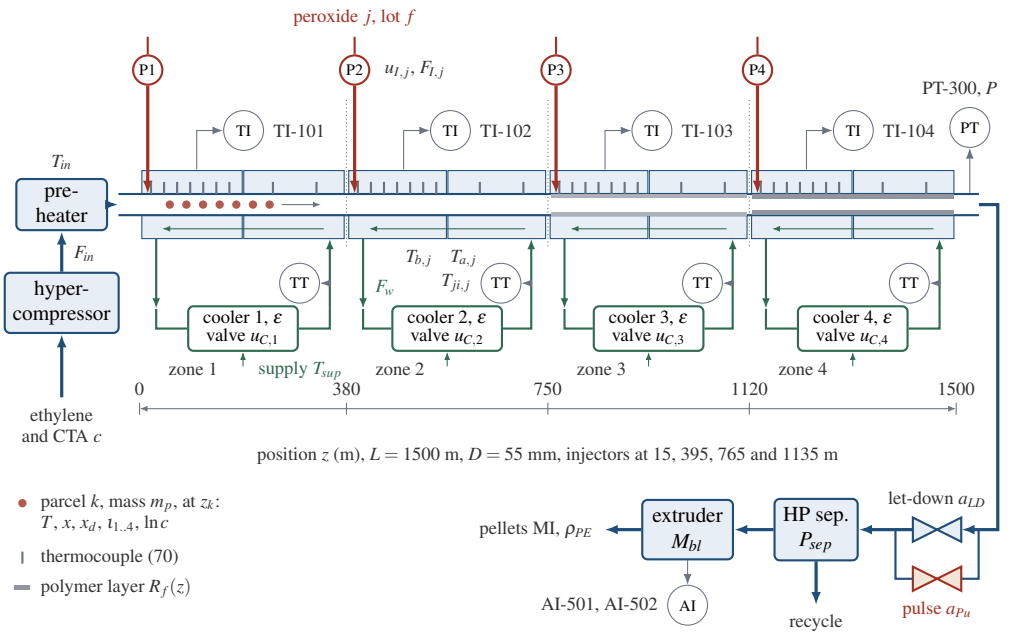


Figure 10.1 High-pressure tubular LDPE reactor as modeled. Ethylene with its chain-transfer agent (CTA) enters at F_{in} and T_{in} and crosses four zones of tube as parcels k of mass m_p at positions z_k. Pumps P1 to P4 inject peroxide $F_{I,j}$ at stroke $u_{I,j}$ from lots of efficiency f. Each zone's jacket water F_w enters its downstream section at $T_{ji,j}$, crosses sections a and b counter-current to the gas and returns through a cooler of effectiveness ε whose valve $u_{C,j}$ sets the share cooled by supply water at T_{sup}. Seventy thermocouples feed TI-101 to TI-104, the hottest of each zone, PT-300 reads the pressure P, TT-201 to TT-204 the jacket inlets, and AI-501 and AI-502 the pellets that leave the separators and extruder hold-up M_{bl}. The let-down valve a_{LD} and the pulse valve a_{Pu} discharge to the separator at P_{sep}. Labels drawn on zone 2 apply to every zone, and the polymer layer $R_f(z)$ is drawn thickest where the model grows it, in zones 3 and 4. The outlet line runs down the right edge to the valves, the separator and the extruder, drawn in a second row under the tube.

> **DID YOU KNOW? A Kilometer or Two of Thick-Walled Pipe**
>
> Commercial tubular reactors are typically 1000 to 2500 m long, built of high-pressure tubes 10 to 15 m long laid in a serpentine inside a concrete bay. The outside diameter of a tube is 2.1 to 2.5 times its inside diameter. Such a tube converts up to 36 % of its ethylene, an autoclave about 20 % [18].

Table 10.1 sorts the variables by role. The state vector holds 1021 entries, 12 states in each of 78 parcel slots, 20 lumped states, 5 ledgers and 60 wall segments. Inside the physics the units are SI, with temperatures in °C and pressures in bar, while the engine's clock runs in minutes.

10.3.1 Parcels That Ride the Gas

The tube is cut into $N = 70$ parcels of equal mass. Parcel k owns the slice of the cumulative feed between km_p and $(k+1)m_p$, so its center lies where Equation (10.1) puts it.

$$z_k(t) = \frac{M_{in}(t) - (k+\tfrac{1}{2})\,m_p}{\rho(P)\,A}, \qquad \frac{\mathrm{d}M_{in}}{\mathrm{d}t} = F_{in}$$
$$\rho(P) = \rho_0\left[1 + \kappa\,(P - P_{ref})\right], \qquad m_p = \frac{\rho_0 A L}{N} \tag{10.1}$$

Table 10.1 Variables by Role, With Their Values at the Design Point of Cases 2 and 3. Strokes, Valves and Ranges of MVs in Percent

Tag or symbol	Role	Design point	Range
TI-101 to 104	CV, hottest TC	290 °C SP	250–335
TT-201 to 204	CV, jacket inlet	175 °C SP	140–240
PT-300	CV, pressure	2500 bar SP	2000–3000
AI-501	CV, melt index	2.0 SP	0.5–8
Δ_{dec}	constraint, truth	44.7 K	≥ 0
$u_{I,1..4}$	MVs, pumps	36.3, 34.5, 36.5, 35.8	0–100
$u_{C,1..4}$	MVs, coolers	32.7, 35.5, 35.8, 36.3	0–100
a_{LD}	MV, let-down	50.0	0–100
c	MV, CTA (mol ppm)	1500	100–5000
a_{Pu}	scheduled, pulse	0, 0.25 open	—
f	DV, lot, unmeasured	100 % of 0.6	25–150
T_{sup}	DV, supply water	140 °C	100–200
T_{in}	DV, feed	165 °C	140–190
—	DVs, fouling, events	100 %, missed pulse, kick	0–500
$T, x, x_d, \iota_{1..4}$	states, parcel	see text	—
$\ln c, Q_r, Q_j, \Lambda, \Phi$	states, parcel	see text	—
P, M_{in}	states	2500 bar	—
$a_{LD}, a_{Pu}, s_{1..4}$	states, actuators	as above	—
$T_{a,j}, T_{b,j}, T_{ji,j}$	states, jackets	181, 188, 175 °C	—
$R_{f,1..60}$	states, wall	0 at reset	—

where $A = \pi D^2/4 = 2.376 \times 10^{-3}\,\mathrm{m}^2$, $\rho_0 = 550\,\mathrm{kg/m}^3$ at $P_{ref} = 2500\,\mathrm{bar}$ and $\kappa = 6.3 \times 10^{-5}\,\mathrm{bar}^{-1}$, so $m_p = 28.0\,\mathrm{kg}$ and each parcel is 21.4 m long. At the design flow the gas moves at 13.78 m/s and stays 108.9 s. When the pressure falls, ρ falls with it and every z_k grows in proportion, so parcels near the outlet move out fastest, which is the velocity profile of a compressible plug. Parcels are created at the inlet at T_{in} carrying the feed's CTA and leave once their rear has passed the outlet, and 78 slots hold them.

A fixed grid of well-mixed cells was tried and rejected. A cell of 21 m holds its radicals for its whole 1.5 s residence, while the initiator near a peak lives 25 to 190 ms, since its decomposition constant between 290 and 320 °C lies between 5.3 and 40 s^{-1}. At the initiator flows that give 290 °C peaks in plug flow, grids of 60, 70, 80 and 200 upwind cells have no steady state in their first cell short of decomposition. Parcels keep the plug-flow kinetics exact, because each one is a batch reactor that never mixes with its neighbors.

10.3.2 Initiators, Radicals and Heat

Each parcel carries four initiator concentrations, its conversion, the fraction of its ethylene decomposed, its temperature and the logarithm of its CTA, with the radicals in quasi-steady balance with termination, as shown in Equation (10.2).

$$\begin{aligned}
\frac{\mathrm{d}\iota_j}{\mathrm{d}t} &= -k_{d,j}\,\iota_j, \qquad j = 1,\ldots,4 \\
w = \frac{\mathrm{d}x}{\mathrm{d}t} &= G(1-x-x_d)\sqrt{2f\rho\textstyle\sum_j k_{d,j}\,\iota_j} \\
\frac{\mathrm{d}x_d}{\mathrm{d}t} &= k_{dec}\,(1-x-x_d) \\
c_p\,\frac{\mathrm{d}T}{\mathrm{d}t} &= \frac{-\Delta H_p}{M_w}\,w + \frac{-\Delta H_{dec}}{M_w}\,\frac{\mathrm{d}x_d}{\mathrm{d}t} - \frac{4U}{\rho D}\,(T - T_j) \\
\frac{\mathrm{d}\ln c}{\mathrm{d}t} &= -\frac{C_s\,w}{1-x-x_d}
\end{aligned} \tag{10.2}$$

where ι_j is initiator j in mol/kg, f its efficiency, x the conversion, x_d the fraction decomposed, c the CTA in mol/kg, $M_w = 28.05\,\mathrm{g/mol}$, $c_p = 2600\,\mathrm{J/(kg\,K)}$, $-\Delta H_p = 93.6\,\mathrm{kJ/mol}$, $-\Delta H_{dec} =$

120 kJ/mol, $C_s = 0.3$ and T_j is the jacket water the parcel passes. The rate constants follow Equation (10.3), with R the gas constant, T in kelvin and $P - P_{ref}$ in pascals inside the exponentials.

$$\begin{aligned} k_{d,j} &= \frac{\ln 2}{1\,\mathrm{s}} \exp\!\left[\frac{E_d}{R}\left(\frac{1}{T_{h,j}} - \frac{1}{T}\right) - \frac{\Delta V_d\,(P - P_{ref})}{RT}\right] \\ G &= G_{ref} \exp\!\left[\frac{E_G}{R}\left(\frac{1}{T_G} - \frac{1}{T}\right) - \frac{\Delta V_G\,(P - P_{ref})}{RT}\right] \\ k_{dec} &= k_{dec,0} \exp\!\left[\frac{E_{dec}}{R}\left(\frac{1}{T_D} - \frac{1}{T}\right)\right] \end{aligned} \tag{10.3}$$

Here $G = k_p/\sqrt{k_t}$ is one lumped constant, $G_{ref} = 0.30\,(\mathrm{m^3/(mol\,s)})^{1/2}$ at $T_G = 280\,^\circ\mathrm{C}$ with $E_G = 29\,\mathrm{kJ/mol}$ and $\Delta V_G = -29.5\,\mathrm{cm^3/mol}$, the four peroxides share $E_d = 90\,\mathrm{kJ/mol}$ and $\Delta V_d = 6\,\mathrm{cm^3/mol}$ and have one-second half-lives at $T_{h,j} = 212$, 228, 232 and 236 °C, and $k_{dec,0} = 5 \times 10^{-3}\,\mathrm{s^{-1}}$ at $T_D = 335\,^\circ\mathrm{C}$ with $E_{dec} = 450\,\mathrm{kJ/mol}$. Decomposition is left out below 260 °C, where it runs at less than 4×10^{-6} of its rate at 335 °C. Three consequences follow from these constants. The adiabatic rise $-\Delta H_p/(M_w c_p)$ is 12.83 K per percent of conversion. The square root rewards a slow supply of radicals, so a dose decomposed quickly makes less polymer per mole than the same dose decomposed slowly. And the negative activation volume makes a pulse that drops 300 bar slow the polymerization by 17 % at 290 °C.

The wall's coefficient is $U = [1/U_c + R_f(z)]^{-1}$, where the clean value $U_c = U_0\,[\varphi_{in} + (\varphi_{out} - \varphi_{in})\,z/L]$ follows the velocity with $\varphi = (F/F_{in,0})^{0.8}$ evaluated at the inlet and outlet flows, $F_{in,0} = 18.0\,\mathrm{kg/s}$ being the design feed, and $U_0 = 800\,\mathrm{W/(m^2\,K)}$. For a clean wall $4U/(\rho D) = 105.8\,\mathrm{W/(kg\,K)}$, which cools a parcel with a time constant of 24.6 s. Each parcel also integrates the heat it has made Q_r, the heat it has given the jacket Q_j, and the polymer-weighted integrals Λ and Φ of the quality correlations below, which makes 12 states.

10.3.3 Pressure, Valves and Pumps

The tube's mass balance is its pressure equation, as shown in Equation (10.4).

$$C\,\frac{\mathrm{d}P}{\mathrm{d}t} = F_{in} - C_v\,(a_{LD} + a_{Pu})\sqrt{P - P_{sep}} \tag{10.4}$$

where $C = \rho_0 A L \kappa = 0.1235\,\mathrm{kg/bar}$, and the valve coefficient $C_v = 0.759\,\mathrm{kg/(s\,bar^{1/2})}$ is set so that the let-down passes the design flow at P_{ref} with an opening of $a_{nom} = 0.5$. With the let-down held, the pressure answers a change in flow with a time constant of 30.9 s. The let-down follows its command through a 0.5 s lag, the pulse valve through 0.3 s to an extra opening of 0.25 while it is open, and the pump strokes s_j through 1.0 s. A pump delivers $F_{I,j} = s_j F_{I,max,j}$, with 13.0 mmol/s at full stroke for pump 1 and 3.8 mmol/s for pumps 2 to 4, and the panels convert moles at 216 g/mol. At the design point the pumps deliver 4.71, 1.31, 1.39 and 1.36 mmol/s.

10.3.4 Jackets and the Polymer Layer

Each zone's water runs counter-current through two well-mixed sections and returns through a cooler whose valve sets the share of it that is cooled, as shown in Equation (10.5).

$$\begin{aligned} m_s c_w\,\frac{\mathrm{d}T_{a,j}}{\mathrm{d}t} &= F_w c_w\,(T_{ji,j} - T_{a,j}) + Q_{a,j} \\ m_s c_w\,\frac{\mathrm{d}T_{b,j}}{\mathrm{d}t} &= F_w c_w\,(T_{a,j} - T_{b,j}) + Q_{b,j} \\ \tau_J\,\frac{\mathrm{d}T_{ji,j}}{\mathrm{d}t} &= T_{b,j} - u_{C,j}\,\varepsilon\,(T_{b,j} - T_{sup}) - T_{ji,j} \end{aligned} \tag{10.5}$$

where section a is the downstream half that the water enters first, $Q_{a,j}$ and $Q_{b,j}$ are the rates at which the parcels gave up heat in each section over the step, $m_s = 2000\,\mathrm{kg}$, $c_w = 4186\,\mathrm{J/(kg\,K)}$,

$F_w = 60\,\mathrm{kg/s}$, $\varepsilon = 0.8$ and $\tau_J = 20\,\mathrm{s}$. A parcel sees as T_j the time-weighted mean of the sections its center crosses during the step, and a parcel already past the outlet sees no jacket. At the design point the inlets hold 175 °C, the downstream sections run near 181 °C and the water returns at 187.4 to 189.3 °C.

A polymer layer grows on each of 60 wall segments of 25 m, where the wall is colder than the cloud point of the polymer in the gas, as shown in Equation (10.6).

$$\begin{aligned} \frac{\mathrm{d}R_{f,i}}{\mathrm{d}t} &= g_0 \,\frac{T_{cl} - T_w}{10\,\mathrm{K}}\, \min\!\left(2, \frac{x}{0.2}\right) \\ T_{cl} &= T_{c0} + T_{c1}\,x, \qquad T_w = \tfrac{1}{2}\,(T + T_j) \end{aligned} \tag{10.6}$$

applied while $T_w < T_{cl}$ and $x > 0.005$, once a second, with $g_0 = 4 \times 10^{-7}\,\mathrm{m^2\,K/(W\,s)}$ scaled by the fouling-rate disturbance, $T_{c0} = 150\,^{\circ}\mathrm{C}$ and $T_{c1} = 300\,\mathrm{K}$. Each completed pulse that lowered the pressure by ΔP_p multiplies every $R_{f,i}$ by $1 - \min(0.9,\, \phi_p \Delta P_p / 300\,\mathrm{bar})$ with $\phi_p = 0.3$. The law is illustrative.

10.3.5 Decomposition as an Event

A parcel held above $T_{dec} = 335\,^{\circ}\mathrm{C}$ for $t_{dwell} = 1.0\,\mathrm{s}$ decomposes. The event reports a local temperature of $T + (-\Delta H_{dec}/M_w c_p)(1 - x - x_d)$ and a pressure 700 bar above the operating one, both illustrative, bursts the rupture discs, shuts the plant down and stops the run. The threshold and the dwell are teaching values. The kinetics of Equation (10.3) give the choice a physical reading. At a conversion of 27 % the decomposition heats a spent parcel by 0.005 K/s at 290 °C, 0.63 K/s at 320 °C, 6.0 K/s at 335 °C and 12.4 K/s at 340 °C, and at 335 °C the clean jacket removes about 6 K/s from such a parcel, so above the line the decomposition wins. The limits of a real reactor come from its licensor's process-safety data, from the plant's own decomposition history and from measured decomposition boundaries such as those of ethylene and its comonomers [4], not from this model. The margin $\Delta_{dec} = T_{dec} - T_{hot}$ is judged on the hottest parcel in the tube, the truth, and the scorecard keeps its worst value over the run.

10.3.6 Product Quality and the Instruments

Melt index and density are illustrative correlations of the CTA, of the temperature at which the polymer is made and of the pressure, as shown in Equation (10.7).

$$\begin{aligned} \ln \mathrm{MI} &= \ln \mathrm{MI}_{ref} + a_C \ln \frac{c}{c_{ref}} + a_T\,(T - T_Q) \\ \rho_{PE} &= \rho_{ref} - b_T\,(T - T_Q) + b_P\,(P - P_{ref}) \end{aligned} \tag{10.7}$$

Each parcel accumulates $\mathrm{d}\Lambda/\mathrm{d}t = w \ln \mathrm{MI}$ and $\mathrm{d}\Phi/\mathrm{d}t = w\rho_{PE}$, so the polymer it carries has the melt index $\exp(\Lambda/x)$ and the density Φ/x of all it has made. The constants are $\mathrm{MI}_{ref} = 2.0\,\mathrm{g/10\,min}$ at $c_{ref} = 1500\,\mathrm{mol\,ppm}$ and $T_Q = 261.5\,^{\circ}\mathrm{C}$, $a_C = 1.0$, $a_T = 0.025\,\mathrm{K^{-1}}$, $\rho_{ref} = 0.9235\,\mathrm{g/cm^3}$, $b_T = 3.5 \times 10^{-4}\,\mathrm{g/(cm^3\,K)}$ and $b_P = 4 \times 10^{-6}\,\mathrm{g/(cm^3\,bar)}$. Parcels leaving the tube mix into one hold-up of $M_{bl} = 2500\,\mathrm{kg}$ of polymer for the separators and the extruder, each moving the pellets' ln MI and density toward its own by the fraction $\min(1, m_p x / M_{bl})$. At the design rate of 17.8 t/h the hold-up is 8.4 min of production, and the pellets are at 1.379 g/10 min and $0.92806\,\mathrm{g/cm^3}$.

No loop reads a parcel. Thermocouples sit every 12 m from 6 m to 150 m after each injector, then every 40 m from 190 m after it to the end of the zone, 70 in all. Each samples a parcel's temperature as that parcel's center crosses it, interpolated quadratically in time within the step, and adds a 1.5 s thermowell lag and 0.3 K of white noise at each scan, and TI-10j is the hottest of zone j. PT-300 has a 0.3 s lag and 1.5 bar of noise, and TT-201 to TT-204 have 3 s and 0.1 K. The melt indexer AI-501 and the laboratory density AI-502 are the framework's shared sampled analyzer. AI-501 draws from the hold-up every 6 min through a 2 min sample line and reports 6 min later with 0.02 g/10 min of noise, so its reading is at least 8 min old, and the laboratory reports density 30 min after an hourly sample with $0.0002\,\mathrm{g/cm^3}$ of noise.

Table 10.2 Model Constants. Visible Ones Can Be Moved in the Show Model Panel, Hidden Ones Only in the Source

Symbol	Meaning	Value	In panel
F_{in}	ethylene feed	64.8 t/h	visible
ρ_0, κ	density, compressibility	550, 6.3×10^{-5}	hidden
P_{ref}, P_{sep}	reference, separator	2500, 250 bar	hidden
a_{nom}	let-down at design	0.5	hidden
c_p	heat capacity	2600 J/(kg K)	visible
$-\Delta H_p$	heat of polymerization	93.6 kJ/mol	visible
f	initiator efficiency	0.6	visible
G_{ref}, E_G	$k_p/\sqrt{k_t}$ at 280 °C	0.30, 29	visible
ΔV_G	its activation volume	−29.5 cm^3/mol	visible
E_d	peroxide activation energy	90 kJ/mol	visible
$T_{h,1..4}$	one-second half-life	212, 228, 232, 236 °C	visible
ΔV_d	peroxide activation volume	6 cm^3/mol	hidden
C_s	chain-transfer constant	0.3	visible
T_{dec}, t_{dwell}	decomposition, dwell	335 °C, 1.0 s	visible
$k_{dec,0}$, E_{dec}	rate, activation	5×10^{-3}, 450 kJ/mol	visible
$-\Delta H_{dec}$	heat of decomposition	120 kJ/mol	hidden
U_0, F_w	clean wall, water	800, 60 kg/s	visible
m_s, τ_J	section water, cooler lag	2000 kg, 20 s	hidden
ε	cooler effectiveness	0.8	visible
g_0, ϕ_p	fouling growth, pulse strip	4×10^{-7}, 0.3	visible
T_{c0}, T_{c1}	cloud point	150 °C, 300 K	hidden
MI_{ref}, c_{ref}, T_Q	quality reference	2.0, 1500, 261.5	hidden
a_C, a_T	melt-index slopes	1.0, 0.025 K^{-1}	visible
ρ_{ref}	density reference	0.9235 g/cm^3	hidden
b_T, b_P	density slopes	3.5×10^{-4}, 4×10^{-6}	visible
M_{hl}	product hold-up	2500 kg	hidden
$F_{I,max}$	pump 1, pumps 2 to 4	13.0, 3.8 mmol/s	hidden
—	pump, let-down lags	1.0, 0.5 s	hidden
—	pulse stroke, longest	0.25, 10 s	both

Units where not shown: ρ_0 in kg/m^3, κ in bar^{-1}, G_{ref} in $(m^3/(mol\,s))^{1/2}$, E_G in kJ/mol, $k_{dec,0}$ in s^{-1}, U_0 in W/(m^2 K), g_0 in m^2 K/(W s), MI_{ref} in g/10 min, c_{ref} in mol ppm, T_Q in °C, b_T in g/(cm^3 K), b_P in g/(cm^3 bar).

10.3.7 Numerics, Initialization and Checks

The parameters are collected in Table 10.2. The tube advances on a fixed step of 0.25 s. Within a step the hydraulics of Equation (10.4) and the actuator lags are advanced first, with one classical fourth-order Runge-Kutta step, every parcel then moves between its exact start and end positions, and the jackets of Equation (10.5) are advanced last with the parcels' heat for the step. Near a peak the initiator decay is stiff, with $k_d\,\Delta t$ up to 10, so each parcel is advanced by Lawson's integrating-factor form of the Runge-Kutta method with $k_{d,j}$ frozen over a substep, and the substep is shortened until T moves at most 10 K across it at its starting rate. Case 3 needs at most four substeps. A parcel with no initiator below 300 °C is cooled by the exact exponential and its slow decomposition added explicitly. The initiator injected since the previous parcel passed an injector enters the next parcel at the instant its center passes, inside the step. The controllers run every 1 s, at the start of the physics step that begins each whole second, a scripted event acts at the start of the step at its time, the historian logs one row a second, and the random sequence is seeded at 20260927, so every run replays bit for bit, as Section 1.6.1 describes for every framework app.

Each scenario opens on the steady tube of its own configuration, and a setting changed before Run, or carried through Reset, rebuilds the steady tube for the settings in force, so a case started with its peak loops at 310 °C starts from 310 °C peaks. A setting no steady tube can hold, such as a closed cooler or a setpoint at the line, starts the tube from the scenario's own settings and then acts as a step. One parcel is marched from the inlet with the engine's own step, the two sections of each jacket are iterated to their balance, and in each zone under automatic control the initiator flow is found by regula falsi so that the zone's hottest thermocouple sits on its setpoint. Every parcel is

then marched from its own entry on the same step grid. Held there in MANUAL with the fouling off, no thermocouple moves by more than 0.18 K in a minute. The parcel, tube and jacket energy ledgers close to 3.8×10^{-15} relative through pulses, fouling and the decomposition of case 5, and $C\,\Delta P$ matches the integrated feed less the let-down to 5.6×10^{-16}. The same initiator flows on 60 or 80 parcels move the steady thermocouple peaks at 300 °C by at most 0.073 K (0.23 K at 290 °C) and the conversion by 0.007 points, halving the step moves the steady peaks by 0.021 K and both the dip and the overshoot of case 3's first pulse by 0.10 K, and a parcel with no cooling heats by 12.834 K per percent of conversion. These checks are among the 55 that the application passes. The speed selector runs from 0.05 to 60 simulated minutes per second, with 0.2 as the default, and the top rung is set by the 68 800 steps a second the browser sustains. At the default speed a pulse of 5.75 s passes in under half a second, and the four-hour challenge plays in four seconds at the top speed.

10.3.8 Assumptions

The tube is plug flow in parcels that are each well mixed, with no axial dispersion, and a parcel receives its injected initiator all at once. This breaks down wherever turbulence mixes neighboring gas over the length of a reaction front, and it makes the drawn profile's tip move by about 2 K from frame to frame as parcels pass the peak.

The kinetics are illustrative, with one lumped $k_p/\sqrt{k_t}$, radicals in quasi-steady balance, four peroxides that share one activation energy, and no transfer to polymer, long-chain branching, molecular-weight distribution or thermal initiation. The lot efficiency is carried with each dose, so a lot change reaches only the initiator pumped after it, and the switch between lots is instantaneous. The kinetics give peaks, conversions and initiator use of the right order and are calibrated to no plant, so a question about molecular weight, branching or a real peroxide's half-life lies outside the model.

The density follows the pressure but not the temperature, so the velocity varies along the tube only while the pressure moves, and the expansion cooling of a pulse is left out, although a 300 bar pulse expands the gas by 1.9 %. The polymer's separation from ethylene enters only as the cloud point that grows the layer, and the model stops being valid below about 2000 bar, above about 340 °C and above about 36 % conversion.

Each jacket is two well-mixed sections with a velocity-scaled clean coefficient, too coarse to resolve the water's profile along a section, and the fouling law is illustrative. The decomposition is a declared event with no model of what follows it, so nothing after the event is physical. The quality correlations are illustrative and hold only near the grade they were written for, the separators and extruder are one well-mixed hold-up, and the analyzers never fail. Pumps and valves are first-order lags without stiction, the hyper-compressor delivers a fixed mass flow whatever the pressure does, and the sizes and limits describe one teaching reactor rather than a design basis.

10.4 How a Peak Forms and What Moves It

A peak is a small runaway limited by its initiator and lit on purpose. At the design point the gas reaches injector 2 at 225.8 °C, where its peroxide decomposes at 0.63 s^{-1}. The polymerization heats the gas, the hotter gas decomposes the rest of the peroxide faster, 7.5 s^{-1} at 290 °C, and within 28.2 m, about 2 s of travel, the initiator is spent and the jacket takes over. Zone 1's gas arrives at only 167.9 °C, where its faster peroxide decomposes at 0.075 s^{-1}, and its peak forms 53.5 m after the injector. The conversion climbs in steps, 9.94, 15.63, 21.58 and 27.51 % at the ends of the four zones, and the gas leaves at 224.8 °C.

A larger dose heats the gas faster, so the rest of the initiator decomposes sooner and the front burns out earlier. The peak therefore rises and moves toward its injector, as shown in Figure 10.2. Between 5 and 80 % of stroke, zone 2's hottest thermocouple rises from 245.4 to 319.4 °C, and the hottest gas moves from 55.8 to 17.9 m after the injector. The gain falls as the stroke rises, 1.9 K per percent at 10 to 15 % and 0.6 K at 45 to 55 %, so one tuning is a compromise across a pump's range. The measurement adds its own distortion. The hottest thermocouple jumps from the one 54 m after

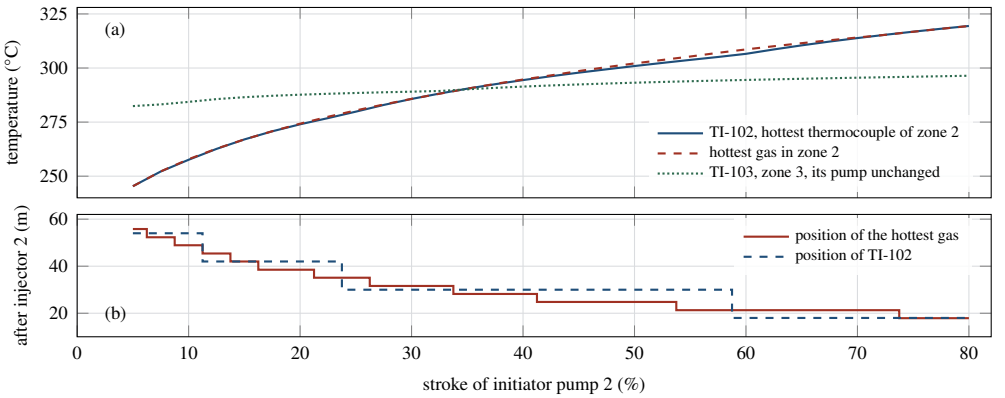


Figure 10.2 Steady peak of zone 2 against the stroke of its pump, from the application's steady solver with the other pumps at their design strokes and the jacket inlets at 175 °C. The measured peak rises with a slope that falls from 2.7 to about 0.5 K per percent while the hottest gas moves from 56 to 18 m after the injector, and the hottest thermocouple hops between readings 12 m apart. The position of the hottest gas is resolved to the 3.4 m a parcel moves in one step. In (a) TI-102 is solid, the hottest gas dashed and TI-103 dotted, and in (b) the hottest gas is solid and TI-102 dashed.

the injector to those at 42, 30 and 18 m as the peak moves, and at 55 % of stroke it reads 303.8 °C while the gas between two thermocouples reaches 305.3 °C.

🕮 **Pause.** Try Exercise 10.2 before reading on.

The zones are coupled one way. With its own pump unchanged, zone 3's hottest thermocouple rises from 282.4 to 296.4 °C as pump 2 goes from 5 to 80 %, because zone 2's hotter tail is the gas into which zone 3's initiator is injected. Open-loop steps in MANUAL from the design point measure the plant each loop sees, each read against an otherwise identical unstepped run. A 5 % step of pump 2 raises the lagged TI-102 by 4.06 K at 180 s, 0.81 K per percent, with the first 6 % of the change at the scan 3 s after the step, 41 % at 5 s and 63 % by 7 s, so the peak loop's plant is roughly 4 s of dead time and 2 s of lag. Zone 3 feels the same step only after 30 s, most of it the travel from zone 2's peak to injector 3, and gains 1.49 K by 180 s as jacket 2 warms.

A jacket acts mainly on the zone after it. Opening cooler 2 by 10 % lowers jacket 2's inlet by 8.9 K, 63 % of it in 2.0 min, and 10 min after the step, with the pumps held, zone 2's peak is 0.83 K lower but zone 3's 3.08 K lower. With the loops closed and the pulses off, a jacket 2 inlet setpoint 10 K warmer moves pump 3 from 36.5 to 31.1 % within 5 min and pump 2 only from 34.5 to 33.4 %. The jacket is a slow handle on the next zone's pump, not on its own.

The pulse moves everything at once. The gas expands, its velocity rises, the fronts are carried downstream, and the negative activation volume slows the polymerization while the pressure is low, so every peak dips. The thermocouples see the gas late when it moves fastest. Before the first pulse of case 3 the hottest gas runs at most 0.77 K ahead of the hottest thermocouple, while 42.5 s into the run, as the pressure recovers, the gas in zone 4 reaches 293.4 °C and no thermocouple reads above 282.5 °C, 10.9 K lower, because the peak is rising faster than a 1.5 s thermowell and a sample at each passing parcel can follow.

10.5 Implemented Controller

Thirteen PI loops and five pieces of logic run every $\Delta t_c = 1\,\text{s}$, four physics steps, in the order instruments, high-high trip, pulse scheduler, feedforward, peak loops, jackets with mid-ranging, pressure, quality trim and supervisor. In MANUAL the operator holds the four pump strokes, the four cooler valves, the let-down and the CTA, and every loop tracks what the operator sets. Within each

Table 10.3 The Thirteen PI Loops With Their Directions and Default Tunings

Tag	CV	MV	γ	K_c	τ_I, output
TIC-101..104	TI-10j	$u_{I,j}$	+1	0.5	6 s, 0–100
TIC-201..204	TT-20j	$u_{C,j}$	−1	3	30 s, 0–100
VPC-602..604	$u_{I,k}$	$T_{ji,k-1,\mathrm{SP}}$	−1	0.5	300 s, 140–240
PIC-300	PT-300	a_{LD}	−1	0.1	10 s, 0–100
AIC-501	AI-501	c	+1	300	900 s, 100–5000

Gains in % per K, % per K, K per %, % per bar and ppm per g/10 min.

physics step the controller runs before the integration, which runs before the post-step corrections, the outputs and the historian. An optional model predictive controller, Section 10.5.6, takes the four pumps in place of the peak loops' algorithm when it is selected, while every other loop and piece of logic runs as described here.

10.5.1 The PI Algorithm

Every loop runs the framework's shared velocity-form PID of Section 1.6.2, with its derivative term unused here, as shown in Equation (10.8).

$$\begin{aligned} e_k &= \gamma(\mathrm{SP}_k - \mathrm{PV}_k), \qquad P_k = K_c\, e_k \\ S_k &= S_{k-1} + (P_k - P_{k-1}), \qquad v_k = S_k + I_{k-1} \\ u_k &= \mathrm{clamp}(v_k, u_{min}, u_{max}) \\ I_k &= I_{k-1} + \left[\frac{K_c}{\tau_I}\, e_k + \frac{u_k - v_k}{\tau_I}\right]\Delta t_c \end{aligned} \tag{10.8}$$

where $\gamma = +1$ where a larger output must follow a measurement below its setpoint and -1 where it must follow one above. These are Equations (1.14) to (1.17) with γ for the action a, no output bias, no derivative and a tracking time equal to τ_I. The running sum S_k is never clamped, and windup is handled on the integral alone by back-calculation, which the shared algorithm omits in a loop with no integral action. No loop here uses the derivative filter or a rate limit. The integral is seeded at reset with the output the steady tube needs, and in MANUAL, in fixed-stroke operation or while a feedforward window or a trip holds a loop, the loop tracks by setting $I_k = u_{op} - S_k$, which makes its output the held value, so every return to automatic is bumpless. Each loop's pairing, direction and default tuning appear in Table 10.3.

Under the ISA convention the peak loops and the melt-index trim are reverse acting and the jacket, pressure and mid-ranging loops direct acting. A cold peak raises its pump, a warm jacket inlet opens its cooler, a pressure above setpoint opens the let-down, a low melt index raises the CTA, and a pump above its target warms the jacket upstream of it.

10.5.2 Peak Loops and the Pulse Feedforward

TIC-101 to TIC-104 hold each zone's hottest thermocouple with that zone's pump, with one shared tuning or, in advanced mode, one per zone. In fixed-stroke operation the pumps hold the strokes on their cards while the jacket and pressure loops run. The pulse scheduler XV-310 opens the pulse valve every $t_p = 180$ s until PT-300 has fallen by the depth $\Delta P_p = 300$ bar from its value at the opening, or for at most 10 s, and holds PIC-300 at its last output until the valve has closed. It checks PT-300 once a second while the pressure falls about 60 bar a second, so a pulse can overrun its depth by up to a second of fall, to 317 bar in case 3 and 362 bar in case 4. Because the pulse is scheduled, FF-310 knows it in advance. From t_ℓ before each scheduled pulse to t_h after it, each peak loop tracks the output u_j^* it had when the window opened, and its pump receives that output reduced as shown in Equation (10.9).

$$u_{I,j} = (1 - \delta\,\omega)\,u_j^*, \qquad \omega = \min\left(1, \frac{t_p + t_h - t}{r}\right) \tag{10.9}$$

where the window runs from $t_p - t_\ell$ to $t_p + t_h$, $r = \min(5\,\text{s}, (t_\ell + t_h)/2)$ ramps the cut out at its end, and the defaults are $\delta = 20\,\%$, $t_\ell = 3\,\text{s}$ and $t_h = 30\,\text{s}$. The loops therefore neither fight the dip nor wind up against it, and they resume from u_j^* without a bump. The feedforward is keyed to the schedule, not to the valve, so it also cuts the initiator for a pulse that fails to open.

🕮 **Pause.** Try Exercise 10.3 before reading on.

10.5.3 Jackets and Mid-Ranging

TIC-201 to TIC-204 hold each jacket inlet with its cooler valve. Because a jacket mainly sets the temperature at which the next zone's initiator is injected, VPC-60k keeps pump k near a target stroke $u_{mid} = 50\,\%$ by moving the setpoint of jacket $k-1$, for $k = 2$, 3 and 4. Pump 1 has no mid-ranging, since its lever would be the feed preheater, which the model does not control. When a cooler is pinned in the direction mid-ranging would push it, wide open for a pump that wants colder water or shut for one that wants warmer water, the mid-ranging loop tracks its present output instead of integrating, which is conditional integration against a limit it cannot move [22].

10.5.4 Pressure, Trip and Restart

PIC-300 holds 2500 bar with the let-down valve. The high-high trip TSHH compares every zone's hottest thermocouple with T_{HH}, 325 °C by default, at each scan, and once it fires it latches, stops all four pumps, opens the let-down wide and suspends the pulses until it is reset. The permissive PSL-300 keeps the pumps at zero while PT-300 reads below 1500 bar, and when they are released each peak setpoint ramps back from the lower of its peak and its setpoint at 1 K/s, because in a counterfactual run without them a reset of case 6's trip decomposes the plant 18.25 s later.

10.5.5 Quality Trim and Supervisor

AIC-501 moves the CTA on each fresh melt-index report, with Δt_c of Equation (10.8) replaced by the 6 min report period, and holds while the analyzer is stale. The optional supervisor XY-700 walks each peak setpoint toward the highest value whose recent excursion stays a declared margin Δ_{set}, 20 K by default, below the line, as shown in Equation (10.10), which is Equation (1.13) with $\hat{e}_j$ as the excursion, $2\sigma_{TC}$ as the measurement error and Δ_{set} as the reserve.

$$\begin{aligned} \hat{e}_j &\leftarrow \max\left(\hat{e}_j\, \mathrm{e}^{-\Delta t_c/\tau_e},\ \mathrm{PV}_j - \mathrm{SP}_j\right) \\ \mathrm{SP}_j^{w} &= T_{dec} - \Delta_{set} - \max(0, \hat{e}_j) - 2\sigma_{TC} \\ \hat{\rho} &= \rho_{lab} - b_T\,(\bar{T}_{pk} - \bar{T}_{pk,lab}) \end{aligned} \tag{10.10}$$

where $\tau_e = \max(60\,\text{s}, 2t_p)$, $\sigma_{TC} = 0.3\,\text{K}$, and each setpoint moves toward SP_j^{w} by at most 1 K/min upward and four times that downward, between 250 °C and $T_{dec} - \Delta_{set}$. The density estimate $\hat{\rho}$ is the laboratory report moved by the change in the mean measured peak $\bar{T}_{pk}$ since its sample was drawn, a bias update of the kind Section 1.4.6 describes, and a rise is cut to the room left before $\hat{\rho}$ reaches the lowest density accepted, 0.9235 g/cm^3. While the melt-index trim is saturated with the melt index high, the supervisor lowers the setpoints instead.

10.5.6 Model Predictive Control

The control architecture offers a third setting for the initiator pumps beside fixed strokes and the four peak loops, one model predictive controller (MPC) that moves all four pumps every $T_s = 2\Delta t_c$ over a horizon of $N_p = 90$ decisions (180 s) and keeps every predicted peak under one ceiling, the trip setting less a margin, $T_{ceil} = T_{HH} - \Delta_{ceil}$ with $\Delta_{ceil} = 5\,\text{K}$ by default. It reads the signals TIC-101 to TIC-104 and FF-310 read, with TT-201 to TT-204, the trip setting and the strokes it applied, and nothing of the parcels, the kinetics or the margin. Every other loop and every protection runs above it as under the loops, and FF-310 is idle because the plan carries the pulse itself.

The controller's model was fitted to step tests of the simulator at the design point of cases 2 and 3 and is shipped as constants, so a plant the learner has changed is model mismatch, as on a real reactor.

From pump j to the hottest thermocouple of its own zone the path is one lag and a dead time with a gain that falls with the stroke, while the three cross paths, the pressure and the jacket inlets enter as output offsets simulated at the 1 s scan from the strokes already sent and the measured signals, as shown in Equation (10.11).

$$\begin{aligned}
\tau_j \frac{\mathrm{d}\hat{s}_j}{\mathrm{d}t} &= u_{I,j}(t-D_j) - \hat{s}_j, \quad \frac{\mathrm{d}F_j}{\mathrm{d}\hat{s}_j} = A_j\, \hat{s}_j^{-g_j} \\
\tau_x \frac{\mathrm{d}\hat{\zeta}_j}{\mathrm{d}t} &= u_{I,j}(t-D_x) - \hat{\zeta}_j, \quad \tau_P \frac{\mathrm{d}\hat{p}_j}{\mathrm{d}t} = \Delta P(t-D_P) - \hat{p}_j \\
\tau_w \frac{\mathrm{d}\hat{w}_j}{\mathrm{d}t} &= T_{ji,j}(t-D_w) - \hat{w}_j \\
\tau_w \frac{\mathrm{d}\hat{w}'_j}{\mathrm{d}t} &= T_{ji,j}(t-D'_w) - \hat{w}'_j \\
\hat{T}_j &= F_j(\hat{s}_j) + K_{P,j}\,\hat{p}_j + K_{w,j}\,\hat{w}_j + b_j \\
&\quad + K_{x,j-1}\,\hat{\zeta}_{j-1} + K'_{w,j-1}\,\hat{w}'_{j-1}
\end{aligned} \tag{10.11}$$

where a hat marks a state of the controller's model, $\hat{s}_j$ is the effective stroke in percent, F_j the static peak it gives, ΔP the measured PT-300 less its setpoint in bar, $T_{ji,j}$ the measured TT-20j, the terms in $j-1$ are absent for zone 1, and b_j is an output bias in kelvin. The own paths have $\tau_j = 2.8$, 1.1, 3.1 and 2.4 s, $D_j = 6$, 6, 4 and 6 s, $A_j = 28.12$, 19.37, 17.46 and 14.69 and $g_j = 0.890$, 0.863, 0.835 and 0.775. The cross paths have $K_{x,j} = 0.204$, 0.241 and 0.123 K per percent with $\tau_x = 4$ s and $D_x = 32$ s, the 24 to 25 s the gas takes from one peak to the next injector plus the own path, the pressure path has $K_{P,j} = 0.0713$, 0.0457, 0.0465 and 0.0523 K/bar with $\tau_P = D_P = 1$ s, and the jacket paths have $K_{w,j} = 0.149$, 0.098, 0.133 and 0.107 and $K'_{w,j} = 0.398$, 0.485 and 0.287 K/K with $\tau_w = 30$ s, $D_w = 35$ s and $D'_w = 27$ s. Refitted with the noise off, the own paths leave residuals of 0.7 to 2.2 % of the response at the design strokes and the other paths 0.5 to 8.7 %, and the design gains of 1.32, 0.88, 0.95 and 0.83 K per percent lie within 13 % of the schedule, with a delay plus lag of 8.8, 7.0, 7.0 and 7.6 s, the transport from each injector to its hottest thermocouple plus the pump lag and the thermowell.

The pulse enters through ΔP. With the preview on, as case 9 ships it, each scheduled pulse enters the prediction of ΔP as 91 one-second values of PT-300's measured deviation through a pulse of case 3, scaled to the depth setting, and what the template does not explain decays with PIC-300's recovery constant of 6.9 s, as the whole measured deviation does with the preview off. The bias b_j is the measured peak less the model's, filtered with $\tau_b = 5$ s at every scan under whichever structure acts, the output-disturbance form of offset-free control [23]. While $|\Delta P|$ exceeds 30 bar, and for 15 s after, the bias is not updated and the plan does not track its targets, which is FF-310's hold in the controller's own terms. After the pumps have been blocked by the trip or the permissive the model is put back on the measurements with the bias at zero.

Each decision solves the quadratic program of Equation (10.12) over the changes of the four strokes, taken as offsets from the strokes applied now, in twelve move blocks, four of one decision, then 2, 2, 3 and 4, then 6, 9, 15 and 45, 48 moves and four slacks on 15 states, the four lags and their delay chains.

$$\begin{aligned}
\min_{\Delta u,\,\varepsilon} \; & \sum_{k=1}^{N_p} q_k \sum_j \left(\hat{T}_{j,k} - r_j\right)^2 + \lambda \sum_i \sum_j \Delta u_{I,j,i}^2 \\
& + \sum_j \left(10^4\, \varepsilon_j^2 + 2\times 10^4\, \varepsilon_j\right) \\
\text{s.t. } & 0 \le u_{I,j,i} \le 100, \qquad \varepsilon_j \ge 0 \\
& \hat{T}_{j,k} \le T_{ceil} + \max(0,\, \hat{T}_{j,0} - T_{ceil})\, \mathrm{e}^{-kT_s/\tau_f} + \varepsilon_j
\end{aligned} \tag{10.12}$$

where $r_j = \min(\mathrm{SP}_j, T_{ceil})$ is the target, the request or the ceiling, whichever is lower, q_k is 1 except on the steps where the predicted $|\Delta P|$ exceeds 30 bar and for 15 s after them, where it is zero, $\lambda = 5$ per percent squared is the move price, i counts the move blocks, $\hat{T}_{j,0}$ is the model's present output and $\tau_f = 10\,\mathrm{s}$ is a funnel through which a peak already above the ceiling is asked back. The ceiling is a soft constraint priced 10^4 per K^2 and 2×10^4 per kelvin against 1 per K^2 of tracking, with one slack ε_j per zone over the whole horizon. The target is clipped rather than left at the request, because a request above the ceiling pulls the plan into that shared slack and lets the peaks ride above the ceiling. The stroke bounds are the peak loops' own and are hard. The framework's dual active-set solver [24] computes each plan with a ridge of $10^{-9}(1 + 2N_p K_{max}^2 + 2\lambda)$, K_{max} being the largest present gain, and only the first block's moves are applied.

A plan is accepted only when the solver reports an optimum and every move, prediction, cost and slack is finite, with the slacks nonnegative and the moves inside 0 to 100 %. Otherwise the historian is marked and the four peak loops, which track the applied strokes at every scan, take the pumps until the next valid plan. With the noise off a forced rejection at 120 s of case 9 moves no stroke at the hand-over, and one at 243 s, inside a pulse window, moves 0.06 points, because a window entered from a fallback holds the strokes without the feedforward's cut. In Chrome a plan takes 2.1 to 2.9 ms, 6.4 to 6.6 % of a core at the 1 min/s rung of case 9, and the 60 min/s rung slows to 17 to 21 min/s.

10.5.7 Simulation, Identified and Internal Models

Three models are kept apart here. The parcel model of Section 10.3 is what the plant does. Under the peak loops nothing inside the application fits a control model, and the open-loop steps of Section 10.4 serve as one, measuring the plants the loops see, 0.81 K per percent with a few seconds of dead time for a peak loop at mid-stroke and 0.89 K per percent with 2.0 min to 63 % for a jacket loop. Under the loops the controllers carry almost no internal model. The feedforward knows the schedule and a fixed cut, the scheduler knows the measured pressure, the supervisor knows T_{dec}, b_T and the laboratory, and none of them contains the parcels, the kinetics or the margin itself. The MPC's identified model, Equation (10.11), fitted once by the same kind of step test, contains none of them either.

10.6 Nine Cases and the Challenge, as Measured

Table 10.4 sets out the nine cases and the four-hour challenge, and Table 10.5 their measured outcomes. Each case starts from the four peak loops at 290 °C, the trip at 325 °C, pulses every 180 s from the first minute and the feedforward, mid-ranging, trim and supervisor off, and changes only what its row names. Every number below was read from the running engine at the default seed, times are simulated, and a controller action is dated by the scan at which it acts. Where a discrete outcome could turn on the measurement noise, the spread over six other seeds is given.

10.6.1 A Peak Lit by Hand

Case 1 starts with every station in MANUAL and pump 2 stopped. The tube converts 24.0 %, zone 2's gas passes its idle injector at 223.3 °C and only cools, and zone 3's peak is 267.4 °C because its gas arrives colder. Pump 2 starts at 20 % at 30 s, zone 2's thermocouples pass 260 °C 9.0 s later, and at 1.0 min the peak is 270.8 °C at the thermocouple 42 m after the injector. At 40 % from 90 s it is 293.0 °C at 3 min, at the one 30 m after it. Zone 3's peak, whose pump never moves, climbs to 280.2 °C by 2 min as zone 2's heat arrives with the gas and to 289.3 °C by 8 min as jacket 2's inlet warms from 159.0 to 173.3 °C. Zone 4's peak dips from 290.7 to 285.7 °C at 1.63 min because the zones before it have left it less ethylene, and the conversion rises to 28.3 % at 3 min and settles back to 27.8 % at 8 min.

10.6.2 Four Loops Coupled Downstream

Case 2 closes the four loops with the pulses off. At 30 s zone 2's setpoint steps from 290 to 300 °C, and TIC-102 moves pump 2 from 34.5 to 48.5 % by 3 min. TI-102 approaches 300 °C from below, stays within 1 K from 46 s after the step, and overshoots by no more than the noise of the hottest

Table 10.4 The Nine Cases and the Challenge

#	Scenario and events	Teaching point
1	MANUAL, pump 2 at 0, 20 at 0.5 min, 40 at 1.5 min	a peak forms and moves
2	pulses off, zone 2 to 300 °C at 0.5 min	one-way coupling
3	first pulse at 30 s, feedforward off	windup, feedforward
4	fixed strokes, jackets 160 °C, pulses every 15 min from 25 min	fouling
5	setpoints 315, 322, 328 °C at 1, 3, 5 min, trip 330 °C	the trip's dead time
6	300 °C, feedforward, trip 320 °C, lot 50 % at 1 min, 100 % at 10 min	gain change
7	feedforward and trim on, 310 °C at 2 min	two handles, late analyzers
8	300 °C, feedforward, mid-ranging at 55 %, supply 140 to 170 °C at 15 min	cooling runs out
9	MPC on the pumps, feedforward, 315, 322, 328 °C at 1, 3, 5 min	a request and a constraint
10	4 h, supply 165 °C at 60 min, lot 120 % at 150 min	the margin

Table 10.5 Measured Outcomes of Each Case and Variant

Case, configuration	Measured
1 as shipped	zone 2 peak 270.8 then 293.0 °C, 42 then 30 m after the injector
2 as shipped	in 1 K from 46 s, no overshoot above noise, zone 3 +2.06 K
3 feedforward off	dip 270.1, overshoot 299.7 and 299.9 °C, worst margin 33.1 K
3 feedforward on	dip 262.7, overshoot 292.2 and 292.8 °C, worst margin 41.9 K
3 hold 10 s	overshoot 294.2 and 295.8 °C, worst margin 38.2 K
4 fixed strokes	U/U_0 0.68, zone 4 peak 279.4 to 293.2 °C
4 peak loops	zone 4 at 290.0 °C, pump 4 at 29.4 %
5 trip 330 °C	trip at 7.350 min, decomposition at 7.375 min
5 trip 325 °C	trip at 4.283 min, worst margin 8.7 K
5 feedforward on	trip at 8.083 min, worst margin 4.8 K
6 trip on	trip 25 s after the lot, worst margin 12.9 K
6 trip off	decomposition 35.25 s after the lot
7 as shipped	in grade after 13.8 min, 4.54 t off grade
8 mid-ranging on	mean conversion 29.4 %, coolers 1 to 3 at 100 %
8 mid-ranging off	mean conversion 28.9 %, coolers 91 to 94 %
9 MPC, then loops	hottest 322.1 °C, margin 12.8 K, 31.54 %, no trip, then trip at 5.083 min, 19.25 %

of 17 thermocouples, its highest reading over the next 5 min being 300.8 °C. Its hotter tail reaches zone 3's injector and pushes TI-103 to 292.1 °C, 2.06 K above its setpoint, 37 s after the step, and TIC-103 cuts pump 3 from 36.5 to 33.3 % by 3 min. The conversion rises from 27.5 to 27.9 %. Each loop rejects what the zone before it sends, so a zone tuned hot becomes a disturbance to every zone after it.

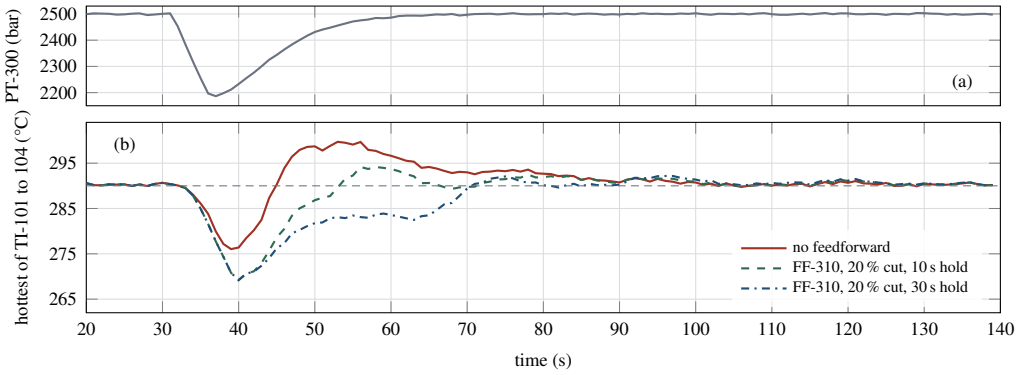


Figure 10.3 First pulse of case 3 ridden through three ways, one logged sample a second at the default seed. The pressure (a) is the same in all three runs. The hottest of the four peak measurements (b) overshoots to 299.7 °C without feedforward (solid), to 294.2 °C with a 20 % cut held 10 s (dashed) and to 292.2 °C with the default 30 s hold (dash-dotted), against the 290 °C setpoints marked by the thin gray dashed line. The lowest of the four, not drawn, dips to 270.1 °C without feedforward and to 262.7 °C with it.

10.6.3 Riding the Pulse

In case 3 the first pulse is scheduled at 30 s and opens at the scan at 30 s. The scheduler holds it open for 5 s, the valve is more than 2 % open for 5.75 s, the pressure falls 317.0 bar to 2184.0 bar, the gas leaves at 20.3 m/s instead of 13.8, and the mean velocity along the tube is 20.2 % higher while the valve is open. The pressure is back above 2490 bar 29.8 s after the scheduled start. The zones' hottest thermocouples move 12 to 72 m downstream, and the peaks dip to 270.1 °C. The loops see an error of 20 K and wind their pumps up, pump 1 to 53.5 %, and when the pressure returns that initiator takes TI-101 to 299.7 °C, 9.7 K above its setpoint, with the hottest gas at 301.6 °C. The conversion at the outlet swings between 26.05 and 28.16 %. The second pulse, at 210 s, repeats the pattern with an overshoot to 299.9 °C and the gas at 301.9 °C, the state shown in Figure 10.4, and it sets the worst margin of the two pulses at 33.1 K, against 33.4 K after the first.



Figure 10.4 The pulse valve, case 3, at $t = 3.90$ min (234 s) in the Profile view, 24 s after the second pulse was due, with no control changed. (1) The badges read a worst margin of 33.1 K, a conversion of 27.4 %, a melt index of 1.38 and a density of 0.9280, both flagged against the grade, U/U_0 of 0.98 and PT-300 at 2464 bar, with the next pulse 156 s away. The unrolled tube shows the fluid temperature of the parcels with four peaks, (2) the hottest thermocouple of each zone ringed, TI-101 at 299.9 °C at the top of its second overshoot, TI-102 at 293.4, TI-103 at 294.7 and TI-104 at 293.8 °C against setpoints of 290 °C, (3) below the dotted amber trip line at 325 °C and the dashed red decomposition line at 335 °C marked as a teaching value. Beneath them lie (4) the jacket water of the eight sections near 181 and 188 °C, the conversion climbing zone by zone on its own axis, and (5) the tube with its injectors, pump strokes and the let-down and pulse valves at the outlet.

> **TRY IT IN THE APP** **3 · The Pulse Valve**
>
> Load the scenario, press Run and watch the four ringed peaks on the Profile view. At 30 s the pulse valve opens, the pressure falls 317.0 bar and the peaks dip to 270.1 °C. Keep watching after the pressure returns: the wound-up loops carry TI-101 to 299.7 °C, almost 10 K above its setpoint.

The feedforward removes most of the overshoot, as shown in Figure 10.3. With a 20 % cut from 3 s before each pulse to 30 s after it, and the loops held meanwhile, the dip of the first pulse deepens to 262.7 °C, the overshoot stops at 292.2 °C, the hottest gas reaches only 292.8 °C, and over the two pulses the worst margin rises from 33.1 to 41.9 K. A hold of 10 s ends before the pressure has recovered, and the overshoot reaches 294.2 °C after the first pulse and 295.8 °C after the second, with a margin of 38.2 K. The margin is bought with conversion at fixed setpoints. Over 30 min the mean conversion is 27.41 % without the feedforward and 26.96 % with it, while the worst margin is 31.9 and 41.9 K, and the challenge shows what those 10 K are worth once the setpoints are raised to spend them. A missed pulse with the feedforward on shows its other side, because the cut still arrives on schedule and the peaks dip to 279.6 °C with no pulse at all.

10.6.4 Fouling Between Sparse Pulses

Case 4 runs the jackets at 160 °C, holds the pumps at fixed strokes and delays the first pulse to 25 min. The layer grows where the wall is below the cloud point, and by 24.9 min its mean resistance is 1.72×10^{-3} m^2 K/W in zone 4, 6.1×10^{-4} in zone 3, 5.0×10^{-5} in zone 2 and none in zone 1. U falls

to 0.82 of its clean value in 10 min, 0.76 in 15, 0.72 in 20 and 0.68 by 24.9 min. Less heat leaves zone 3's tail, so zone 4's initiator meets warmer gas and its peak creeps from 279.4 to 293.2 °C while zones 1 to 3 move by less than 2 K, and the conversion slips from 28.6 to 28.1 %. The pulse at 25 min stays open 6 s, because the scan 5 s into it read PT-300 1 bar above its closing value, so it falls 362 bar and strips 36.2 % of the layer, and U is back to 0.76 half a minute later. In case 3, with the jackets at 175 °C and a pulse every three minutes from 30 s, U is still 0.95 at 24.9 min. With the loops closed in case 4, zone 4 stays at 290.0 °C while pump 4 falls to 29.4 %. Parametric sensitivity to the wall coefficient [5] appears here as a peak that drifts toward the line or a pump that drifts toward its stop. The butyl rubber reactor of Chapter 11 fouls its jacket with its own product in the same way, without a pulse to strip it.

10.6.5 An Honest Decomposition

Case 5 raises the setpoints to 315, 322 and 328 °C at 1, 3 and 5 min, pulsing without feedforward, with the trip moved to 330 °C. At the steady tube each kelvin of peak buys about 0.2 points of conversion, from 27.51 % at 290 °C to 29.65 % at 300, 31.56 % at 310 and 33.54 % at 320 °C. After the pulse at 7 min zone 1's own thermocouple passes 330 °C and trips the plant at 7.350 min, but the gas behind it has already been dosed, and 1.5 s later, at 7.375 min, gas 64 m down zone 1 has been above 335 °C for a second, at 336.7 °C. It decomposes, the app reports about 1760 °C and 3010 bar, and the run stops. The outcome turns on one scan. A trip forced one scan earlier leaves 1.4 K, and over six other noise seeds the trip fires at 7.333 min three times, with 1.1 to 1.3 K to spare, and at 7.350 min three times, each followed by a decomposition. With the trip at 325 °C it fires at 4.283 min with the hottest gas 8.7 K below the line (8.7 to 9.1 K over the seeds), and with the feedforward and the 330 °C trip the plant trips at 8.083 min with 4.8 K to spare (3.9 to 5.1 K). A protection layer has a dead time of its own, and here it is the 1 s scan, the thermowell and the transport of initiator already injected. The surge override of Volume 4, Chapter 2 is another guard that a fast enough excursion crosses.

> **TRY IT IN THE APP 5 · Conversion Pushed Toward the Line**
>
> Press Run and watch the hottest parcel against the dashed decomposition line through each pulse. With the trip at 330 °C it fires at 7.350 min, and gas 64 m down zone 1 decomposes 1.5 s later. Reset, set the Trip temperature to 325 °C and run again: the trip fires at 4.283 min with the hottest gas 8.7 K below the line.

Pause. Try Exercise 10.1 before reading on.

10.6.6 A Weak Lot and the Trip

Case 6 holds 300 °C with the feedforward on and the trip at 320 °C, and the pumps start at 47.7, 46.3, 46.2 and 47.2 %. At 1 min the pumps begin to draw from a lot half as effective, and the loops hold the peaks, but by 9.9 min the strokes are 95.3, 93.0, 92.6 and 90.2 %, with half the gain per percent and almost no room. At 10 min the normal lot returns as a pulse opens, with the feedforward holding the commands a fifth lower, at 72.0 to 76.3 %, and the integrals frozen. The initiator already in the gas keeps the weak lot's efficiency, but every dose pumped after the change makes radicals twice as fast. As the pressure recovers, the four peaks climb past 313 °C on doses the frozen loops cannot trim, and the trip fires on zone 1 at the scan 25 s after the change, with the hottest gas at 322.1 °C, 12.9 K below the line. At 325 °C the same trip fires 34 s after the change, 1.25 s before a decomposition, which is why the case sets it at 320 °C. With the trip off, the feedforward hands the pumps back at 90 to 95 % and zone 1 decomposes 35.25 s after the change, at 61 m and 336.4 °C. Over six other seeds the trip fires 25 to 27 s after the change with 12.2 to 12.8 K left, and the decomposition comes 35.0 to 35.5 s after it. Excess initiator is the first runaway cause the autoclave study names [7], and here it arrives as an unmeasured gain change. A reset at 12 min brings the plant back, since the pumps wait until PT-300 reads 1500 bar, reached 11 s later, and by 22 min every peak reads within 0.5 K of 300 °C.

10.6.7 A Grade Transition

Case 7 moves from a grade made at 290 °C, melt index 1.379 g/10 min and density 0.92806 g/cm^3, to the film grade 2.0 ± 0.3 and 0.924 ± 0.001, with the feedforward and the trim on. At 2 min the setpoints go to 310 °C. Hotter peaks make polymer with more short branches, so the density falls, and a higher melt index. The pellets enter the grade box 13.8 min after the setpoints move and stay in it, and 4.54 t of off-grade polymer is made on the way. The trim raises the CTA from 1500 to 1638 ppm to bring the melt index to 1.942 g/10 min by 60 min, while AI-501 reads 1.904. The pellets are then at 0.92426 g/cm^3 while the laboratory still reports 0.92822, from the sample drawn at the start, and the conversion averages 30.62 % over the hour. The peaks carry the density and the CTA the melt index alone. Section 1.4.5 sets out why the hold-up and the analyzers set the off-grade tonnage, and Chapter 8 measures the same cost in off-specification tonnage on a fluidized bed.

10.6.8 Cooling That Runs Out

Case 8 holds 300 °C with mid-ranging on at a 55 % target. By 14.9 min mid-ranging has lowered jackets 1 to 3 to 166.8, 167.7 and 164.0 °C, their coolers run 43 to 49 % open, pumps 2 to 4 have risen to 52, 52 and 49 %, and the mean conversion is 29.6 % against 29.0 % without mid-ranging. At 15 min the supply water warms from 140 to 170 °C. Coolers 1 to 3 are wide open by 15.95 min, the inlets drift to 173.4 to 173.8 °C, several kelvin above the setpoints mid-ranging chose, mid-ranging holds instead of winding up, and pumps 2 to 4 fall back to 48, 47 and 44 %. By 29.9 min the mean conversion is 29.4 % against 28.9 % without mid-ranging, whose coolers run 91 to 94 % open and hold 175 °C. The setpoints are infeasible, and the Zones view reports the cooling as limited rather than met.

10.6.9 Four Peaks Under One Ceiling

Case 9 asks for the 315, 322 and 328 °C of case 5 at 1, 3 and 5 min, pulsing every three minutes from 1 min with the trip at 325 °C, and loads with the MPC on the pumps at a ceiling of 320 °C. Its comparison is the run after Reset with the peak loops and the feedforward on the same requests. Table 10.6 measures cases 9, 5 and 4 under the shipped structure and, with the settings case 9 ships and no retuning, under the MPC, with the same seed, instruments, noise and duration in every row, beside the stronger classical rows: the loops without the feedforward, the loops with the requests clipped by hand to the ceiling, and the best fixed tuning of a 35-point grid chosen in hindsight on each case. Figure 10.5 shows case 9 under both structures.

The loops follow the request into the trip. With the feedforward on, zone 4's hottest thermocouple passes 325 °C at the 5.08 min scan, 5 s after the 328 °C request reaches the pumps, and the run converts 19.25 % over its ten minutes. The MPC takes the 315 °C request, all four peaks within 1 K of it at 2.02 min, stops the 322 °C request at its ceiling, within 1 K of 320 °C at 3.52 min, and refuses the 328 °C one. The strokes hold through the pulses at 4 and 7 min, the peaks dip to 297.8 and 298.0 °C and come back to 320.8 °C after each, and from 7.7 min the four peaks average 320.0 to 320.2 °C. The hottest reading, 322.1 °C in zone 4 at 5.48 min, is the scatter of about 2 K between the parcels a thermocouple samples, the reason the ceiling sits 5 K below the trip. The hottest gas stays 12.8 K below the line, the run converts 31.54 %, and none of its 300 plans is rejected.

Against the operator's own remedy, the loops with the requests clipped by hand to 320 °C, the MPC's lead narrows to 0.45 points of conversion, 1.0 K of hottest reading and a third of the stroke travel, and retuning those loops in hindsight recovers only 0.07 points. Most of what the MPC adds is therefore the ceiling itself, and the rest is the strokes held still through the pulses where the loops integrate against the dip. The scorecard's IAE, 272.8 K min for the MPC, counts the refused request as error.

The MPC loses one comparison. A hindsight-tuned loop without the feedforward and with the requests clipped ($K_c = 1.5$, $\tau_I = 24$ s) converts 0.24 points more by running 0.4 K from the trip with 7.7 K of margin against 12.8 K, which is margin spent rather than control. By design the MPC also

Table 10.6 Shipped Structure Against the MPC on Cases 9, 5 and 4, Default Seed, Full Duration. IAE and Travel Are the Scorecard's, IAE_c Is Against the Lower of the Request and the Ceiling, and the Zone-Seconds Count Measured Peaks Near the Trip (Within 5 K) and Over the Ceiling

Case	Structure	IAE (K·min)	IAE_c (K·min)	Hottest (°C)	Near trip (zone·s)	Over ceiling (zone·s)	Margin (K)	Conv. (%)	Travel (%)	Outcome	Plans, rejected
9, 10 min	loops, FF-310 (shipped)	2963.3	2800.1	325.3	242	219	9.8	19.25	760	trip 5.08 min	—
trip 325,	loops, no FF	3345.3	3176.8	325.1	165	146	8.7	17.12	744	trip 4.28 min	—
ceiling 320	MPC as loaded	272.8	105.7	322.1	679	180	12.8	31.54	216	none	300, 0
	MPC, preview off	267.7	100.4	322.1	674	176	12.8	31.56	215	none	300, 0
	loops, FF, clipped to 320 °C	200.7	200.7	323.1	647	221	11.9	31.09	673	none	—
	clipped, hindsight K_c 1, τ_I 6 s	186.9	186.9	323.1	677	203	11.8	31.16	948	none	—
	no FF, clipped, hindsight 1.5, 24 s	75.9	75.9	324.6	1101	682	7.7	31.78	1577	none	—
5, 10 min	loops, FF-310	1124.9	1109.3	330.2	562	532	4.8	29.48	990	trip 8.08 min	—
trip 330,	loops, no FF (shipped)	85.4	96.1	331.2	560	506	−1.0	31.71	805	decomp. 7.37 min	—
ceiling 325	MPC	164.1	109.8	327.1	494	124	7.9	31.92	244	none	300, 0
	loops, FF, clipped to 325 °C	204.0	204.0	328.0	497	150	7.3	31.47	711	none	—
	clipped, hindsight K_c 0.5, τ_I 3 s	189.0	189.0	328.0	563	180	6.3	31.60	861	none	—
	no FF, clipped, hindsight 1, 12 s	77.7	77.7	329.6	748	342	4.2	32.19	996	none	—
4, 30 min	loops, FF-310	69.9	69.9	292.6	0	0	42.1	29.03	708	none	—
trip 325,	loops, no FF	53.3	53.3	302.0	0	0	30.7	29.07	752	none	—
ceiling 320	MPC	52.2	52.2	291.7	0	0	42.9	29.05	112	none	900, 0
	loops, FF, hindsight K_c 0.35, τ_I 6 s	67.6	67.6	292.3	0	0	42.3	29.03	497	none	—

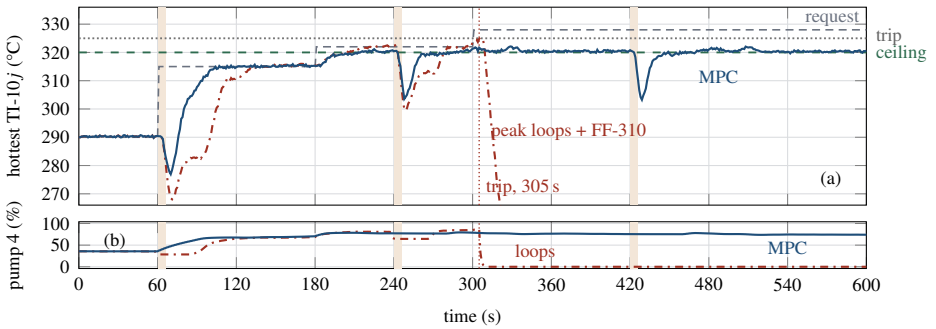


Figure 10.5 Case 9 as loaded under the MPC and, after Reset, under the peak loops with the feedforward, default seed, with the pulse openings shaded. (a) The hottest of TI-101 to TI-104 under the MPC (solid) and the loops (dash-dotted) against the requests of 315, 322 and 328 °C (gray, densely dashed), the ceiling at 320 °C (dashed) and the trip at 325 °C (dotted). The MPC stops at the ceiling, and the loops cross the trip at 5.08 min and leave the panel as the peaks collapse to 172.9 °C by 10 min. (b) Pump 4's stroke, in the same line styles, 76.6 under the MPC at 5.5 min against 87.3 % as the loops trip, and zero after it.

spends 679 zone-seconds within 5 K of the trip against 242 for the shipped loops, because it holds the peaks there while the loops trip and leave.

Case 5, with the trip at 330 °C and the ceiling at 325 °C, gives the same ranking. The MPC finishes at 31.92 % without a trip, where the loops trip with the feedforward and, as the case ships, decompose the plant without it, and again only the hindsight loop without the feedforward converts more, 0.27 points, at 0.4 K from the trip. In case 4, run under the peak controllers, the MPC's IAE is matched

Table 10.7 Challenge Configurations Over 240 min. MI and Density Columns Give the Pellets' Worst Deviation From the Grade After 60 min

Configuration	Conv. (%)	Margin (K)	MI dev.	ρ_{PE} dev.	Result
as shipped	27.72	35.31	0.638	0.00416	fail
suggested[a]	30.79	16.46	0.048	0.00057	pass
feedforward off	30.81	13.55	0.050	0.00062	fail
setpoints 312 °C	30.86	13.84	0.056	0.00052	fail
setpoints 305 °C	30.58	20.34	0.116	0.00152	fail
mid-ranging off	30.80	16.52	0.056	0.00029	pass
trim off	30.79	16.46	0.254	0.00057	pass
supervisor, 20 K	30.91	11.71	0.057	0.00074	fail
supervisor, 25 K	30.74	18.46	0.082	0.00112	fail
MPC on the pumps	30.80	16.46	0.048	0.00030	pass
MPC, else as shipped[b]	27.16	36.97	0.642	0.00419	fail

[a] peak loops at 310 °C, feedforward, mid-ranging at 55 %, trim. Other rows change the suggested configuration by one item, [b] the shipped one.

only by the loops without the feedforward (53.3, and 52.2 retuned in hindsight), which overshoot the pulse at 25 min to 302.0 °C (299.7 retuned), and it moves the pumps a sixth as far as the loops with the feedforward.

The pulse preview is credited with nothing, since switching it off moves the MPC's rows by at most 0.03 points and 0.1 K. Halving the physics step changes no verdict or ranking, and over four other noise seeds the loops trip at 5.08 to 5.10 min while the MPC never trips. After a trip's reset the pressure rule also holds the plan while PIC-300 restores the pressure, so the pumps stay at zero for 46 s after their release and then step by 11 %, the peaks topping out at 322.4 °C where the loops restart in 12 s and re-trip at 326.9 °C.

> ✦ **DID YOU KNOW? The Controller That Lives Near the Trip Never Trips**
>
> From the simulator: in case 9 of Table 10.6 the MPC holds the measured peaks within 5 K of the trip for 679 zone-seconds, against 242 for the shipped loops. Yet the loops trip at 5.08 min and convert 19.25 %, while the MPC never trips and converts 31.54 %.

10.6.10 The Four-Hour Challenge

The challenge runs 240 min with pulses every three minutes from 90 s, warms the supply water to 165 °C at 60 min, and brings a stronger initiator lot of 120 % at 150 min. Its target is a mean conversion of at least 30.5 %, a hottest gas never within 15 K of the line, pellets within 2.0 ± 0.3 in melt index and 0.924 ± 0.001 in density from 60 min, and no trip or decomposition, all scored on the truth. It ships with fixed strokes and the loops, feedforward, mid-ranging and trim off. The configurations measured against that target are collected in Table 10.7, and Figure 10.6 draws its conversion and margin columns against the target.

As shipped the plant stays 35.31 K from the line but converts only 27.72 %, and the pellets miss the grade by up to 0.638 in melt index and 0.00416 g/cm^3 in density. The suggested configuration converts 30.79 %, holds the melt index within 0.048 and the density within 0.00057, never trips, and comes closest to the line at 150.07 min, 4 s after the stronger lot arrives, leaving 16.46 K. That is 0.29 points above the conversion floor and 1.46 K more margin than required, and the run passes whether the configuration is set before Run or carried through Reset. The lot change decides the margin, and the feedforward is what lets the peaks sit at 310 °C. Without it the pulses take the margin to 13.55 K at 187.9 min, and at 312 °C the lot change takes it to 13.84 K. Over five other noise seeds every row keeps its verdict, and the suggested margin stays between 16.35 and 16.63 K. At 305 °C the margin

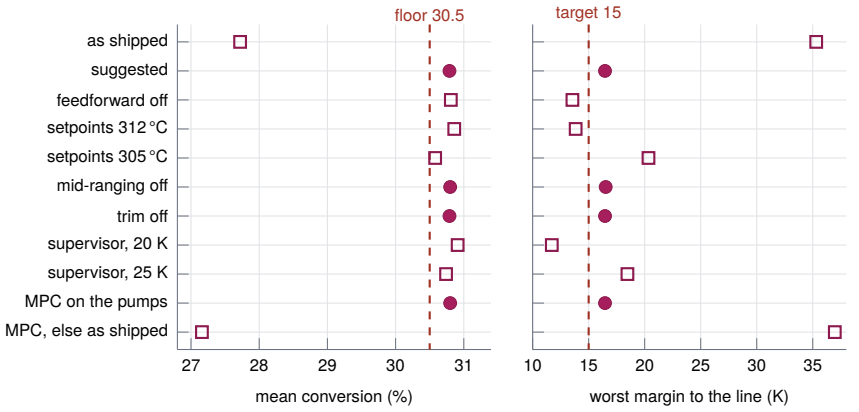


Figure 10.6 The conversion and margin columns of Table 10.7 as dots, filled for a configuration that passes the challenge and open for one that fails. The dashed lines are the conversion floor of 30.5 % and the 15 K the hottest gas must keep from the line. Notice that every passing configuration sits just right of both lines, and that the rows at 305 °C and with the supervisor at 25 K clear both lines yet fail, on density.

is ample but the density leaves the grade by 0.00152 g/cm^3, so the grade, not the line, sets the floor. Neither mid-ranging nor the trim decides the result, since the run passes without one, the other or both, although without the trim the melt index comes within 0.046 of its tolerance. The supervisor set at 20 K walks the peaks to 312 to 314 °C and leaves 11.71 K at the lot change, and at 25 K it keeps 18.46 K but lets the density leave the grade, so a margin chosen without the lot change in view fails either way.

The MPC in place of the suggested loops also passes with the same 16.46 K, because the lot change sets the margin 4 s after the lot arrives, before any controller acts, and it does so at a tenth of the loops' stroke travel, 1435 against 12 213 %. Of the unscored limits it reaches only the coolers' stops, for 14.2 % of the zone-scans against 23.4 % under the loops, and the pumps never. With every other setting as shipped it fails in the manner of the fixed strokes, holding 290 °C where they drift upward as the water warms and the stronger lot arrives.

10.7 Technology in Practice

What Measures It

Every peak loop of this chapter reads a row of thermocouples, and its measurement is the hottest of them. Section 10.3 gives each element a 1.5 s thermowell lag and 0.3 K of noise, so the reading hops from one element to the next as the peak moves, and Section 10.4 shows the gas running 10.9 K ahead of every thermocouple as the pressure recovers from a pulse. Figure 10.7 draws the element and its well, and the box below describes them.

> **TECHNOLOGY** **Sensor: Thermocouples in Thermowells Along the Tube**
>
> Temperature elements installed along the length of a tubular reactor follow the progress of the polymerization [18]. A thermocouple is the most rugged and wide-ranging contact sensor, and its accuracy depends on its type and its installation. Its pressure-tight thermowell lets it be replaced without depressurizing the process, but the well's mass adds a first-order lag, an air gap at the bottom of its bore adds a second, and a delayed reading can upset feedback. The most common failure is an open junction, called burnout, and the instrument's burnout mode decides whether a broken element then reads high or low [25]. On a trend a slow well reads a climbing peak late and low, as the model's 1.5 s lag does after a pulse.

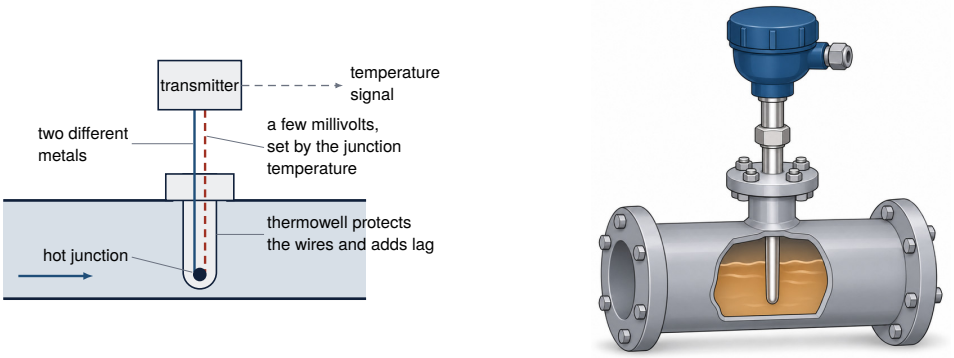


Figure 10.7 A thermocouple in a thermowell, the sensor behind TI-101 to TI-104. Notice the mass of metal between the gas and the junction: it is the 1.5 s lag of the model, and it is why the hottest gas can run ahead of every reading while a peak climbs.

What Moves It

Each peak has one final element, the initiator pump of its zone. The cooler valves move the jackets, the let-down valve holds the pressure, and the pulse valve opens on a timetable rather than on a controller's demand. The model gives every pump a stroke that delivers in proportion and follows its command through a 1.0 s lag, with no stiction.

> **TECHNOLOGY** **Final Element: High-Pressure Initiator Pumps**
>
> Where a tube runs on peroxides, the initiator added at each injection point is set by the speed of high-pressure pumps, and the pressure calls for reciprocating machines. The peroxide travels dissolved in a hydrocarbon solvent [18]. A positive-displacement pump discharges a fixed volume with every revolution, so at constant speed it delivers a fixed flow whatever the discharge pressure, and a blocked discharge locks it. A metering pump spans its flow from zero to a maximum set on the pump as its control signal goes from 0 to 100 %, and a plunger type delivers that flow as discrete pulses rather than a continuous stream [25]. The chapter's pumps, whose delivery is their stroke times a fixed maximum after a 1.0 s lag, are that behavior without the pulses.

Where the Controller Runs

Figure 10.8 draws one peak loop of Section 10.5 with hardware in place of the schematic's symbols. A distributed control system holds loops like these at a supervisory level that sends set points to field controllers, with loops nested or cascading and cycle times from milliseconds to minutes [26]. The hottest of a row of transmitters reaches the controller through a high-select function block, which passes only the greatest of its inputs. A textbook exothermic reactor holds its hottest measured temperature at setpoint in exactly this way [25]. In the app the thirteen PI loops, the feedforward and the trip logic execute every 1 s, four physics steps, the feedforward reads the pulse scheduler rather than the valve, and the MPC of case 9 plans every 2 s in place of the four peak blocks. Where the trip belongs is the subject of the In practice box below.

What Is Modernizing It

Model predictive control is accepted in industry for its multivariable control and its explicit handling of constraints, and for the tubular reactor a tracking nonlinear predictive controller was shown to keep the reactor stable through persistent cycles of fouling and cleaning while holding the melt index tightly [20, 27]. A 2003 survey counted polymers among the areas with the most nonlinear predictive control applications and expected their number to grow where linear control had proven difficult, such

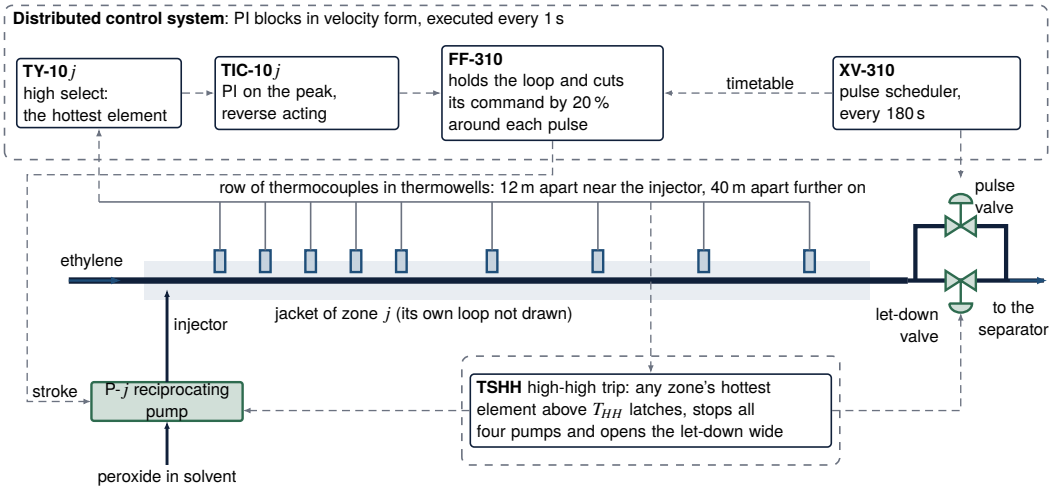


Figure 10.8 One peak loop and the trip with their hardware. Blue marks are sensing devices, the row of thermocouples in thermowells along zone j. Green symbols are final elements: the zone's reciprocating initiator pump, the let-down valve and the pulse valve at the outlet. Dashed arrows are signals. Notice that the controller never sees a single temperature: a high select passes the hottest element, and the feedforward stands between the peak controller and the pump around each scheduled pulse. The trip reads the same row of elements. The other three zones, the jacket loops with mid-ranging, PIC-300, the melt-index trim, the supervisor and the MPC are left out. Not to scale, and not a piping diagram.

as polymerization [13]. Plant data show the wall fouling, so the thickness of the layer can be inferred from the measured heat-transfer coefficient and a heat-transfer model, the basis of soft sensors for it [27]. The MPC of case 9 is the linear, identified form of the predictive idea, with the margin of this chapter written into its plan as a ceiling. How far a wall estimate can be trusted is the subject of the Open challenge box in Section 10.8.

> **IN PRACTICE** **A Trip With Its Own Sensors and a Relief Path**
>
> In service a high-high trip such as TSHH is a safety instrumented function. Its sensors may be transmitters separate from the regulatory control system, its logic solver is separate as well, and one piece of hardware should not both regulate and shut down, since a single fault would then disable both [25]. The standard for such systems is ANSI/ISA-84.00.01-2004, *Functional Safety: Safety Instrumented Systems for the Process Industry Sector*. Behind the trip, the reactor is protected by pressure relief devices that release its contents at once if ethylene runs away, and they vent to the air because the response must be fast [18]. In the chapter the trip reads the same thermocouples as the peak loops.

10.8 Limitations

The kinetics, the decomposition threshold and dwell, the fouling law and the quality correlations are illustrative or teaching values fitted to no plant, and nothing is modeled after a decomposition. The instruments misread only through lag, sampling and the spacing of the thermocouples, and the analyzers never fail. The supervisor is offered untuned and fails the challenge at its default margin, and case 2 runs without pulses, so its wall fouls over a long run. The weak lot of case 6 changes its strength in one step at a declared minute, which no plant would announce, so that a gain change can be told from everything else the tube does.

The MPC's model is four identified paths and a set of offsets. It leaves out the parcels, the kinetics, the margin, the decomposition and the fouling, which reach it only through the bias, the shortening of

the dead time as the stroke rises, the gains of the cross and jacket paths away from the design point, the lot, which arrives as an unmeasured gain change for the bias to carry, and the plant below 15 % of stroke, where the gain schedule is clamped. Its cross paths and jackets are offsets rather than states the plan can move, so a plan's own effect on the next zone is left to the next plan. The scatter of about 2 K between the parcels a thermocouple samples is not modeled and is the reason for the 5 K margin. After a trip's reset the pressure rule keeps the pumps at zero for 46 s after their release, and the one comparison the MPC loses is to a tuning chosen in hindsight that runs 0.4 K from the trip.

OPEN CHALLENGE Seeing the Wall Foul From Outside the Tube

The polymer layer on the inside wall of an LDPE tube is difficult to assess and has been described in only a few technical papers. Its prediction is not systematically formulated in practice, and when the product leaves its quality range the process is adjusted by hand, which is slow. Plants strip the layer online by pressure cleaning or thermal shock, and the reactor has to stay stable through every cycle of fouling and cleaning. A 2022 study pairs a soft sensor of the layer's thickness with a predictive controller that starts the cleaning when the layer passes a limit, tested on a process simulation [27]. Progress would be a wall estimate proved on a running tube.

10.9 Conclusion

A tubular LDPE reactor is run on a margin that its excursions spend, and the simulator of this chapter measures that margin on the truth while its loops see thermocouples, a pressure gauge and delayed analyzers. The tube is 70 parcels of 28 kg riding a 1500 m flow at 2500 bar, and at four 290 °C peaks it converts 27.51 % with 44.7 K to the teaching line at 335 °C. A peak's gain falls from 1.9 to 0.6 K per percent of stroke as it moves toward its injector, and each zone's tail is the next zone's feed.

The scheduled pulse winds the peak loops up and costs 9.7 K of overshoot, which a feedforward on the schedule reduces to 2.2 K, raising the worst margin over two pulses from 33.1 to 41.9 K. A trip set 5 K below the line fires 1.5 s before a decomposition that one scan earlier it would have prevented. Over four hours the suggested configuration converts 30.79 % with 16.46 K to spare against 27.72 % as shipped. An optional model predictive controller that carries the ceiling in its plan takes the request that trips the loops at 5.08 min and holds the four peaks at 320 °C, converting 31.54 % with 12.8 K to spare against 31.09 % for the loops with the same requests clipped by hand.

The model is plug flow in well-mixed parcels with illustrative kinetics and a declared decomposition. A fuller model would add axial dispersion, a temperature-dependent density with the expansion cooling of a pulse, a molecular-weight distribution, analyzer faults and a supervisor that anticipates the lot change. As it stands, the simulator is a place to learn to size a safety margin against the excursions a reactor actually makes.

KEY POINTS

- Each injection of initiator lights its own hot peak, and the gas it heats becomes the next zone's feed.
- A peak's gain falls from 1.9 to 0.6 K per percent of stroke as the peak moves toward its injector.
- The scheduled pulse winds the peak loops up and costs 9.7 K of overshoot, which a feedforward on the schedule reduces to 2.2 K.
- A trip set 5 K below the line fires 1.5 s before a decomposition it does not prevent, because it stops the pumps and not the initiator already in the gas.
- Excursions set the margin, and the setpoint is what they leave.

Where else this applies. A slow handle that keeps a fast one in range is also the mid-ranging of Volume 4, Chapter 10, and a guard that a fast excursion can cross is also the surge override of Volume 4, Chapter 2.

References

[1] C. Kiparissides, G. Verros, and J. F. MacGregor, "Mathematical modeling, optimization, and quality control of high-pressure ethylene polymerization reactors," *Journal of Macromolecular Science, Part C: Polymer Reviews*, vol. 33, no. 4, pp. 437–527, 1993.

[2] R. C. M. Zabisky, W.-M. Chan, P. E. Gloor, and A. E. Hamielec, "A kinetic model for olefin polymerization in high-pressure tubular reactors: a review and update," *Polymer*, vol. 33, no. 11, pp. 2243–2262, 1992.

[3] R. Geyer, J. R. Jambeck, and K. L. Law, "Production, use, and fate of all plastics ever made," *Science Advances*, vol. 3, no. 7, p. e1700782, 2017.

[4] J. Albert and G. Luft, "Thermal decomposition of ethylene–comonomer mixtures under high pressure," *AIChE Journal*, vol. 45, no. 10, pp. 2214–2222, 1999.

[5] O. Bilous and N. R. Amundson, "Chemical reactor stability and sensitivity: II. Effect of parameters on sensitivity of empty tubular reactors," *AIChE Journal*, vol. 2, no. 1, pp. 117–126, 1956.

[6] C. Kiparissides, "On the elucidation of polymer fouling mechanisms and ethylene decomposition in high-pressure LDPE tubular reactors," *Macromolecular Reaction Engineering*, vol. 16, no. 6, p. 2200023, 2022.

[7] S. X. Zhang, N. K. Read, and W. H. Ray, "Runaway phenomena in low-density polyethylene autoclave reactors," *AIChE Journal*, vol. 42, no. 10, pp. 2911–2925, 1996.

[8] B. J. Allison and A. J. Isaksson, "Design and performance of mid-ranging controllers," *Journal of Process Control*, vol. 8, no. 5–6, pp. 469–474, 1998.

[9] D. E. Seborg, T. F. Edgar, D. A. Mellichamp, and F. J. Doyle, III, *Process Dynamics and Control*, 4th ed. Hoboken, NJ: John Wiley & Sons, 2016.

[10] C. H. Chen, J. G. Vermeychuk, J. A. Howell, and P. Ehrlich, "Computer model for tubular high-pressure polyethylene reactors," *AIChE Journal*, vol. 22, no. 3, pp. 463–471, 1976.

[11] A. Brandolin, M. H. Lacunza, P. E. Ugrin, and N. J. Capiati, "High pressure polymerization of ethylene. An improved mathematical model for industrial tubular reactors," *Polymer Reaction Engineering*, vol. 4, no. 4, pp. 193–241, 1996.

[12] M. Asteasuain, S. Pereda, M. H. Lacunza, P. E. Ugrin, and A. Brandolin, "Industrial high pressure ethylene polymerization initiated by peroxide mixtures: A reduced mathematical model for parameter adjustment," *Polymer Engineering & Science*, vol. 41, no. 5, pp. 711–726, 2001.

[13] S. J. Qin and T. A. Badgwell, "A survey of industrial model predictive control technology," *Control Engineering Practice*, vol. 11, no. 7, pp. 733–764, 2003.

[14] R. O. Gibson, E. W. Fawcett, and M. W. Perrin, "The effect of pressure on reactions in solution I—Sodium ethoxide and ethyl iodide to 3000 kg/cm^2 II—Pyridine and ethyl iodide to 8500 kg/cm^2," *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, vol. 150, no. 869, pp. 223–240, 1935.

[15] E. W. Jenkins, "The discovery of polythene—a case history," *School Science and Mathematics*, vol. 68, no. 2, pp. 135–140, 1968.

[16] American Chemical Society, "Discovery of polypropylene and the development of a new high-density polyethylene," National Historic Chemical Landmark booklet, Office of Communications, Washington, DC, 1999, designated at Phillips Petroleum Company, Bartlesville, Oklahoma, 12 November 1999; acs.org/education/whatischemistry/landmarks/polypropylene.html, read November 2026.

[17] K. Ziegler, "Consequences and development of an invention," Nobel Lecture, Stockholm, 12 December 1963, 1963, nobelprize.org/uploads/2018/06/ziegler-lecture.pdf, read November 2026.

[18] European IPPC Bureau, "Reference document on best available techniques in the production of polymers," European Commission, Joint Research Centre, Institute for Prospective Technological Studies, Seville, Tech. Rep., Aug. 2007.

[19] M. H. Lacunza, P. E. Ugrin, A. Brandolin, and N. J. Capiati, "Heat transfer coefficient in a high pressure tubular reactor for ethylene polymerization," *Polymer Engineering & Science*, vol. 38, no. 6, pp. 992–1013, 1998.

[20] V. M. Zavala and L. T. Biegler, "Optimization-based strategies for the operation of low-density polyethylene tubular reactors: nonlinear model predictive control," *Computers & Chemical Engineering*, vol. 33, no. 10, pp. 1735–1746, 2009.

[21] M. Häfele, A. Kienle, M. Boll, and C.-U. Schmidt, "Modeling and analysis of a plant for the production of low density polyethylene," *Computers & Chemical Engineering*, vol. 31, no. 2, pp. 51–65, 2006.

[22] K. J. Åström and T. Hägglund, *Advanced PID Control*. Research Triangle Park, NC: ISA – The Instrumentation, Systems, and Automation Society, 2006.

[23] G. Pannocchia and J. B. Rawlings, "Disturbance models for offset-free model-predictive control," *AIChE Journal*, vol. 49, no. 2, pp. 426–437, 2003.

[24] D. Goldfarb and A. Idnani, "A numerically stable dual method for solving strictly convex quadratic programs," *Mathematical Programming*, vol. 27, no. 1, pp. 1–33, 1983.

[25] T. R. Kuphaldt, *Lessons in Industrial Instrumentation*, version 2.33 ed. Open textbook, Creative Commons Attribution 4.0 license, ibiblio.org/kuphaldt/socratic/sinst, 2024.

[26] K. Stouffer, M. Pease, C. Tang, T. Zimmerman, V. Pillitteri, S. Lightman, A. Hahn, S. Saravia, A. Sherule, and M. Thompson, "Guide to operational technology (OT) security," National Institute of Standards and Technology, Gaithersburg, MD, Special Publication 800-82r3, 2023.

[27] F. S. Rohman, M. R. Othman, D. Muhammad, A. Azmi, I. Idris, R. A. Ilyas, S. E. Elkhatif, and M. N. Murat, "Nonlinear control of fouling in polyethylene reactors," *ACS Omega*, vol. 7, no. 44, pp. 39 648–39 661, 2022.

10.10 Exercises

10.1 ⌕ Concept check · 2 min

In case 5 the peak setpoints are 328 °C and the high-high trip is set at 330 °C, 5 K below the decomposition line. After the pulse at 7 min the trip fires on zone 1, and 1.5 s later gas further down zone 1 decomposes. Why does the trip not prevent it?

(a) The trip stops the pumps, but the initiator already in the gas still reacts as it is carried to the peak

(b) The trip opens the let-down valve wide, and the falling pressure speeds up the polymerization in the peak

(c) The thermocouple noise of 0.3 K hides the approach of the peak until the scan that fires the trip

(d) The trip compares only the last zone's thermocouple with its setting, so zone 1 is not protected at all

10.2 ⌕ Concept check · 2 min

Between 10 and 15 % of stroke, zone 2's steady peak rises by about 1.9 K per percent of pump stroke, and between 45 and 55 % by only 0.6 K per percent. Which explanation is right?

(a) The pump's delivery flattens near full stroke, so each extra percent injects less peroxide

(b) A larger dose heats the gas faster, so the rest of the dose decomposes sooner and the front burns out earlier

(c) The decomposition of ethylene removes heat from the gas once the peak passes about 300 °C

(d) The pressure loop lowers the reactor pressure as the conversion rises, which slows the polymerization

10.3 Concept check · 2 min

The pulse feedforward FF-310 is on, and the pulse valve fails to open at its next scheduled time. What happens to the peaks?

(a) Nothing, because the feedforward watches the valve position and stays idle when the valve does not move

(b) They overshoot their setpoints, because the loops wind up against a pressure dip that never comes

(c) They dip with no pulse at all, because the cut is keyed to the timetable and still arrives on schedule

(d) The trip fires, because the pressure stays high while the pumps run at their full strokes

10.4 Theory and calculation · 5 min

The heat of polymerization is $-\Delta H_p = 93.6\,\mathrm{kJ/mol}$, the molar mass of ethylene $M_w = 28.05\,\mathrm{g/mol}$ and the heat capacity of the gas $c_p = 2600\,\mathrm{J/(kg\,K)}$. The tube is fed 64.8 t/h of ethylene at 165 °C and converts 27.51 % of it.

(a) Find the adiabatic temperature rise per percent of conversion. *Checkpoint:* 12.83 K.

(b) Find the outlet temperature if the whole conversion happened in one adiabatic front, and compare it with the decomposition line at 335 °C. *Checkpoint:* A rise of 353 K, to about 518 °C.

(c) Find the polymer production rate and how many minutes of production a product hold-up of 2500 kg holds. *Checkpoint:* 17.8 t/h and 8.4 min.

10.5 Theory and calculation · 6 min

The tube is $L = 1500\,\mathrm{m}$ long with a bore of 55 mm and holds $N = 70$ parcels. The gas density is $\rho_0 = 550\,\mathrm{kg/m^3}$ at $P_{ref} = 2500\,\mathrm{bar}$, its compressibility $\kappa = 6.3 \times 10^{-5}\,\mathrm{bar^{-1}}$, and the feed $F_{in} = 18.0\,\mathrm{kg/s}$. The separator is at 250 bar, and the let-down passes the design flow at P_{ref} with an opening of 0.5.

(a) Find the mass and length of one parcel, the gas velocity and the residence time. *Checkpoint:* 28.0 kg, 21.4 m, 13.78 m/s and 108.9 s.

(b) Find the capacity $C = \rho_0 A L \kappa$ and the valve coefficient C_v of Equation (10.4). *Checkpoint:* 0.1235 kg/bar and 0.759 kg/(s bar$^{1/2}$).

(c) Linearize Equation (10.4) about the design point with the let-down held, and find the time constant of the pressure. *Checkpoint:* 30.9 s.

10.6 Theory and calculation · 6 min

Ethylene decomposition in the model has $k_{dec,0} = 5 \times 10^{-3}\,\mathrm{s^{-1}}$ at $T_D = 335\,°\mathrm{C}$, an activation energy $E_{dec} = 450\,\mathrm{kJ/mol}$ and a heat of decomposition $-\Delta H_{dec} = 120\,\mathrm{kJ/mol}$. Take $M_w = 28.05\,\mathrm{g/mol}$, $c_p = 2600\,\mathrm{J/(kg\,K)}$, $R = 8.314\,\mathrm{J/(mol\,K)}$ and a spent parcel with $1 - x - x_d = 0.73$.

(a) Find the rate at which decomposition heats the parcel at 335 °C. *Checkpoint:* 6.0 K/s.

(b) Find the same rate at 320 °C. *Checkpoint:* 0.63 K/s, about 9.5 times slower.

(c) A clean wall cools a parcel with a time constant of 24.6 s. With the jacket water at 181 °C, find the cooling rate of a parcel at 335 °C and say what happens to a parcel held just above the line. *Checkpoint:* About 6.3 K/s.

10.7 App challenge · 9 min

Load scenario 3, “3 · The pulse valve”, at the default seed. The four peak loops hold 290 °C and the first pulse is scheduled at 30 s. Run at 1 min/s until the clock passes 5 min, pause and export the CSV. Temperatures and margins within 0.2 K of the key count as correct.

(a) With Pulse feedforward Off, find the highest value of the columns `Tpk1_meas_C` to `Tpk4_meas_C` between 0.5 and 3.4 min, and read the Worst decomposition margin tile at the end of the run. *Checkpoint:* 299.7 °C and 33.1 K.

(b) Pause, press Reset, set Pulse feedforward to On on the XV-310 card before Run, and repeat the run and the two readings. *Checkpoint:* 292.2 °C and 41.9 K.

(c) Take the supervisor's rule, Equation (10.10), with $\hat{e}_j$ equal to the overshoot above 290 °C that you found, $\Delta_{set} = 20$ K and $\sigma_{TC} = 0.3$ K. Find the highest peak setpoint it allows without and with the feedforward. *Checkpoint:* 304.7 °C and 312.2 °C.

10.8 App challenge · 8 min

Load scenario 5, "5 · Conversion pushed toward the line", at the default seed. The peak setpoints rise to 315, 322 and 328 °C at 1, 3 and 5 min, the pulses come every three minutes from 1 min without feedforward, and the trip is at 330 °C. Run at 1 min/s. Margins within 0.1 K and times within 0.05 min of the key count as correct.

(a) Run as shipped until the run stops. Read the Plant and Worst decomposition margin tiles. *Checkpoint:* Decomposed at 7.4 min, −1.0 K.

(b) Press Reset, set the Trip temperature (hottest thermocouple) to 325 °C on the Control architecture card, and run until the clock passes 10 min. Read the same two tiles, and find the first row of the exported CSV with `tripped` equal to 1. *Checkpoint:* Tripped, 8.7 K, at 4.30 min.

(c) The trip at 330 °C sat 5 K below the line. Explain why it was not enough and what the 325 °C setting buys. *Checkpoint:* The trip's dead time and the dosed gas.

10.9 App challenge · 10 min

Load the graded challenge, "Challenge · the most conversion inside the margin", at the default seed. It runs 240 min with pulses every three minutes, warmer jacket water at 60 min and a 120 % initiator lot at 150 min. Make every change before Run, then run at 60 min/s until the clock reaches 240 min. Conversions within 0.02 points and margins within 0.1 K of the key count as correct.

(a) Set Initiator pumps to Peak loops, all four peak setpoints to 310.0 °C, Pulse feedforward On, Mid-ranging (VPC) On with a Target pump stroke of 55 %, and Melt-index trim On. Read the Mean conversion, Worst decomposition margin and Challenge target tiles. *Checkpoint:* 30.79 %, 16.5 K, met.

(b) Press Reset, set Pulse feedforward Off, change nothing else, and run again. *Checkpoint:* 30.81 %, 13.5 K, not met.

(c) Press Reset, set Pulse feedforward On again and all four peak setpoints to 312.0 °C, and run again. From the CSV column `metric_worst_margin_K`, say when the worst margin is set in part (a)'s run and in this one. *Checkpoint:* 30.86 %, 13.8 K, not met. Both just after the lot change at 150 min.

10.10 Application area · 3 min

Tubular LDPE reactors open a pulse valve every few minutes on purpose.

(a) What does a pulse do for the wall, and what happens to the heat transfer when the pulses are sparse? Use case 4. *Checkpoint:* It strips the polymer layer. U falls to 0.68 of clean in 24.9 min without a pulse.

(b) Name two costs of pulsing, and say how the pulse period should be chosen. *Checkpoint:* A dip and an overshoot each time, and a pressure upset.

10.11 Application area · 3 min

The model draws the decomposition line at 335 °C with a dwell of 1.0 s, and every loop sees the peaks through thermocouples.

(a) Where should the decomposition limit and the trip setting of a real reactor come from? *Checkpoint:* Licensor data, plant history, measured boundaries.

(b) Give two reasons the hottest thermocouple can read well below the hottest gas, with a number from the chapter for one of them. *Checkpoint:* Spacing and lag. Up to 10.9 K after a pulse.

10.12 Review the agent · 5 min

An AI assistant is asked how close to the decomposition line the peaks can run. It answers: “In case 2 the zone 2 loop takes a step to 300 °C and its highest reading over the next five minutes is only 300.8 °C, so the loops hold the peaks within about 1 K. Set all four peaks to 328 °C and the trip to 330 °C. The peaks then stay 7 K below the line, the trip covers the last kelvin of loop error, and the conversion gains several points.” Find the flaw and say how you would check it in the app.