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CHAPTER 8

Fluidized-Bed Polyethylene Simulator for Cascade Control and Grade-Transition Economics

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Edited by John D. Hedengren

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CHAPTER 8

Fluidized-Bed Polyethylene Simulator for Cascade Control and Grade-Transition Economics



The controller moves 1 cooling-water valve, for the cooler outlet 2 ethylene valve, for the pressure 3 hydrogen valve, for melt index 4 hexene valve, for density 5 catalyst feeder, for the production rate 6 discharge valve, for the bed level

The controller reads 1 bed temperature 2 cooler outlet temperature 3 reactor pressure 4 bed level 5 gas analyzer, hydrogen and hexene ratios 6 quality laboratory, melt index and density 45 to 105 minutes late

What disturbs it 1 warmer cooling water 2 a fouling cooler 3 a recycle compressor that loses capacity

Notice that the gas mix can change in minutes while the bed of powder holds four hours of product and the laboratory reports long after its sample was drawn, and that in the chapter the catalyst enters the bed itself, not the space above it. Illustration, not to scale.

IN PLAIN TERMS A Fast Gas Steering a Slow Bed

The main idea. Plastic grains for film and molded parts grow in a tall vessel, kept floating by a stream of gas that also carries away the heat. The mix of gases decides what kind of plastic is being made, and that mix can be changed within minutes.

The challenge. The vessel holds about four hours of grains, all stirred together, so the plastic that leaves changes only slowly. A switch to a new product therefore makes a long run of plastic that fits neither order.

Why it matters. In the simulated plant, better tuning and a smaller bed cut that waste by more than half.

THREE WAYS TO READ THIS CHAPTER

Explore	12 min	This page, the Did you know? and History boxes of the Background section, the Try it boxes in Sections 8.4 and 8.6, the Did you know? box in Section 8.7, and Key points in Section 8.10. No equations.
Study	65 min	The whole chapter in order, stopping at the three pause points, then Exercises 1 to 12.
Practice	15 min	This page, Section 8.7 with Figure 8.4, Section 8.8, and Section 8.9 with its Open challenge boxes.

The control question The gas in a fluidized-bed polyethylene reactor settles in minutes to hours, while melt index and density are averages over a four-hour bed of powder. How should cascades that span two decades of time scale be tuned, and what do tuning and bed preparation save in off-specification tonnes during a grade change?

Learning objectives

- Compute the time constants of the gas, thermal, catalyst and resin inventories from the model and rank them.
- Identify the inner cooler loop and the outer temperature loop from step tests, and explain why the outer plant is lead-lag.
- Derive the off-grade tonnage of a grade change and show that the production rate cancels from it.
- Reduce the off-grade tonnage of a transition with quality-loop tuning and bed level, and judge a rate cut by measurement.
- Read the cooling-water valve and the cooling utilization as early warnings of the heat-removal limit.

Prerequisites Sections 1.4.4 (heat removal), 1.4.5 (grade transitions), 1.4.6 (laboratory and bias update), 1.6.1 and 1.6.2 (engine and velocity-form PID). Section 1.6.3 is needed only for the predictive controller.

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See also Volume 3, Chapter 2 and Volume 3, Chapter 3 for cascade structure and the speed an inner loop needs. Volume 9, Chapter 4 for offset-free predictive control with a disturbance estimate. Volume 5, Chapter 3 and Volume 5, Chapter 4 for control through a slow analyzer and a late laboratory.

8.1 Introduction

Most teaching examples in process control carry one dominant time constant, and the controller is tuned against that number. A gas-phase polyethylene reactor carries two populations that respond about two decades apart. The gas above and inside the bed turns over in minutes, so ethylene inventory, hydrogen ratio and comonomer ratio are fast, measurable and reachable with a valve. The powder in the bed turns over in four hours, and the molecular weight and density of the resin leaving the discharge valve are the mass-weighted average of everything produced over the preceding residence time. No control action on the gas changes the resin already stored in the bed.

The consequence is a control problem that no amount of loop tuning removes. Melt index and density are the variables the customer buys and they cannot be manipulated directly. They are reached only through a gas-composition setpoint, which makes the quality loops the outer half of a cascade whose inner half settles between one and two orders of magnitude faster. The cooler outlet temperature in the simulator of this chapter answers its water valve in about 0.5 min, the 1-hexene inventory turns over in 4.0 min, the ethylene inventory in 6.7 min, the bed thermal lag is 11.3 min, the hydrogen inventory turns over in 142 min, the active catalyst inventory in 176 min and the resin property in 240 min. A melt-index controller tuned as though it acted on the hydrogen valve saturates a ratio the plant has already reached and then cycles for hours afterward.

The second consequence is economic rather than dynamic. A grade change is not a disturbance to be rejected. It is a scheduled excursion whose cost is the tonnage discharged while the resin sat outside its specification band. Integral absolute error is a poor objective for a transition, because the setpoint moved on purpose and hours of transient were always going to be spent. The relevant measure is the tonnage discharged at the wrong melt index, and the variables that reduce it differ from those regulatory tuning rules address.

The physics behind the model are the standard conservation statements of the process control curriculum. Material balances on the gas-phase species, an energy balance on the bed and a mixing balance on the solids inventory follow the forms of the introductory texts [1, 2], propagation follows Arrhenius kinetics, and each bed-average resin property is a first-order lag whose time constant is the solids residence time. The experiments built on that model show cascade structure, time-scale separation, integrating level dynamics, feedforward, anti-windup, override control and the difference

between an instantaneous and an inventory-averaged quality [1, 3]. Each of these behaviors appears in industrial polymer service, where off-grade production during transitions is a direct and recurring cost [4].

Gas-phase polyethylene reactors have carried a large modeling and control literature for exactly these reasons, covering the production processes and property correlations [5], the dynamics of a fluidized bed with solid catalyst [6], industrial copolymerization kinetics [7], the question of whether a two-phase description is needed at all [8], and the inferential and nonlinear control of resin properties in a running plant [9, 10]. The simulator of this chapter turns those questions into experiments. Nine loops can be opened one at a time, a grade change can be repeated with a single condition altered, and the off-specification tonnage is accumulated at the discharge valve during the run.

This chapter defines a fluidized-bed polyethylene reactor completely enough for it to be reconstructed, and measures what its two separated time scales cost during a grade transition. The plant is a thirteen-state model with nine independent controller stations, six non-defeatable overrides and a complete data export. Section 8.3 sets out the balances, the constants and the solved design point. Section 8.4 measures the seven process time constants that span the plant and shows that catalyst deactivation turns the outer temperature loop's plant from first order into lead-lag. Section 8.5 describes the nine loops, the cascades, the feedforward, the overrides and the optional predictive controller. Section 8.6 runs the rate, condensing-agent, cooling and impurity scenarios. Section 8.7 derives and tests the result that off-grade tonnage during a transition does not depend on production rate, runs one grade change in the ten ways of Table 8.9, measures its cost in tonnes of off-specification resin, and compares the cascades with the predictive controller. Section 8.8 names the hardware and the practice behind the model, and Sections 8.9 and 8.10 state the limitations and the conclusions.

8.2 Background

Polyethylene was made first at high pressure and then in solution and slurry, and each of those routes carries a diluent that has to be removed from the product. The gas-phase route eliminates the diluent. A vertical vessel holds a bed of polymer powder fluidized by its own recycled monomer, solid catalyst is metered into the side of the bed, and granules grow around the catalyst particles until they are withdrawn. Because nothing has to be filtered or distilled, the process took a large share of world polyethylene capacity, and its economics are dominated by the heat the recycle gas can carry away rather than by separation [5], which Section 1.4.4 works through for the running example of Chapter 1.

> **+ DID YOU KNOW? One Vessel, Hundreds of Thousands of Tonnes**
>
> The fluidized-bed reactor of a polyethylene plant is a vertical pressure vessel up to 40 m tall, and a 2007 European reference document gives 450 kt a year as the largest capacity of a gas-phase line for linear low-density polyethylene [11]. Fluidized-bed polymerization, introduced in 1968, accounts for 40 % of world polyethylene capacity [12].

The control problem that arrived with the technology was one of measurement rather than actuation. Bed temperature, pressure and level have had instruments since the first plants and melt index and density have not. Both are laboratory determinations on a sample pulled every hour or two and reported after the granules have been pressed, conditioned and run through an extrusion plastometer, so an operator holding melt index with hydrogen manipulated a four-hour inventory against a measurement that was several hours old.

Two developments closed the measurement gap, an inferential sensor and model-based control built on top of it, as the first History box below tells. Polymer units appear throughout the industrial model predictive control population that was inventoried a decade after the second of them [13].

> ⧖ HISTORY **Reading Melt Index Between Samples, 1991 and 1993**
>
> In 1991 an article named the lack of suitable on-line measurements of polymer properties as a major difficulty for quality control in industrial polymerization reactors. It predicted melt index and density in a fluidized-bed ethylene copolymerization reactor from the on-line temperature and gas composition, updated the models' adjustable parameters from the infrequent laboratory measurements by recursive estimation, and illustrated the scheme on operating data from an industrial reactor [9]. In 1993 a nonlinear model-based controller moved the hydrogen and butene feeds to regulate the instantaneous melt index and density and to carry them through grade changeovers, with an extended Kalman filter estimating the disturbances. Tested in simulation on a mechanistic model of the process, it handled both tasks, where an analogous linear controller was inadequate at changing operating conditions and during changeovers [10].

Grade transitions became the natural target once the properties could be estimated online. Optimal transition trajectories for polyolefin reactors were computed as dynamic optimization problems and showed that the shortest path is not the direct one [4], that the choice of control structure and the transition policy interact and should be selected together [14], and that the resulting policies can be commissioned on a plant with commercial real-time optimization software [15]. Alongside this, condensed-mode operation raised the ceiling on production by putting part of the recycle stream into the liquid phase and letting it evaporate in the bed, which requires the reactor model to carry a dew point and a condensed fraction rather than a sensible-heat balance alone [16]. The simulator of this chapter carries a reduced-order version of each of these pieces and exposes the loops that connect them. The second History box below tells where the fluid bed and its condensing cooler came from.

> ⧖ HISTORY **From a Low-Pressure Fluid Bed to Condensed Mode, 1975 to 1985**
>
> A patent application of 1975 copolymerized ethylene with other alpha-olefins in a fluid bed reactor at low pressure to make low- and medium-density polymers, which were then usually made by homopolymerizing ethylene at very high pressures with free-radical catalysts. Its recycle gas passed an external exchanger that stripped the heat of reaction before the gas returned to the bed [17]. A patent filed in 1984 and issued in 1985 started from the observation that the polymer a reactor of a given size can make is directly related to the heat that can be withdrawn. It cooled the recycle stream below its dew point and returned the two-phase mixture below the bed, raising the dew point with pressure or with an inert condensable fluid such as a butane, pentane or hexane, and keeping the liquid entrained in the gas until it vaporized [18].

8.3 Reactor Model

One fluidized-bed reactor with an external cycle gas loop is simulated, and Figure 8.1 carries every symbol the equations below use. Recycle gas leaves the top of the disengaging section, passes a compressor and a water-cooled exchanger, and returns below the distributor plate carrying whatever condensed in the cooler, with ethylene, hydrogen, 1-hexene and cyclohexane added to it as make-up.

8.3.1 Controlled Variables, Inputs and Disturbances

Nine variables are controlled, six valves and three inner setpoints are manipulated, and ten disturbances are available. Table 8.1 classifies them with their enforced ranges.

Only three of the nine loops produce performance statistics on the scorecard of Section 1.6.4, namely reactor temperature with a 1.0 °C band, bed level with a 3 % band and melt index with a band of $\pm 10\,\%$ of its setpoint, which is the specification band of Section 8.7. The other six are measured and logged but do not produce integral absolute error, overshoot or settling numbers.

8.3.2 Gas-Phase Balances and Pressure

The gas in the reactor, the disengaging section and the recycle loop is treated as one perfectly mixed volume. Four species are carried as molar holdups and nitrogen with the accumulated light ends is a fixed inert holdup n_I, so the balance for species $i \in \{C_2, H_2, C_6, ICA\}$ is Equation 8.1.

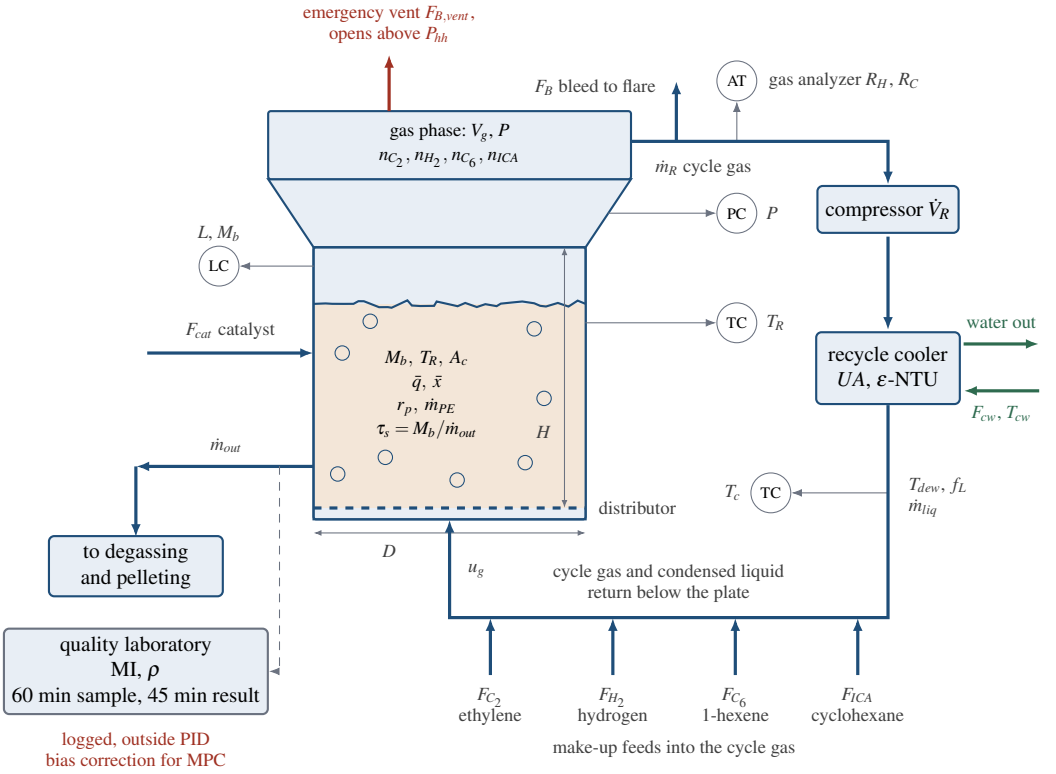


Figure 8.1 Fluidized-bed polyethylene reactor with its cycle gas loop, make-up feeds, instruments and quality laboratory. The vessel is drawn schematically and not to scale. Every symbol shown appears in (8.1)–(8.15), and the dashed path marks the laboratory, which is sampled, delayed, displayed and logged. It remains outside the PID loops and corrects the optional MPC estimate.

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = F_i - r_i - y_i F_B, \quad y_i = \frac{n_i}{n_g}, \quad n_g = n_I + \sum_j n_j \tag{8.1}$$

where F_i is the make-up feed, r_i is the consumption by reaction and F_B is the total gas leaving through the bleed. Only ethylene, hydrogen and 1-hexene react, so $r_{ICA} = 0$. Cyclohexane is an inert condensable whose only purpose is to raise the dew point of the recycle stream. The bleed carries all four away in proportion to their mole fractions, which is what makes the direction of a hydrogen move asymmetric.

The make-up flows are valve positions against fixed capacities, with the ethylene flow additionally scaled by the square root of the supply header pressure as shown in Equation 8.2.

$$F_{C_2} = F_{C_2}^{max} \frac{v_{C_2}}{100} \sqrt{\frac{\phi_h}{100}} \tag{8.2a}$$

$$F_{H_2} = F_{H_2}^{max} \frac{v_{H_2}}{100}, \qquad F_{C_6} = F_{C_6}^{max} \frac{v_{C_6}}{100} \tag{8.2b}$$

$$F_B = F_{B0} \frac{\phi_B}{100} + k_{vent} \max(0, P - P_{hh}) \tag{8.2c}$$

Table 8.1 Variable Classification and Panel Ranges

Symbol	Meaning	Unit	Range (default)
Controlled variables			
T_R	bed temperature	°C	78–100 (88)
T_c	cooler outlet temperature	°C	22–70 (40)
P	reactor pressure	bar	18–23 (21.7)
L	bed level	%	35–85 (65)
R	production rate	t/h	12–42 (30)
R_H	H_2/C_2 ratio $\times 100$	—	4–80 (20)
R_C	C_6/C_2 ratio $\times 100$	—	0.02–2.5 (1.5)
MI	melt index	g/10 min	0.2–12 (1.0)
ρ	resin density	g/cm^3	0.915–0.955 (0.918)
Manipulated variables			
v_{CW}	cooling-water valve	%	0–100 (50.0)
v_{C_2}	ethylene make-up valve	%	0–100 (57.6)
v_{dis}	product discharge valve	%	0–100 (41.7)
v_{cat}	catalyst feeder	%	0–100 (40.0)
v_{H_2}	hydrogen valve	%	0–100 (11.6)
v_{C_6}	1-hexene valve	%	0–100 (36.3)
$T_{c,\mathrm{SP}}$	cooler outlet setpoint	°C	22–70
$R_{H,\mathrm{SP}}$	H_2/C_2 setpoint	—	4–80
$R_{C,\mathrm{SP}}$	C_6/C_2 setpoint	—	0.02–2.5
Operator handle with no loop on it			
F_{ICA}	cyclohexane feed	mol/min	0–600 (216)

Symbol	Meaning	Unit	Range (default)
Disturbances			
T_{cw}	cooling-water inlet	°C	18–42 (30)
ϕ_f	cooler fouling	%	0–45 (0)
ϕ_K	recycle compressor capacity	%	55–110 (100)
ϕ_h	ethylene header pressure	%	40–115 (100)
ϕ_B	gas bleed to flare	%	20–320 (100)
z	feed impurity	ppm-eq	0–0.6 (0)
ϕ_a	catalyst activity bias	%	−30–30 (0)
ϕ_d	discharge restriction	%	0–60 (0)
ϕ_m	melt-index analyzer bias	%	−20–20 (0)
ϕ_n	measurement noise multiplier	—	0–4 (1)
States			
$n_{C_2}, n_{H_2}, n_{C_6}, n_{ICA}$	gas-phase molar holdups	mol	positive
A_c	active catalyst inventory	—	non-negative
M_b	bed mass	kg	2000–193798
T_R	bed temperature	°C	—
T_c	cooler outlet temperature	°C	—
$\bar{q}$	bed-average ln MI	—	—
$\bar{x}$	bed-average incorporated C_6	—	0–0.2
v_{CW}, v_{dis}, F_{cat}	actuator positions	%	0–100

where F_{ICA} is set directly in mol/min by the operator. The second term of (8.2c) is a hard-wired overpressure vent that no controller can inhibit, and because it discharges the whole gas mixture it moves every composition at once while it is open.

Pressure is not a state. It is an algebraic output of the ideal gas law applied to the moles present in the free volume, and that free volume shrinks as the bed grows, as shown in Equation 8.3.

$$P = \frac{n_g R T_R}{V_g}, \qquad V_g = V_{tot} - \frac{M_b}{\rho_s} \tag{8.3}$$

where R is the gas constant, T_R is absolute bed temperature, V_{tot} is the total gas and solids volume of the reactor and loop and ρ_s is the resin particle density. Equation 8.3 couples the level loop to the pressure loop, because moving 10 % of bed level moves 20.5 m^3 of free gas volume out of 400 m^3.

8.3.3 Catalyst, Kinetics and Production

Propagation is first order in ethylene concentration and in active catalyst inventory, with an Arrhenius temperature dependence referenced to 88 °C, a mild comonomer enhancement and a poisoning term, as shown in Equation 8.4.

$$r_p = k_{p,ref} \mathrm{e}^{-\frac{E_p}{R}\left(\frac{1}{T_R} - \frac{1}{T_{ref}}\right)} \frac{A_c n_{C_2}}{V_g} \frac{1 + k_{com} R_C}{1 + K_z z} \left(1 + \frac{\phi_a}{100}\right) \tag{8.4}$$

where $R_H = n_{H_2}/n_{C_2}$ and $R_C = n_{C_6}/n_{C_2}$ are the gas-phase mole ratios, T_R and $T_{ref} = 88\,^\circ\mathrm{C}$ are in kelvin inside the exponential, z is the feed impurity and ϕ_a is a catalyst activity bias. The reduced-order form follows the industrial gas-phase copolymerization kinetics of [7] with the site distribution collapsed into one lumped activity. Comonomer and hydrogen consumption and the polymer production rate are then given by Equation 8.5.

$$x_{inst} = \frac{K_C R_C}{1 + K_C R_C} \tag{8.5a}$$

$$r_{C_6} = r_p \frac{x_{inst}}{1 - x_{inst}}, \qquad r_{H_2} = \zeta\, r_p R_H \tag{8.5b}$$

$$\dot{m}_{PE} = \frac{M_{C_2} r_p + M_{C_6} r_{C_6}}{1000} \tag{8.5c}$$

where x_{inst} is the mole fraction of 1-hexene incorporated into the chain, K_C is the competitive incorporation constant, ζ is the chain-transfer hydrogen consumption per unit of propagation, M_{C_2} and M_{C_6} are molar masses in g/mol, and $\dot{m}_{PE}$ is in kg/min.

Catalyst does not act at the moment it is fed. It accumulates in the bed, deactivates thermally and leaves with the product, as shown in Equation 8.6.

$$\frac{\mathrm{d}A_c}{\mathrm{d}t} = k_a F_{cat} - A_c \frac{\dot{m}_{out}}{M_b} - k_d A_c, \quad k_d = k_{d0}\, \mathrm{e}^{\beta_d (T_R - 88)} \tag{8.6}$$

where F_{cat} is the feeder position in percent, k_a is a hidden activation factor and T_R is in °C inside the exponential. At the design point $\dot{m}_{out}/M_b = 4.168 \times 10^{-3}$/min and $k_d = 1.5 \times 10^{-3}$/min, so the active inventory has a time constant of 176 min. No controller gain shortens that number, so production is the slowest loop on the plant that is paired with its own valve.

8.3.4 Solids Inventory and Residence Time

The bed is a pure integrator. Nothing on the right-hand side of Equation 8.7 depends on how full the bed is, so the discharge rate is independent of head and any imbalance integrates without bound [3].

$$\frac{\mathrm{d}M_b}{\mathrm{d}t} = \dot{m}_{PE} - \dot{m}_{out} \tag{8.7a}$$

$$\dot{m}_{out} = \dot{m}_{dis}^{max} \frac{v_{dis}}{100} \left(1 - \frac{\phi_d}{100}\right) \tag{8.7b}$$

$$L = \frac{100\, M_b}{\rho_b A H}, \quad A = \frac{\pi D^2}{4}, \qquad \tau_s = \frac{M_b}{\dot{m}_{out}} \tag{8.7c}$$

where ρ_b is the fluidized bulk density, A is the bed cross-sectional area, H is the bed height at 100 % level and τ_s is the solids residence time. At the design point $M_b = 119970$ kg and $\dot{m}_{out} = 500$ kg/min, so $\tau_s = 240$ min. That single number sets the length of every grade change.

8.3.5 Energy Balance and the Condensing Cooler

The reaction heat leaves through the recycle gas and nowhere else. Sensible heat is carried by the gas warming from the distributor to the bed, latent heat by whatever condensed in the cooler and boils again in the bed, as shown in Equation 8.8.

$$\begin{aligned}(M_b c_{p,s} + C_{metal}) \frac{\mathrm{d}T_R}{\mathrm{d}t} = {} & (-\Delta H_p) r_p - \dot{m}_R c_{p,g} (T_R - T_c) \\ & - \dot{m}_{liq} \Delta H_{vap} - Q_{loss}\end{aligned} \tag{8.8}$$

where $c_{p,s}$ is the resin heat capacity, C_{metal} is the lumped heat capacity of the vessel steel, $-\Delta H_p$ is the heat of polymerization, $\dot{m}_R$ is the recycle mass flow, $c_{p,g}$ is the recycle gas heat capacity, $\dot{m}_{liq}$ is the condensed flow, ΔH_{vap} is its heat of vaporization, and $Q_{loss} = U A_{wall} (T_R - T_{amb})$. At the design point the three removal terms are 19.85 MW sensible, 5.90 MW latent and 0.32 MW of wall loss

against 26.07 MW of reaction heat. The dry recycle gas alone cannot carry the reaction heat, and that deficit is the motivation for condensed-mode operation.

Pause. Try Exercise 8.1 before reading on.

The recycle flow follows from the gas density and the compressor displacement, and the condensed fraction from how far the cooler outlet sits below the dew point, as shown in Equation 8.9.

$$\dot{m}_R = \frac{P\overline{M}}{RT_R}\dot{V}_R\frac{\phi_K}{100}, \qquad \overline{M} = \sum_i y_i M_i \tag{8.9a}$$

$$T_{dew} = T_{dew,0} + a_P(P-21.7) + a_I(100y_{ICA}-12) + a_6(100y_{C_6}-0.6) + a_2(100y_{C_2}-40) \tag{8.9b}$$

$$\Delta T_{sub} = w\ln\left(1+\mathrm{e}^{(T_{dew}-T_c)/w}\right) \tag{8.9c}$$

$$f_L = f_{L,max}\left(1-\mathrm{e}^{-\Delta T_{sub}/\Delta T_{ref}}\right), \quad \dot{m}_{liq} = f_L\dot{m}_R \tag{8.9d}$$

where $\overline{M}$ is the mixture molar mass including the inert, $\dot{V}_R$ is the compressor volumetric displacement, and w is a smoothing width that rounds the corner of the positive part in (8.9c) over about one kelvin. A hard $\max(0,\cdot)$ puts a kink in the condensation curve that a fourth-order Runge-Kutta step integrates straight through, and the rounded version is also more realistic because a real cooler condenses a small mist fraction before the bulk dew point is reached. Equation 8.9b couples the condensed fraction to the grade being made, because 1-hexene raises the dew point and low-density grades carry more of it.

The exchanger itself is a counterflow effectiveness-NTU calculation whose hot-side capacity rate is inflated to account for the latent duty, as shown in Equation 8.10.

$$UA = UA_0\left(1-\frac{\phi_f}{100}\right)\left(\frac{F_{cw}}{F_{cw,ref}}\right)^{n_{UA}} \tag{8.10a}$$

$$C_h = \dot{m}_R c_{p,g}\varphi, \quad \varphi = \mathrm{clamp}\left(1+\frac{Q_{vap}}{Q_{sens}},1,4\right) \tag{8.10b}$$

$$C_c = F_{cw}c_{p,w} \tag{8.10c}$$

$$\varepsilon = \frac{1-\mathrm{e}^{-N(1-C_r)}}{1-C_r\mathrm{e}^{-N(1-C_r)}}, \; N = \frac{UA}{C_{min}}, \; C_r = \frac{C_{min}}{C_{max}} \tag{8.10d}$$

$$T_c^* = T_R - \frac{\varepsilon C_{min}\max(0,T_R-T_{cw})}{C_h} \tag{8.10e}$$

$$\frac{\mathrm{d}T_c}{\mathrm{d}t} = \frac{T_c^*-T_c}{\tau_{HX}} \tag{8.10f}$$

where $n_{UA}=0.8$ is the flow exponent, $F_{cw}=F_{cw}^{max}v_{CW}/100$, $Q_{sens}=\dot{m}_R c_{p,g}(T_R-T_c)$, $Q_{vap}=\dot{m}_{liq}\Delta H_{vap}$, C_{min} and C_{max} are the smaller and larger of C_h and C_c, and τ_{HX} is the thermal lag between the solved outlet temperature and the measured one. The exchanger solution is clamped so that T_c can never fall below the water inlet temperature or rise above the bed temperature, C_h and C_c are floored at 500 kJ/(min K), ε reverts to $N/(1+N)$ when C_r exceeds 0.999, and F_{cw} is floored at 200 kg/min inside (8.10a) so that a closed valve does not produce a zero UA.

Two derived quantities are computed continuously. The first is the production rate the cooler could carry with the water valve wide open, obtained by evaluating (8.10) at $F_{cw}=F_{cw}^{max}$ and dividing the resulting duty by the heat of polymerization, as shown in Equation 8.11.

$$R_{max} = \frac{Q_{max}-Q_{loss}}{-\Delta H_p}\left(M_{C_2}+M_{C_6}\frac{x_{inst}}{1-x_{inst}}\right)\frac{0.06}{1000} \tag{8.11}$$

where the factor 0.06 converts kg/min to t/h. The second is the cooling utilization $100R/R_{max}$, which reads 88.3 % at the design point.

8.3.6 Quality Correlations and the Bed Average

Melt index is an inverse measure of molecular weight and hydrogen is the chain-transfer agent that shortens the chains. The instantaneous property of the resin currently being produced follows the reduced-order form used throughout the polyethylene inference literature [9], given in Equation 8.12.

$$\ln \mathrm{MI}_{inst} = a_T \left(\frac{1}{T_R} - \frac{1}{T_{ref}} \right) + m \ln(a_0 + a_H R_H + a_C R_C + a_z z) \tag{8.12a}$$

$$\rho_{inst} = \rho_{HD} - K_\rho x_{inst} + K_{MI} \ln \mathrm{MI}_{inst} \tag{8.12b}$$

where a_0, a_H, a_C and a_z weight the intercept, the hydrogen ratio, the comonomer ratio and the impurity, m is the exponent, a_T carries the temperature effect, ρ_{HD} is the homopolymer density base and K_ρ converts incorporated comonomer into a density decrement. The bracket in (8.12a) is floored at 0.05 to keep the logarithm defined. The design ratios $R_H = 0.20$ and $R_C = 0.015$ make the bracket exactly 1.000 and the temperature term exactly zero, so $\mathrm{MI}_{inst} = 1.00$ and $\rho_{inst} = 0.91801\,\mathrm{g/cm^3}$ without any fitting residual.

Neither of those is what leaves the reactor. The bed is one well-mixed solids volume, so the product of bed mass and bed-average property obeys a mixing balance, and expanding it against (8.7a) leaves the first-order form of Equation 8.13.

$$M_b \frac{\mathrm{d}\bar{q}}{\mathrm{d}t} = \dot{m}_{PE} (\ln \mathrm{MI}_{inst} - \bar{q}), \quad M_b \frac{\mathrm{d}\bar{x}}{\mathrm{d}t} = \dot{m}_{PE} (x_{inst} - \bar{x}) \tag{8.13}$$

where $\bar{q}$ is the bed-average logarithm of melt index and $\bar{x}$ the bed-average incorporated comonomer, from which $\mathrm{MI}_{bed} = \mathrm{e}^{\bar{q}}$ and $\rho_{bed} = \rho_{HD} - K_\rho \bar{x} + K_{MI} \bar{q}$. Equation 8.13 is a first-order lag of time constant $M_b/\dot{m}_{PE}$, the form of Equation (1.8), which is 240 min at design against gas time constants of 4 min to 142 min. This single lag is the source of the two-decade separation. Averaging the logarithm rather than the melt index itself follows the property that mixes additively in the reduced-order correlation, and it also reduces the transition analysis of Section 8.7 to one closed-form expression.

8.3.7 Sticking Limit and Fluidization

Two constraints bound the operating window and neither has a controller. Polyethylene softens over a range rather than melting at a point, and a bed whose particles have begun to soften agglomerates into sheets and then into one lump. The temperature at which that starts depends on the resin, as shown in Equation 8.14.

$$T_{stick} = \min\left(128,\; T_{s0} + k_\rho 10^3 (\rho_{bed} - 0.920) - k_I 10^2 y_{ICA} - k_{MI} \bar{q}\right) \tag{8.14}$$

where T_{s0} is the base sticking temperature, k_ρ, k_I and k_{MI} are sensitivities to density, cyclohexane content and molecular weight, and the reported sticking margin is $T_{stick} - T_R$. It reads 8.01 °C at the design point. Low-density film grades stick at the lowest temperatures, and the cyclohexane that adds heat-removal capacity lowers the limit further, so added condensing agent costs temperature margin.

The second constraint is fluidization. Below minimum fluidization the bed slumps and heat transfer collapses, so the superficial gas velocity and the minimum fluidization velocity are computed at every step from Equation 8.15.

$$u_{mf} = \frac{d_p^2(\rho_s - \rho_g)g}{1650\,\mu}, \qquad u_g = \frac{\dot{m}_R}{60\,\rho_g A} \tag{8.15}$$

where d_p is the mean particle size, ρ_g is the gas density, g is gravitational acceleration and $\mu = 1.4 \times 10^{-5}$ Pa s is the gas viscosity, with $\rho_s - \rho_g$ floored at 50 kg/m^3. At the design point $u_g = 0.583$ m/s and $u_{mf} = 0.182$ m/s, a ratio of 3.20.

8.3.8 Instruments, Actuators and the Quality Laboratory

Five measurements carry band-limited noise from a first-order-filtered Gaussian process whose innovation is scaled to give the quoted stationary standard deviation, all multiplied by the noise multiplier ϕ_n. Bed temperature uses $\tau = 1.5$ min and $\sigma = 0.06\,^{\circ}$C, pressure 1.0 min and 0.012 bar, level 2.0 min and 0.35 %, the hydrogen ratio 1.5 min and 0.09, and the comonomer ratio 1.5 min and 0.008. The cooler outlet temperature is read exactly. Production is not measured directly, because no instrument weighs 500 kg/min of powder in real time. The reported rate is the mass-balance inference $\dot{m}_{PE}$ passed through a first-order filter of time constant 3 min, and a second independent estimate from the heat balance, $(Q_{hot} + Q_{loss})/(-\Delta H_p)$ converted to tonnes per hour with $Q_{hot} = Q_{sens} + Q_{vap}$, is reported beside it. The two agree on a settled plant, both reading 30.00 t/h at the design point, so a disagreement between them indicates an instrument fault or a transient rather than a steady process change.

Three actuators carry their own first-order lags as states, namely the cooling-water valve at $\tau_V = 0.25$ min, the discharge system at $\tau_{Vd} = 0.4$ min and the catalyst feeder at $\tau_{feed} = 5.0$ min. The ethylene, hydrogen and 1-hexene valves are applied without lag.

The quality laboratory is modeled and corrects the optional MPC estimate, although it remains outside the nine PID loops. A sample is taken every $t_{lab} = 60$ min, holding the bed-average melt index and density at the instant of sampling, and the result is posted $\theta_{lab} = 45$ min later. The posted value is then held until the next result arrives, so the reported laboratory value is between 45 min and 105 min old. That value is displayed beside the inferred properties and exported with its age. It is not the measurement either cascaded quality controller uses. The melt-index controller reads $\mathrm{MI}_{bed}(1 + \phi_m/100)$ and the density controller reads ρ_{bed}, both taken from the plant states with no delay and no reconstruction. For the cascades the laboratory illustrates the measurement problem without participating in its solution, and the consequence is stated in Section 8.9.

8.3.9 Constants, Initialization and Numerics

Every constant appears in Table 8.2. Most are adjustable in the application, and the entries marked hidden appear only in the source code, which is deliberate because inferring a catalyst activation factor or a chain-transfer coefficient from a step test is part of the identification work.

The initial state is not hard-coded. Every scenario solves for the equilibrium of whatever setpoints and disturbances it declares, using two scalar bisections on monotone functions. The first finds the cooler outlet temperature at which $Q_{sens} + Q_{vap}$ equals the reaction heat less the wall loss, and the second finds the cooling-water valve position that produces exactly that outlet temperature through (8.10). Everything else follows in closed form. A built-in test evaluates all thirteen derivatives at the solved state and requires the largest relative rate to fall below 10^{-9}, so a scenario that starts at a different grade, level or production rate starts at a true equilibrium where the requested thermal line-up is feasible. If a learner chooses an infeasible disturbance before Run, the solve retains its closest bounded state and the app discloses the thermal mismatch. The disturbance remains a starting condition rather than becoming a hidden later step. A setpoint or disturbance chosen before Run is therefore part of the starting state, and the same setting carried through Reset gives the same run. A manual station set by hand before Run is treated differently. The start-up solve does not read it, so the plant starts lined out at the solved position and the edited station is applied when control begins, which survives Reset as well. A step meant to be watched on a setpoint is therefore made after Run, while a valve step on a station in Manual can be made before it.

Table 8.2 Model Constants. Hidden Constants Are Not Adjustable in the Application

Symbol	Meaning	Value	Unit
D	reactor diameter	5.0	m
H	bed height at 100% level	23.5	m
V_{tot}	gas and solids volume of reactor and loop	533.3	m^3
ρ_b	fluidized bulk density	400	kg/m^3
ρ_s	resin particle density	900	kg/m^3
d_p	mean particle size	700	µm
n_I	inert holdup	113899	mol
$k_{p,ref}$	propagation constant at 88 °C	54.79	m^3/min
E_p	propagation activation energy	14000	J/mol
k_{com}	comonomer rate enhancement	3.0	—
k_a	catalyst activation factor, hidden	1.41667×10^{-4}	1/(%·min)
k_{d0}	catalyst decay at 88 °C	0.0015	1/min
β_d	decay temperature sensitivity	0.05	1/K
K_z	poison sensitivity	1.6	—
ζ	chain-transfer H_2 use, hidden	0.005618	—
$-\Delta H_p$	heat of polymerization	94.5	kJ/mol
$F_{C_2}^{max}$	ethylene valve capacity	30000	mol/min
$F_{H_2}^{max}$	hydrogen valve capacity	1400	mol/min
$F_{C_6}^{max}$	1-hexene valve capacity	1200	mol/min
F_{B0}	bleed at 100% setting	1800	mol/min
$\dot{m}_{dis}^{max}$	discharge capacity	1200	kg/min
$\dot{V}_R$	compressor volumetric flow	686.4	m^3/min
$c_{p,g}$	recycle gas heat capacity	1.515	kJ/kg·K
ΔH_{vap}	condensate heat of vaporization	360	kJ/kg
UA_0	cooler UA at reference water flow	63139	kJ/min·K
F_{cw}^{max}	cooling water at 100% valve	80000	kg/min
$F_{cw,ref}$	reference water flow, hidden	40000	kg/min
n_{UA}	UA flow exponent, hidden	0.8	—
$c_{p,w}$	water heat capacity, hidden	4.19	kJ/kg·K
τ_{HX}	cooler thermal lag	0.4	min
UA_{wall}	vessel heat loss UA, hidden	300	kJ/min·K
T_{amb}	ambient temperature, hidden	25	°C
$c_{p,s}$	resin heat capacity, hidden	2.0	kJ/kg·K
C_{metal}	vessel steel heat capacity, hidden	40000	kJ/K

Symbol	Meaning	Value	Unit
$T_{dew,0}$	dew point at the design gas	43.287	°C
a_P	dew point per bar	0.9	°C/bar
a_I	dew point per mol% cyclohexane	1.3	°C/mol%
a_6	dew point per mol% 1-hexene	2.0	°C/mol%
a_2	dew point per mol% ethylene	−0.15	°C/mol%
$f_{L,max}$	maximum condensed fraction	0.25	—
ΔT_{ref}	subcooling scale	12	K
w	dew-point smoothing width, hidden	0.7	K
a_0	melt-index intercept	0.3287	—
a_H	melt index per H_2/C_2	3.244	—
a_C	melt index per C_6/C_2	1.5	—
a_z	melt index per impurity, hidden	0.8	—
a_T	melt-index temperature term	−5000	K
m	melt-index exponent, hidden	3.5	—
K_C	comonomer incorporation constant	1.709	—
ρ_{HD}	homopolymer density base	0.9585	g/cm^3
K_ρ	density per incorporated C_6	1.62	—
K_{MI}	density per ln MI, hidden	0.0025	—
T_{s0}	sticking base temperature	102.0	°C
k_ρ	sticking per 0.001 density	0.9	°C
k_I	sticking per mol% cyclohexane	0.35	°C
k_{MI}	sticking per ln MI	1.0	°C
P_{hh}	emergency vent pressure	23.5	bar
k_{vent}	vent capacity, hidden	9000	mol/min·bar
τ_V	cooling-water valve lag	0.25	min
τ_{Vd}	discharge system lag	0.4	min
τ_{feed}	catalyst feeder lag	5.0	min
t_{lab}	laboratory sample interval	60	min
θ_{lab}	laboratory turnaround	45	min
ε_{MI}	melt-index specification band	±10	%
ε_ρ	density specification band	±0.0015	g/cm^3

Solving rather than tabulating the design point produces the numbers in Table 8.3, and each of them can be checked by hand from Table 8.2.

Four training grades are provided and each pair of ratios was inverted out of (8.12), so loading a grade and letting the cascades line out reproduces its melt index and density to better than 2 % and 0.001 g/cm^3, which a built-in test enforces. Table 8.4 lists them. These are training grades calibrated to make the simulation behave like a polyethylene plant. They are not commercial specifications and no number in them is taken from any licensor's process.

A classical fourth-order Runge-Kutta step of $\Delta t = 0.05$ min advances the thirteen states, controllers execute every $\Delta t_c = 0.1$ min, and the historian logs four samples per minute of plant time. The order of work in one step and the separation of the clocks from the display are those of the shared engine in Section 1.6.1, with the post-step corrections below applied after the integration. The speed setting offers 1, 2, 5 and 10 simulated minutes per second of real time, with 5 as the default. Noise comes from a seeded mulberry32 generator with Box-Muller normal deviates, seed 20260825, so a scenario replays bit for bit.

Post-step corrections clamp the four molar holdups positive, the active catalyst inventory non-negative, bed mass to 2000 kg to 193798 kg which is 105 % level, the three actuator states to 0 % to 100 % and $\bar{x}$ to 0 to 0.2. The same pass integrates the off-grade accounting and services the laboratory sampler. Six annunciator conditions are raised and cleared there as well, namely sticking margin below 2 °C, the high-temperature interlock below 0.5 °C, the vent open, gas velocity below $1.6\,u_{mf}$, level above 92 % and level below 28 %.

Table 8.3 Solved Design Point for Film A at 65% Bed Level

Quantity	Value	Unit
Bed temperature, pressure	88.00, 21.70	°C, bar
Bed mass, level, height	119970, 65.0, 15.28	kg, %, m
Free gas volume V_g	400.0	m^3
Total gas holdup n_g	289083	mol
Gas $C_2/H_2/C_6$/ICA/inert	40.0/8.0/0.60/12.0/39.4	mol%
Propagation rate r_p	16550	mol/min
Production $\dot{m}_{PE}$	500.0 (30.00)	kg/min (t/h)
Residence time τ_s	240.0 (4.00)	min (h)
Recycle flow $\dot{m}_R$	16382	kg/min
Cooler outlet, dew point	40.00, 43.29	°C
Condensed fraction f_L	6.00	%
Reaction heat	26.07	MW
Sensible, latent, wall loss	19.85, 5.90, 0.32	MW
Heat-removal ceiling R_{max}	33.97	t/h
Cooling utilization	88.3	%
Melt index, density	1.000, 0.91801	g/10 min, g/cm^3
Sticking temperature, margin	96.01, 8.01	°C
u_g, u_{mf}, ratio	0.583, 0.182, 3.20	m/s
Valves CW/C_2/discharge	50.0, 57.6, 41.7	%
Valves catalyst/H_2/C_6	40.0, 11.6, 36.3	%

Table 8.4 Training Grade Slate. Not Commercial Specifications

Grade	MI g/10 min	ρ g/cm^3	Rate t/h	T_{SP} °C	$R_{H,SP}$	$R_{C,SP}$
A Film LLDPE	1.00	0.918	30	88	20.000	1.500
B Film LLDPE	2.00	0.925	32	88	26.843	1.301
C Molding MDPE	8.00	0.935	28	88	45.219	1.055
D HDPE	0.30	0.952	25	92	10.736	0.126

8.3.10 Modeling Assumptions

The gas phase is one perfectly mixed volume and the bed is another. Real fluidized beds have a bubble phase and an emulsion phase exchanging mass across a boundary, and a real reactor carries a vertical temperature and composition profile. The approximation is defensible because the recycle rate is large and the conversion per pass is a few percent, and it has been tested directly against two-phase models for industrial gas-phase conditions [8]. It stops holding near minimum fluidization, where the bed slumps and the two phases stop exchanging, which is exactly the region the fluidization override protects.

Molecular weight is represented by a single melt-index correlation rather than a population balance and catalyst is one lumped activity with one decay constant, so there is no molecular-weight distribution and no polydispersity. Anything that depends on the shape of the distribution, such as bimodal products, long-chain branching or rheology beyond melt index, is outside this model, and a real Ziegler-Natta or chromium catalyst has several site types with different reactivity ratios and different hydrogen responses.

Condensation is an effective dew-point correlation with a smooth subcooling curve rather than a rigorous flash. It gives the right qualitative couplings, because the dew point rises with pressure, with cyclohexane and with 1-hexene, but it will not give the right liquid composition and it cannot predict the onset of the entrainment and agglomeration problems that limit real condensed-mode operation [16].

Table 8.5 Dominant Time Constants Across the Plant, Evaluated at the Design Point

Path	Expression	Value min	Measured min
Cooler outlet	$\tau_V + \tau_{HX}$	0.65	0.5
1-hexene inventory	$n_{C_6}/(r_{C_6} + y_{C_6} F_B)$	4.0	—
Ethylene inventory	$n_{C_2}/(r_p + y_{C_2} F_B)$	6.7	—
Bed temperature	$(M_b c_{p,s} + C_{metal})/\dot{m}_R c_{p,g}$	11.3	12.0
Hydrogen inventory	$n_{H_2}/(r_{H_2} + y_{H_2} F_B)$	142	—
Active catalyst	$1/(\dot{m}_{out}/M_b + k_d)$	176	—
Resin property	$M_b/\dot{m}_{PE}$	240	—

The recycle loop has no transport delay, although a real reactor takes tens of seconds to move gas from the cooler outlet to the distributor plate, so a student identifying the inner loop from a step test here finds a pure lag where a plant would show a lag plus dead time. Nitrogen and the accumulated light ends are a fixed inert holdup replaced exactly as the bleed removes them, so inert accumulation never happens even though it is a real operating problem and part of why the bleed exists. Product discharge is a continuous valve rather than the pot-and-lock-hopper cycle that puts a saw-tooth on a real level measurement and a periodic disturbance on the pressure. Sensible heat carried in with cold feed gas and out with warm product is neglected, and both are small next to 26 MW of reaction heat but neither is zero. Every coefficient in the quality, sticking and condensation models was calibrated to make this simulation behave like a polyethylene plant, and none of them is plant data.

8.4 Dynamic Analysis

The separation of time scales is not asserted by the application. It is recoverable from step tests, and the scenario sequence is built so that a student measures the spread rather than reading it from a table. Table 8.5 collects the seven dominant time constants, each evaluated from Table 8.2 at the design point, with the two that a single step test can isolate reported beside them.

8.4.1 Inner Cooler Loop Identification

Scenario 2 opens with the cooler-outlet loop in MANUAL at 50 % on the water valve and its tuning deliberately detuned to $K_c = 1.0$ and $\tau_I = 8$ min. Stepping the valve from 50.0 % to 60.0 % at $t = 5$ min drives the cooler outlet from 40.00 °C to 38.54 °C within two minutes, a gain of $K_p = -0.146\,°\mathrm{C}/\%$. The response reaches 63.2 % of that change 0.51 min after the step, for any valve step from 1 to 20 points, faster than $\tau_V + \tau_{HX} = 0.65$ min suggests. A colder outlet condenses more liquid, raises φ and lowers the effectiveness, so T_c^* in (8.10e) rises 1.01 °C for each degree that T_c falls, which shortens the effective exchanger lag to about 0.2 min. This is by far the fastest loop on the plant, its gain is negative so the controller is direct acting and carries $a = -1$, meaning the water valve opens further as the cooler outlet rises, and both facts are why it is the inner half of a cascade. Those two numbers are also all a model-based rule needs to set the inner tuning, which is the route the scenario asks for [19].

The outlet temperature does not settle completely. It drifts a further 0.16 °C by $t = 20$ min because the bed temperature is falling underneath it, from 88.0 °C to 82.1 °C by $t = 20$ min, and the bed cools because the outer loop cannot act while the inner loop is in MANUAL. The slow tail is the outer loop's process appearing in the inner loop's measurement, and the step test must be read before the tail dominates the fit.

8.4.2 Outer Temperature Loop Identification

With the inner loop tightened to $K_c = 8.0$ and $\tau_I = 0.8$ min, the outer loop can be identified on its own. Taking the reactor temperature controller to MANUAL at $t = 11$ min leaves the cooler outlet setpoint where the controller last put it, at 39.93 °C, and an otherwise identical run without a step

shows the bed drifting from 88.00 °C to 87.66 °C by $t = 300$ min, so the gains below are read from the stepped run minus that unstepped run. Stepping the setpoint to 41.00 °C at $t = 11$ min drives the bed temperature through a peak of 93.47 °C at $t = 51.7$ min, a rise of 5.87 °C over the unstepped run and a peak gain of $+5.47\,°\text{C}/°\text{C}$. The gain then falls to $+4.40\,°\text{C}/°\text{C}$ at $t = 140$ min and recovers to $+4.75\,°\text{C}/°\text{C}$ at $t = 300$ min and $+5.38\,°\text{C}/°\text{C}$ at $t = 1500$ min. The response reaches 63.2 % of its peak rise 12.0 min after the step, close to the 11.3 min thermal lag of Table 8.5.

The dip is neither oscillation nor a numerical artifact. A hotter bed deactivates catalyst faster through k_d in (8.6), the active inventory falls over its 176 min time constant, and part of the temperature rise is given back. The production controller, still in AUTO, then raises the catalyst feeder over its 180 min integral time to restore 30 t/h and takes the gain back up. With the production loop also in MANUAL the catalyst path acts alone and the outer loop sees a lead-lag plant, with a peak gain of $+5.77\,°\text{C}/°\text{C}$ at $t = 58.8$ min that decays to $+4.47\,°\text{C}/°\text{C}$ at $t = 300$ min and $+4.63\,°\text{C}/°\text{C}$ at $t = 1500$ min, so the fast gain is 25 % larger than the slow one. A controller tuned on the peak is sluggish in the long run and one tuned on the slow gain overshoots in the short run.

The order in which the two loops are tuned matters more than either tuning. With the inner loop left at Scenario 2's $K_c = 1.0$ and $\tau_I = 8$ min, the suggested outer tuning of Table 8.6 overshoots a 1 °C setpoint step made at $t = 11$ min by only 0.29 °C, so the cascade appears well tuned. The warm cooling water of Scenario 8 then swings the bed from 86.6 °C to 90.4 °C, against 87.8 °C to 88.2 °C with the inner loop tightened to $K_c = 8.0$ and $\tau_I = 0.8$ min. A slow inner loop passes the cooling disturbance through to the bed before the outer loop can act on it, the same requirement on inner-loop speed that the fermenter cascade of Volume 3, Chapter 3 measures.

8.4.3 Integrating Level Dynamics

Scenario 4 puts the level loop in MANUAL and asks for a slope rather than a settling point. Stepping the discharge valve from 41.7 % to 47.0 % at $t = 5$ min raises the discharge from 500.0 kg/min to 564.0 kg/min, and between $t = 8$ min and 25 min the level falls at a constant −0.0351 %/min. The same run without the step drifts at +0.0003 %/min, so the difference gives an integrating gain of $K_I = -6.65 \times 10^{-3}\,\%/(\text{min}\,\%)$. The analytical value from (8.7b) and (8.7c) is $-\dot{m}_{dis}^{max}/(\rho_b A H) = -6.50 \times 10^{-3}\,\%/(\text{min}\,\%)$, and the difference is the small production shortfall while the bed drains, 498.4 kg/min rather than 500 kg/min by $t = 25$ min. There is no gain to read off a settling point because there is never a settling point.

Tight level control is not the objective. Downstream equipment is insensitive to whether the bed sits at 64 % or 66 % but is sensitive to variation in the discharge rate, so the loop is a classic averaging-level application and the shipped tuning is deliberately gentle at $K_c = 6$ and $\tau_I = 90$ min [1]. The scenario presents two upsets that produce similar level responses and demand different responses, a discharge valve partly plugged at $t = 25$ min, which is a sustained imbalance needing a permanent valve change, and a 4 t discharge surge at $t = 70$ min, which needs no valve change once the level has been returned to its setpoint.

8.4.4 Gas and Resin Time-Scale Separation

Scenario 5 demonstrates the time-scale separation that motivates the application, and it is the operating case shown in Figure 8.3. The melt-index controller is placed in MANUAL and its output, the hydrogen ratio setpoint, is stepped from 20.00 to 30.00 at $t = 20$ min. Four traces then separate on one time axis. The hydrogen valve opens immediately from 11.7 % to 23.7 %. The gas ratio reaches 26.90 by $t = 80$ min and 30.02 by $t = 200$ min, consistent with the 142 min hydrogen inventory. The instantaneous melt index follows the ratio almost without lag, because the instantaneous property depends only on the present gas composition, reaching 2.02 at $t = 80$ min and 2.68 at $t = 200$ min. The bed average moves far more slowly, reaching 1.15 at $t = 100$ min, 1.50 at $t = 200$ min and 1.99 at $t = 360$ min. The laboratory value lags further still, reporting 1.22 at $t = 200$ min and 1.83 at $t = 354$ min from a sample 54 min old.

The bed average is the trace the customer receives, and it drifted outside the $\pm 10\,\%$ band of the original melt index at $t = 81.8\,\text{min}$. By $t = 360\,\text{min}$ the run had discharged 136.8 t of off-specification resin out of 177.0 t made, 77 % of a six-hour shift, from one ratio move with no grade change ordered.

> **TRY IT IN THE APP** **5 · Fast Gas, Slow Resin**
>
> Load the scenario, press Run on the Quality tab and watch the three melt-index cards, Making now, In the bed and Laboratory, after the hydrogen ratio setpoint steps from 20 to 30 at 20 min. The resin being made reads 2.02 by 80 min, while at 200 min the bed average that leaves the reactor reads only 1.50 and the laboratory 1.22.

8.5 Controller Design

8.5.1 PID Implementation

All nine loops run the shared velocity-form PID of Section 1.6.2, Equations (1.14) to (1.17), with the derivative on the measurement and back-calculation on the integral alone [20]. Each executes every $\Delta t_c = 0.1\,\text{min}$ whatever mode the loop is in, with the error $e_k = a\,(\text{SP}_k - \text{PV}_k)$ and the loop action $a = \pm 1$ of Table 8.6. The measurement passes a first-order filter $\hat{y}_k = \hat{y}_{k-1}\alpha + \text{PV}_k(1-\alpha)$ with $\alpha = \mathrm{e}^{-\Delta t_c/\tau_f}$ and $\tau_f = 0.6\,\text{min}$ on all nine loops, and the tracking time is $T_t = \tau_I$. In the symbols of Chapter 1, the running sum S_k accumulates the proportional increment $K_c(e_k - e_{k-1})$ and the derivative increment $-aK_c\tau_D(\hat{y}_k - 2\hat{y}_{k-1} + \hat{y}_{k-2})/\Delta t_c$, the demanded output is $v_k = u_{bias,k} + S_k + I_{k-1}$, and u_k is v_k clipped to the output range. Because $T_t = \tau_I$, the proportional part of the demand cancels from the integral update while the output is clipped, and with no derivative action I relaxes toward $u_{lim} - u_{bias}$ with time constant τ_I whatever the error. Slew limits are unused, and derivative action is enabled only on the reactor temperature loop, where τ_D still defaults to zero.

MANUAL seeds the integral, $I_k = u_{man} - u_{bias,k} - S_k$, and in AUTO each station is set to its controller's output after every execution, which makes transfer bumpless in both directions as in Section 1.6.2. The header master switch throws all nine loops at once and, on the way to MANUAL, copies each controller's present output into its own station first. Every controller is initialized with u_{bias} equal to the output its own loop needs to hold the solved design point and with $I_0 = 0$, so a scenario opens with zero error and zero integral rather than with something quietly winding. Only the pressure loop's bias moves, because the feedforward below rewrites $u_{bias,k}$ at every execution. The temperature cascade carries an external reset. While the water valve sits at a stop and the outer controller asks for a cooler outlet beyond the one reached, its integral is set to $I_k = T_c - u_{bias,k}$, so its output is the measured outlet plus the proportional and derivative terms. In the cooling-fault run of Section 8.6 the setpoint therefore bottoms at 27.2 °C at $t = 271.9\,\text{min}$, when the bed is 7.4 °C above its setpoint, and the valve leaves its stop at $t = 342.4\,\text{min}$, as the bed returns to 88 °C. The two quality cascades carry none, and each of their outer controllers is held only by its own output range.

8.5.2 Loop Pairing and Cascade Structure

Figure 8.2 shows the nine pairings and the tier each belongs to. Two features of that map carry more weight than the count of loops.

The first is that pressure is held with ethylene and inventory with product discharge, and not the other way round. Both pairings are available on paper, because ethylene adds moles and therefore raises pressure, while discharge removes mass and therefore raises the free gas volume of (8.3) and lowers pressure. The chosen pairing points each loop at the handle with the direct, fast and large effect and leaves the cross-effects small, which is what a relative-gain analysis is for [21]. The interactions remain and they are visible. Bed level changes free gas volume and therefore pressure, bed mass changes thermal inertia and therefore the temperature response, and melt index enters the density correlation of (8.12b) directly.

The second is that, under Cascades, no polymer property is controlled directly with a valve. Melt index writes the hydrogen ratio setpoint and density writes the comonomer ratio setpoint, and the

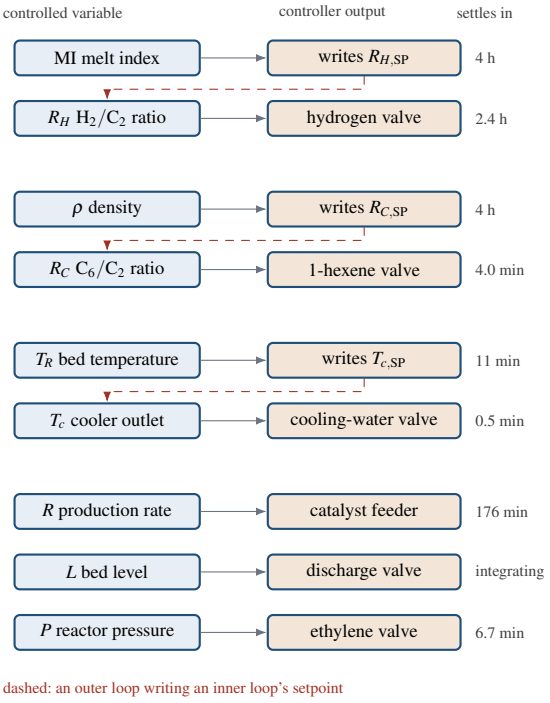


Figure 8.2 Loop pairing map. Three cascades are marked by the dashed links, in which the outer controller's output is the setpoint of the loop below it, and each pair spans roughly two decades of settling time.

Table 8.6 Controller Settings. Shipped Defaults and the Values the Graded Challenge Suggests

		Shipped		Suggested	
Loop	Action	K_c	τ_I min	K_c	τ_I min
Cooler outlet T_c	−1	4.0	1.2	8.0	0.8
Pressure P	+1	30	6	—	—
C_6/C_2 ratio	+1	60	5	—	—
Bed temperature T_R	+1	1.5	45	4.0	15
Bed level L	−1	6	90	—	—
H_2/C_2 ratio	+1	1.2	120	1.8	90
Production R	+1	2.5	180	5.0	120
Melt index MI	+1	7	400	18	260
Density ρ	−1	45	320	100	240

inner ratio loops track them, so a header pressure change, a bleed swing or a sticking valve is rejected before it reaches the quality loop [1]. This remains the default structure, because the property is a four-hour inventory and the chemistry can be reached only through the gas.

Pause. Try Exercise 8.2 before reading on.

Table 8.6 gives the shipped tuning and the tuning the graded challenge suggests. The suggestion also lowers the bed level setpoint from 65 % to 55 %, which Section 8.7 explains. The integral times range from 1.2 min on the cooler to 400 min on melt index, which restates the time-scale separation in tuning terms.

The reactor temperature loop is the one loop where derivative action is useful, because the process

Table 8.7 Non-Defeatable Overrides

Condition	Action	Label
$T_{stick} - T_R < 0.5\,^{\circ}\mathrm{C}$	$u_{cat} = 0$, $u_{CW} = 100$	high temperature
$T_{stick} - T_R < 2\,^{\circ}\mathrm{C}$	$u_{cat} \le 0.7\,u_{bias,cat}$	sticking margin
$u_g < 1.5\,u_{mf}$	$u_{cat} \le 20\,\%$	low fluidization
$L > 95\,\%$	$u_{dis} \ge 85\,\%$	bed level high
$L < 22\,\%$	$u_{dis} \le 10\,\%$	bed level low
$P > P_{hh}$	$v_{C_2} \le 5\,\%$	high pressure

is slow and the measurement noise is small at $\sigma = 0.06\,^{\circ}\mathrm{C}$. It ships with $\tau_D = 0$ and the suggested tuning sets 2.0 min. Raising the noise multiplier to four times the design level quantifies the cost of derivative action on a noisy measurement [20].

8.5.3 Feedforward on the Ethylene Valve

When the production target rises the reactor is about to consume more ethylene. Waiting for the pressure to fall before adding it leaves the pressure controller to find the extra ethylene by feedback alone. Instead the pressure controller's bias term follows the production inference, filtered with a three-minute time constant, as shown in Equation 8.16.

$$r_{p,ff} = \frac{10^6\,\widehat{R}/60}{M_{C_2} + M_{C_6}\,x_{inst}/(1 - x_{inst})} \tag{8.16a}$$

$$u_{bias,P} = \frac{100}{F_{C_2}^{max}} \left(r_{p,ff} + y_{C_2} F_{B0} \frac{\phi_B}{100} \right) \tag{8.16b}$$

where $\widehat{R}$ is the filtered production inference in tonnes per hour, the molar masses are in g/mol, and $r_{p,ff}$ is the propagation rate that inference implies in mol/min, which is 16550 mol/min at the design rate of 30 t/h. The pressure controller then trims the difference. The feedforward is on by default and can be disabled [1]. It follows production as the catalyst inventory changes rather than applying the eventual target's ethylene demand immediately. Pressure feedback corrects inference error. The three-minute filter is short relative to the catalyst's three-hour response.

8.5.4 Protective Overrides

Six protective actions sit between the controllers and the valves, listed in Table 8.7. They are not tuning and they cannot be disabled, because what they prevent ends a run rather than degrading it. When one acts, the loop whose handle it took is immediately told what was actually applied through the same tracking mechanism that MANUAL uses, so its integral does not wind up while the override holds. The active override is recorded in the exported data.

8.5.5 Model Predictive Control

The optional predictive controller follows the pattern of Section 1.6.3 and replaces only the quality and inventory loops. It moves the hydrogen, 1-hexene and discharge valves, and the pressure, temperature and production loops stay in charge of their own valves. Its six states are the gas ratios $h = 100 n_{H_2}/n_{C_2}$ and $c = 100 n_{C_6}/n_{C_2}$, the estimates $\hat{q}$ and $\hat{x}$ of the bed-average quality, the level L and the discharge valve position $\hat{v}_{dis}$. The local nominal balances are

$$\begin{aligned} \dot{\eta}_i &= F_i^{max} u_i/\hat{n}_2 - (k_i \hat{r}_p + F_{B0}\hat{y}_2)\eta_i/\hat{n}_2, \\ \dot{\hat{q}} &= a(q_{inst} - \hat{q}), \quad \dot{\hat{x}} = a(x_{inst} - \hat{x}), \\ \dot{L} &= (100\hat{m} - \dot{m}_{dis}^{max}\hat{v}_{dis})/M_{100}, \\ \dot{\hat{v}}_{dis} &= (u_{dis} - \hat{v}_{dis})/\tau_{Vd}. \end{aligned} \tag{8.17}$$

where $i = H, C$, $\eta_H = h$, $\eta_C = c$, $k_H = \zeta$, $k_C = K_C$, $a = \hat{m}/(M_{100}L/100)$, $M_{100} = \rho_b AH$, the u_i are valve percentages and hats denote estimates. The quality correlations receive $h/100$ and $c/100$ and assume zero impurity.

The ethylene storage $\hat{n}_2$ and its mole fraction $\hat{y}_2$ come from the measured pressure, temperature, ratios and level with the nominal geometry and the design inert and cyclohexane inventories. The controller's own ethylene command through the nominal valve capacity, less the nominal bleed and the change in storage, gives the propagation estimate $\hat{r}_p$ and from it the production $\hat{m}$ in kg/min, filtered over 3 min and bounded at 50–1000. The declared coefficients are frozen and exclude the hidden production and resin states. The quality maps are differentiated at the measured ratios with storage and rate held, the affine offsets are retained, and the model is discretized by an exact zero-order hold. Six noise-free ± 2 valve-point tests over 120 min give maximum RMS residuals across tests of 0.247 and 0.0128 ratio points, 0.00530 in log-MI, 0.0000586 g/cm^3 in density and 0.118 level points. These residuals cover local steps only.

The quality estimates propagate every 0.1 min. Each laboratory result corrects the log-MI and density biases against the estimate at the sample time, as in Equation (1.11), with gain 0.5 and bounds of 2 and 0.02 g/cm^3, respectively [22]. This is a simpler form of the disturbance estimate that the offset-free controller of Volume 9, Chapter 4 carries in a Kalman filter. The program decides every 5 min, including initialization, over 120 min ($N = 24$), with move blocks $[1, 1, 2, 4, 6, 10]$, and minimizes

$$J = \sum_{j=1}^{24} w_j \|y_j - r_j\|_Q^2 + 0.03 \sum_{b=1}^{6} \|\Delta u_b\|^2 + s_L^2 + s_H^2 + 100 s_C^2, \tag{8.18}$$

where $y = (\hat{q}, 1000(\hat{\rho} - \rho_{HD}), L)$ and r holds the corresponding targets. The weights are

$$Q = (5/240)\mathrm{diag}(\ln^{-2}(1.1), 1/1.5^2, 1/25),$$

with $w_{24} = 6$ (the stage weight plus a $5Q$ terminal weight) and $w_j = 1$ otherwise. The valves are bounded hard at 0–100%, with block-move caps of 35, 25 and 10 points. Three nonnegative slacks, each shared over the horizon, soften the level band 28–92%, h at 4–80 and c at 0.02–2.5, so the program has 18 valve variables and three slacks. The first move is applied [23].

With the grade preview On the plan reads the announced grade targets, and with it Off it holds the present targets. A 32-point sweep on the new case only selected the move weight $\lambda = 3$, the gentlest setting within 10% of the best off-grade result, 85.254 versus 81.016 t, and it was not retuned afterward. The five PI loops the controller displaces track the applied valves and the measured ratio setpoints. The protections and any loop the reader holds in Manual stay in force, and the controller stands by when it is not eligible. A plan that is not optimal, not finite or outside its bounds holds the first failed scan and then hands the valves to the tracked cascades until a plan succeeds.

8.6 Results

Table 8.8 lists the eleven shipped scenarios. Each one starts from a solved steady state and carries a guided sequence that asks for a prediction before the run and an explanation after it.

8.6.1 Production Rate Increase

Scenario 6 starts at 25 t/h and steps the production target to 34 t/h at $t = 30$ min. The catalyst feeder command moves immediately from 29.2 % to 51.7 %. The ethylene bias follows the filtered production inference, so the make-up valve remains near 48.3 % at the step, reads 47.9 % one minute later and 62.1 % at $t = 360$ min. Between $t = 25$ min and 150 min, pressure spans 21.68 bar to 21.72 bar. With feedforward switched off, the same window spans 21.65 bar to 21.71 bar. The previous target-based bias opened hours before the gas was consumed and widened that range to 21.65 bar to 22.08 bar. Everything downstream is slow. The active catalyst inventory climbs from 83.3 % to 100.5 % by $t = 120$ min and 108.7 % by $t = 360$ min, and the production rate reaches 30.1 t/h and 32.6 t/h at those two times without arriving at the target within the run.

Table 8.8 Shipped Scenarios and Their Timed Events

Id	Purpose	Events
lined-out	read a steady plant	none
tune-cooler	inner loop step test	loop starts in MANUAL, de-tuned
tune-temp	outer loop after inner	inner pre-tuned to 8.0/0.8
level-integrator	integrating dynamics	valve plugged 12% at 25 min, 4 t surge at 70 min
gas-vs-resin	the two time scales	$R_{H,\mathrm{SP}}$ 20 to 30 at 20 min
rate-up	rate into the heat limit	R_{SP} 25 to 34 t/h at 30 min
condensed	lose the condensing agent	F_{ICA} to 40 mol/min at 20 min, restored at 150 min
cw-upset	three cooling faults	water +6 °C at 40 min, fouling +15% at 140 min, compressor to 82% at 240 min
poison	diagnose an upset	impurity to 0.28 ppm-eq at 45 min, clean at 260 min
mpc-grade	MPC comparison	prepared 55% bed, grade A to C at 90 min
grade-change	the graded challenge	grade A to C at 90 min

The heat balance carries the larger changes. Reaction heat rises from 21.7 MW to 28.4 MW, the water valve opens from 37.0 % to 58.8 %, the cooler outlet falls from 42.2 °C to 38.7 °C, the condensed fraction rises from 2.5 % to 7.9 %, and the latent duty grows from 2.4 MW to 7.7 MW. The latent term, not the sensible term, supplies the added capacity. Cooling utilization moves from 83.3 % to 91.1 %, so the plant is still inside its ceiling. Pushing the target on to 45 t/h at $t = 150$ min finds the limit. The water valve reaches its stop at $t = 381$ min, the bed then warms to 94.0 °C, and at $t = 720.8$ min the sticking-margin override caps the catalyst feeder and production falls from 43.5 t/h to 34.4 t/h.

8.6.2 Loss of the Condensing Agent

Scenario 7 cuts the cyclohexane feed from 216 mol/min to 40 mol/min at $t = 20$ min and restores it at $t = 150$ min. Cyclohexane takes no part in the chemistry, so the response is entirely thermal.

The cyclohexane mole fraction falls from 12.0 % to 6.63 % by $t = 148$ min, because its only route out is the bleed and its inventory time constant is 161 min. The dew point falls with it from 43.29 °C to 35.76 °C. The condensed fraction barely moves, reading 6.00 % at the start and 6.23 % at $t = 148$ min, because the temperature controller drives the cooler outlet down from 40.00 °C to 32.33 °C to follow the falling dew point and condenses very nearly the same fraction at a lower temperature.

The cost appears in two quantities and neither is a controlled variable. The cooling-water valve climbs from 50.1 % just before the cut to a peak of 88.9 %, and the heat-removal ceiling drops from 33.97 t/h to 30.32 t/h. Production does not hold at 30 meanwhile. The cyclohexane leaving the gas raises the ethylene fraction from 40.0 % to 44.6 % at constant pressure, and production drifts up to 31.7 t/h although its controller cuts the catalyst feeder from 39.9 % to 34.5 %, so cooling utilization passes through 100 % and reaches 101.1 %. The bed temperature moves last and least, rising only from 88.0 °C to a peak of 89.7 °C. That ordering is the general signature of an approaching constraint on a well-controlled plant, because the controlled variable is the last place a constraint appears and the valve position is the leading indicator.

8.6.3 Unmeasured Cooling Faults

Scenario 8 applies three cooling faults in sequence at 30 t/h. None of the three has a measurement.

Warmer cooling water at $t = 40$ min takes the inlet from 30 °C to 36 °C, the water valve from 49.8 % to 77.5 %, the ceiling from 33.88 t/h to 30.36 t/h and utilization from 88.3 % to 98.8 %, read

just before this fault and the next. The bed temperature peaks only 1.1 °C high at $t = 43$ min, is within 0.11 °C of setpoint from $t = 60$ min, and the melt index stays between 0.998 and 1.000. Fifteen percent of fouling at $t = 140$ min repeats the pattern, taking the valve to 93.4 %, the ceiling to 29.63 t/h and utilization to 101.2 % by $t = 240$ min, with a bed temperature transient of 0.6 °C.

The compressor stepping down to 82 % at $t = 240$ min is different in kind. The water valve reaches its stop at $t = 243$ min and stays there until $t = 342$ min, saturated for 27.6 % of the run by the logged flag, so the bed temperature peaks at 95.4 °C at $t = 272.3$ min, the sticking margin closes from 8.0 °C to 0.54 °C, just above the 0.5 °C interlock (0.54 on the default seed and 0.61 to 0.72 °C over six additional noise seeds), and from $t = 258$ min the sticking-margin override caps the catalyst feeder and pulls production to 27.0 t/h. The same fault also takes the fluidization ratio from 3.20 to 2.62, which is the constraint that would have bind next. The valve position gives the warning the temperature does not. Lowering the production setpoint to 27 t/h when the fouling arrives keeps the margin above 5.7 °C, while the same cut made at $t = 240$ min lets it fall to 1.7 °C.

> **TRY IT IN THE APP** **8 · Warm Water and a Fouling Cooler**
>
> Press Run on the Heat removal tab and watch the Cooling water valve rather than the bed temperature. Warmer water at 40 min opens the valve from 49.8 to 77.5 % while the bed peaks only 1.1 °C high. After the compressor slows at 240 min the valve reaches its stop, and the sticking margin closes to 0.54 °C.

Pause. Try Exercise 8.3 before reading on.

8.6.4 Feed Impurity Diagnosis

Scenario 9 introduces 0.28 ppm equivalent of feed impurity at $t = 45$ min without saying so. Production falls at once from 29.9 t/h to 20.8 t/h and reaction heat from 26.0 MW to 18.0 MW, and within eight minutes the ethylene valve closes from 57.1 % to 39.0 % and the cooling-water valve from 49.8 % to 26.6 %, while the bed temperature dips to 85.0 °C at $t = 49.0$ min and then returns. Falling production with a closing ethylene valve is the distinguishing signature, because a supply problem starves the reactor and opens the valve while a catalyst problem stops the reactor asking for ethylene.

The quality response is less intuitive. The impurity term sits inside the melt-index correlation through a_z in (8.12a), so the instantaneous melt index rises from 1.00 to 2.01 with no hydrogen move behind it, and the melt-index controller responds by pulling the hydrogen ratio setpoint from 20.0 down to 16.6 to compensate for a disturbance that did not enter through hydrogen. Meanwhile the production controller has raised the catalyst feeder to 54 % and the active inventory to 137 % of design. When the feed cleans up at $t = 260$ min all of that catalyst acts at once. Production jumps from 28.9 t/h to 41.6 t/h, cooling utilization reads 124 % until the water valve catches up four minutes later, the bed reaches 93.1 °C at $t = 265.5$ min, and the hydrogen correction then has to be unwound. The run ends with 122.3 t of off-specification resin from an unannounced disturbance.

8.7 Grade Transition Case Study

8.7.1 Off-Grade Accounting

Resin is on grade when both properties sit inside their bands, as defined in Equation 8.19, and the accounting is integrated at the discharge valve on every physics step.

$$\text{on grade} \iff |\mathrm{MI}_{bed} - \mathrm{MI}_{\mathrm{SP}}| \le \varepsilon_{MI}\mathrm{MI}_{\mathrm{SP}} \quad \text{and} \quad |\rho_{bed} - \rho_{\mathrm{SP}}| \le \varepsilon_{\rho} \tag{8.19a}$$

$$W_{off} = \int \frac{\dot{m}_{out}}{1000}\left[1 - \mathbf{1}_{\text{on grade}}\right] \mathrm{d}t \tag{8.19b}$$

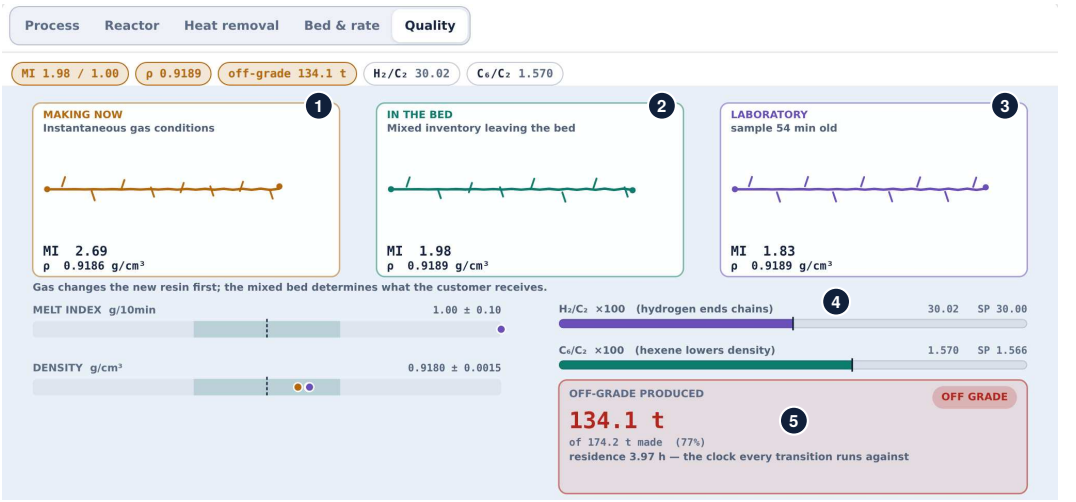


Figure 8.3 The gas-vs-resin scenario as shipped at $t = 354.4\,\text{min}$, on the Quality view. A single step of the hydrogen ratio setpoint from 20 to 30 at $t = 20\,\text{min}$ (4) has driven the instantaneous melt index (1) to 2.69 while the bed average that leaves the discharge valve (2) has reached only 1.98 and the laboratory (3), sampling a 54 min old specimen, reports 1.83. (5) The accumulated off-specification resin is 134.1 t out of 174.2 t made.

where $\varepsilon_{MI} = 10\,\%$ of the melt-index setpoint and $\varepsilon_\rho = 0.0015\,\text{g/cm}^3$, and W_{off} is in tonnes. Counting at the discharge valve rather than in the bed is a design decision and it changes the ranking of transition strategies. A metric evaluated on the bed average alone would reward emptying the reactor. The one that measures what actually reaches the silo does not.

8.7.2 Independence From Production Rate

The derivation repeats that of Section 1.4.5 in the symbols of this reactor. Take the bed mass and the production rate as constant through a transition and let q_{inst} be the logarithm of the instantaneous melt index that the gas composition is holding. Equation 8.13 is then a first-order lag of time constant τ_s, and the bed average crosses the specification edge q_{spec} at the time given by Equation 8.20.

$$\bar{q}(t) = q_{inst} - (q_{inst} - q_0)\mathrm{e}^{-t/\tau_s} \tag{8.20a}$$

$$t_{off} = \tau_s \ln \frac{q_{inst} - q_0}{q_{inst} - q_{spec}} \tag{8.20b}$$

$$W_{off} = \dot{m}_{out} t_{off} = M_b \ln \frac{q_{inst} - q_0}{q_{inst} - q_{spec}} \tag{8.20c}$$

where q_0 is the logarithm of the starting melt index, the last step uses $\tau_s = M_b/\dot{m}_{out}$ from (8.7c), and W_{off} in (8.20c) carries the units of M_b rather than the tonnes of (8.19b). The production rate cancels exactly. Halving the rate halves the tonnage at risk per hour and doubles the residence time in the same proportion, and the product is unchanged. Only two quantities are left. One is the bed mass, which the level setpoint controls. The other is how far past the target the resin being made can be driven and held, which is what the outer loop's gain and output limits decide. The loop reactor of Chapter 9 averages its product over an inventory that turns over in less than an hour, and there the hydrogen overshoot that shortens a transition is limited by the bubble-point margin it spends.

Equation 8.20c is a scaling argument rather than a prediction, because q_{inst} is not a step and the density band binds as well. It nevertheless gets close. For the Film A to Molding C change with

Table 8.9 Film A to Molding C at $t = 90$ min, Measured at $t = 900$ min. Off-Spec Is the Time From the Change to the Last Off-Specification Sample

Preparation	Off-grade t	Off-spec min	Peak R_H	Peak MI_{inst}
Shipped tuning, bed 65%	179.1	399.5	73.8	34.1
Retuned cascade, bed 65%	94.5	219.5	83.3	49.2
Retuned, 20 t/h until change	93.0	233.3	83.0	48.6
Retuned, 20 t/h throughout	128.7	404.5	83.4	49.4
Retuned, bed 55%	80.9	191.0	83.7	50.2
Retuned, bed 50%	84.9	235.0	84.0	50.6
Retuned, bed 40%	87.7	222.8	84.5	52.9
Retuned, drawn to 55%	77.5	189.0	84.2	51.0
Retuned, drawn to 50%	81.4	233.8	84.7	52.0
Retuned, drawn to 40%	83.6	223.5	86.0	56.4

$q_0 = 0$ and $q_{spec} = \ln 7.2 = 1.974$, and with the retuned quality cascade holding the instantaneous melt index near 47, the mean of $\ln \mathrm{MI}_{inst}$ from $t = 150$ min to 250 min being $q_{inst} = 3.85$, (8.20c) predicts 86.3 t at the 120.1 t of bed present at the change in the 65 % run and 70.9 t at the 98.6 t left by a drawdown to 55 %, against measured values of 94.5 t and 77.5 t. The first excursion of every retuned run in Table 8.9 costs between 0.77 and 0.84 t of off-grade resin per tonne of bed at the change, against the 0.72 that the logarithm gives, whatever the level or the production rate.

> ✦ **DID YOU KNOW? Running Slower Through the Change Costs More**
>
> From the simulator: with the retuned cascade, holding production at 20 t/h through the Film A to Molding C change leaves 128.7 t of off-grade resin, against 94.5 t at full rate. The slower bed carries the melt index past its band a second time (Table 8.9).

8.7.3 Ten Runs of One Transition

The graded challenge, Scenario 11, loads Film A, lets the plant line out, and changes the grade target to Molding C at $t = 90$ min. That is a factor of eight in melt index and 0.017 g/cm^3 in density, with ninety minutes of warning in which to prepare, and the grade change also writes the Molding C production target of 28 t/h. The challenge is judged at $t = 360$ min, with the model parameters as given. It passes when Molding C is on specification (MI 8.0 ± 10 %, density 0.935 ± 0.0015 g/cm^3), less than 90 t of off-grade resin has been discharged and the sticking margin never fell below 2 °C. Table 8.9 reports ten runs of the same event, each carried to $t = 900$ min so that the off-grade total has stopped accumulating. Every preparation is made before Run on the scenario as loaded, which makes it part of the starting state. A level chosen before Run starts the bed lined out at that level and a rate starts the plant at that rate, the same run that Reset gives with the setting carried. The three drawn rows instead lower the level setpoint at $t = 1$ min, so the bed is drawn down from 65 % during the warning. The retuned runs use the suggested tuning of Table 8.6 with the bed level setpoint at 65 % unless the table names another level, so the bed 55 % row is the suggestion exactly. Figure 8.4 draws the table's off-grade and off-specification columns as bars.

The shipped tuning costs 179.1 t and keeps the plant off specification for 399.5 min. Its failure is visible in the peak hydrogen ratio, which reaches only 73.8 against an available limit of 80. A melt-index controller with $K_c = 7$ and $\tau_I = 400$ min raises its output, the hydrogen ratio setpoint, no higher than 73.8, which it reaches at $t = 174$ min, 84 min after the change, and it never uses the limit it is permitted. The unused driving force is exactly the logarithm argument in (8.20c).

With the shipped settings the challenge fails at $t = 360$ min, with the bed-average melt index at 6.59, which is 0.61 below the lower band edge of 7.2, and 115.2 t of off-grade resin. The suggested

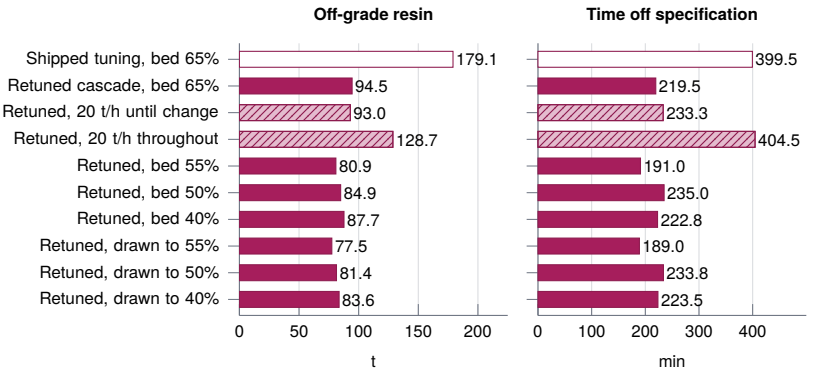


Figure 8.4 The ten runs of Table 8.9 as bars, off-grade resin on the left and the time from the change to the last off-specification sample on the right. Open bar: shipped tuning. Hatched bars: the two rate cuts. Solid bars: the retuned cascade at a chosen bed level. Notice that retuning removes about half of the loss, that every bed prepared below 65 % beats the retuned run at 65 %, and that holding the rate cut through the change is the worst of the retuned runs.

settings, the retuned cascade of Table 8.6 with the bed level setpoint at 55 %, start the bed lined out at 55 % and pass with MI 8.40, density 0.9352, 80.9 t of off-grade resin, 9.1 t inside the limit, and a lowest sticking margin of 7.8 °C. The run is the same whether the settings are applied before Run or carried through Reset.

Retuning the two quality controllers and the loops beneath them to the values in Table 8.6 takes the loss to 94.5 t, a reduction of 47 %, and shortens the excursion to 219.5 min. The retuned outer loop saturates the hydrogen ratio setpoint at its upper limit of 80 at its first execution after the change and holds it there until $t = 295.4$ min, for 3.4 h, and the density controller holds the comonomer ratio setpoint at its lower limit of 0.02 until $t = 124.0$ min. Both saturated outputs are productive, because an outer loop that can demand far more than the final grade requires is the mechanism that puts extra driving force into the transition.

Cutting production to 20 t/h before Run starts the plant at that rate only until the grade change writes 28 t/h, and it changes the loss from 94.5 t to 93.0 t, 2 % less. Holding 20 t/h through the change, which takes a second entry just after $t = 90$ min, leaves 92.9 t in the first excursion, as the cancellation predicts. The residence time is then about six hours, and the melt-index loop tuned for a four-hour bed carries the bed average to 8.89, past the upper band edge, so a second excursion adds 35.8 t and the total reaches 128.7 t. The rate reduction that operating intuition suggests first is the least effective preparation made before the change and the most costly one held through it.

A smaller bed at the change is effective, and the optimum level is not the lowest one available. With the bed started at 55 % the loss falls to 80.9 t and the excursion to 191.0 min, a 14 % improvement over retuning alone. Going further reverses the gain, with 50 % giving 84.9 t and 40 % giving 87.7 t even though the 40 % case has the shortest first excursion of the three, 148.8 min against 177.0 min and 191.1 min. A smaller bed turns over faster, and the melt-index loop tuned for the full bed carries the bed average past the upper band edge after reaching grade, to 8.87 at 50 % and 9.31 at 40 %, so second excursions add 10.5 t and 25.6 t. The 40 % bed also has less thermal inertia and catalyst, and cooling utilization reaches 122.4 %. Drawing the bed down in the first ninety minutes instead does slightly better at every level, 77.5 t, 81.4 t and 83.6 t, because the level overshoots its setpoint and leaves 98.6 t of bed rather than 101.6 t at the change in the 55 % case. The drawdown itself costs nothing, because it runs the discharge at up to the valve's 1200 kg/min capacity while the bed still holds on-grade Film A. Over five other noise seeds the bed started at 55, 50 and 40 % costs 81.0 t to 81.4 t, 84.2 t to 86.3 t and 86.0 t to 87.1 t, and drawn down to them 77.5 t to 78.1 t, 80.3 t to 82.4 t and

Table 8.10 Matched 900 min Comparisons, Seed 20260825. On/Off Denotes Announced-Target Preview. Costs Are Node Decision Times

Case	Control	Off-grade t	Before 90 t	Last off min	Valve travel total points	Outside bands min	Min. margin °C	Solves/fails	Mean cost ms
Shipped	Cascades	179.074	0.000	489.60	3978.7	0.00	7.917	0/0	—
Shipped	MPC On	93.845	23.975	261.75	217.7	95.35	8.008	180/0	0.257
Shipped	MPC Off	106.955	0.000	350.35	255.3	130.15	7.903	180/0	0.215
Prepared	Cascades	80.931	0.000	281.15	4124.7	121.50	7.755	0/0	—
Prepared	MPC On	85.254	24.956	226.80	202.9	38.15	7.938	180/0	0.311
Prepared	MPC Off	96.343	0.000	312.55	254.7	56.05	7.760	180/0	0.222
Drawdown	Cascades	77.498	0.000	279.20	4183.3	122.00	7.877	0/0	—
Drawdown	MPC On	103.944	32.009	235.60	206.5	26.15	7.946	180/0	0.228
Drawdown	MPC Off	106.066	0.000	316.80	270.8	78.05	7.826	180/0	0.230
Impurity	Cascades	122.258	0.000	342.90	3870.7	0.00	2.968	0/0	—
Impurity	MPC On	131.199	0.000	361.80	111.8	0.00	3.453	180/0	0.206
Impurity	MPC Off	131.199	0.000	361.80	111.8	0.00	3.453	180/0	0.206

82.0 t to 83.3 t, so the reversal is robust while the order of the two lower levels is within the noise. The best of the ten runs is a 57 % reduction from the shipped baseline, and both of the levers that produced it are tuning and preparation rather than equipment.

8.7.4 Predictive and Cascade Transition Control

Table 8.10 compares the cascades with the predictive controller of Section 8.5.5 with the grade preview On and Off. Within each triple of rows the initial state, seed, noise, instruments and retained loops are the same. The prepared case, Scenario 10, uses the suggested settings with the bed started at 55%. The drawdown case requests the level move from 65 to 55% at 1 min. Preview Off matches the cascades' grade information, although the cascades read bed quality without delay (Section 8.9).

On the shipped case the predictive controller reduces the loss from 179.074 to 93.845 t, and to 106.955 t with preview Off. It loses to the prepared cascades, 80.931 against 85.254 and 96.343 t, and to the drawdown, 77.498 against 103.944 and 106.066 t. Impurity is also a loss, 122.258 against 131.199 t with either preview setting. Preview reduces the prepared loss from 96.343 to 85.254 t but spends 24.956 t before 90 min, as Figure 8.5 shows: the plan starts moving the gas before the change, while the resin leaving is still Film A. Its earlier final excursion still costs more than the cascades, so an earlier last off-specification sample does not mean less off-grade resin.

Valve travel sums the scorecard travel totals of the physical valves at 0.25 min intervals. The time outside the soft gas and level envelopes falls from 121.50 to 38.15 min in the prepared case and from 122.00 to 26.15 min in the drawdown case with preview On. These envelopes are not protective limits. Paired production differs by less than 0.18 t. The shipped lined-out, rate-step and cooling-upset comparisons each produce zero off-grade under all three variants, and the minimum cooling-upset margin is 0.541/0.516/0.516 °C for Cascades/On/Off. An independent integration of the discharge reproduces the totals, and halving the physics step preserves the rankings within 0.014 t. In the Chrome browser a decision costs 1.386/0.706 ms at 1×/10× over 31/16 s, which occupies 0.0313/0.1455% of wall time with 7/33 plans, zero failures and 60 frames/s.

8.8 Technology in Practice

What Measures It

Figure 8.6 draws the loops of Section 8.5 with the hardware of a fluidized-bed reactor in place of the schematic's symbols. The pressure drop through a fluidized bed is equal to or slightly greater than the weight of the bed divided by its cross-sectional area [18], so a differential-pressure transmitter across the bed reads bed mass, as a liquid column's pressure reads its height [24]. The model's level, computed from bed mass with 0.35 % of noise, stands for that reading. Impulse lines prone to plugging are kept clear by a small, steady purge of clean fluid, often a gas such as nitrogen. Too much

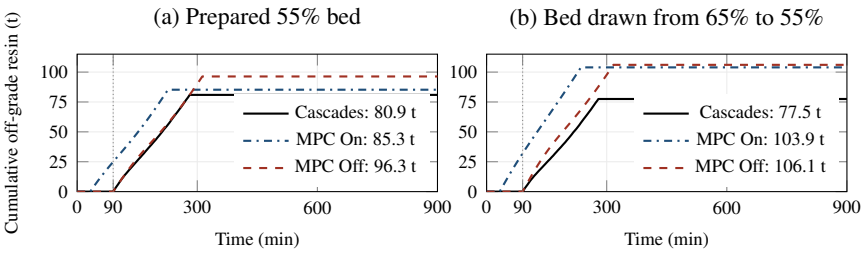


Figure 8.5 Full-duration economic comparisons over all 900 min. Cascades are the thick solid line, MPC with preview On the dash-dotted line and MPC with preview Off the dashed line. The dotted line marks the grade change at 90 min. Preview spends off-grade resin before the event and loses to both prepared cascade strategies over 900 min.

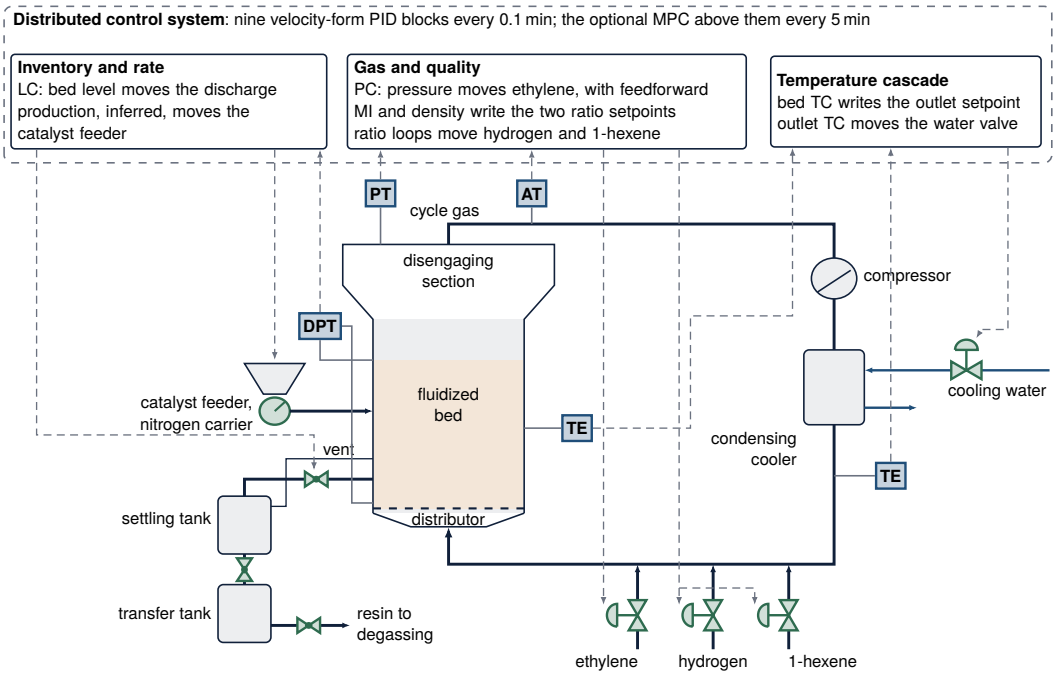


Figure 8.6 The reactor's main loops with their hardware. Blue tags are sensing devices: the bed and cooler-outlet temperature elements TE, the pressure transmitter PT, the differential-pressure transmitter DPT across the bed and the gas analyzer AT. Green symbols are final elements: the cooling-water, ethylene and hydrogen valves, the catalyst feeder and the on/off valves of the discharge tanks. Dashed arrows are signals. Notice that only the cooler outlet, the pressure and the ratio loops touch a valve directly. Melt index and bed temperature act through setpoints, and the laboratory reaches the plant only through the predictive controller's bias update. Not to scale, and not a piping diagram.

purge flow adds its own pressure drop and reads high, and a purge that stops lets the line plug [24]. A gas analyzer on the recycle stream sets the make-up composition that holds the gas steady [18], the instrument behind the model's two ratio measurements. Melt index itself comes from the laboratory, the subject of the box below.

> **TECHNOLOGY** **Sensor: The Melt Flow Test**
>
> Melt index is the mass of molten polymer extruded through a standardized capillary in ten minutes under a prescribed temperature and load, as ISO 1133-1 and ASTM D1238 define it. The test is simple and empirical, yet it classifies commercial grades and releases production lots. A sample has to be carried to the quality laboratory, conditioned, tested, checked and reported before an engineer sees the result, so the result describes the past [25]. A few units fit online melt flow analyzers to report sooner, but these need more equipment investment, read less accurately, and need their sampling molds replaced often, which interrupts production [26]. The chapter's laboratory, with a sample every 60 min and a result 45 min later, is that chain in short form.

What Moves It

Catalyst is carried into the bed by an inert gas such as nitrogen, at a point above the distributor plate, because catalyst injected below the plate could start polymerization there and plug it. The production rate is controlled by adjusting the rate of catalyst injection, and the temperature of the recycle stream entering the reactor is moved up and down to follow the rate of heat generation [18]. Those are the production loop and the temperature cascade of Figure 8.2. The model gives the feeder a 5.0 min lag and treats the discharge as a continuous valve with a 0.4 min lag, where a plant moves resin in batches.

> **TECHNOLOGY** **Final Element: The Discharge Valves and Their Tanks**
>
> Resin leaves a fluidized bed in batches. In one discharge process a settling tank below the bed is joined to it by a solids line near the distributor plate and by a vent line near the top of the bed. Opening the valves sends resin and gas into the tank, the gas vents back to the reactor, and the valves close. The resin then drops into a transfer tank, the pressures equalize, and an outlet valve passes it on at lower pressure. The tanks are sized by the discharge rate and the batch cycle time, and too large a transfer tank wastes reactor gas [27]. Ball, plug and gate valves suit such on/off duty because fully open they leave a nearly unimpeded path [24].

Where the Controller Runs

A distributed control system holds loops like these at a supervisory level that sends set points to field controllers, with loops nested or cascading and cycle times from milliseconds to minutes [28]. In condensed-mode polyethylene reactors, cascades of PID loops for the temperature are well established, and operators assist the critical loops by hand through that system [12]. In the app all nine loops are velocity-form PID blocks that execute every 0.1 min, the six overrides sit between the controllers and the valves, and the predictive controller is a supervisory layer that decides every 5 min and hands the valves back to the cascades when a plan fails.

> **IN PRACTICE** **Keep the Poisons Out of the Loop**
>
> The gas-phase process is highly sensitive to impurities, so purification beds remove sulfur compounds, acetylene and other impurities from the feed ethylene before it is compressed to reaction pressure. A small side stream of the recycle gas, mostly ethylene, is taken off to limit the build-up of impurities and burned as fuel gas or sent back to a cracker. Oxygen is kept very low because it poisons transition-metal catalysts, which are so effective that one gram of the metal makes more than 200 tonnes of product [11]. Scenario 9 shows what an impurity that passes the beds does to production and to melt index.

What Is Modernizing It

Soft sensors estimate product quality where online analyzers are not available [29], the line of work that the first History box traces to an industrial reactor. Online melt flow analyzers shorten the laboratory's delay at a cost in equipment and accuracy [26]. Among the industrial nonlinear predictive control applications counted in 2003, polymers were one of the areas with the largest number [13].

Keeping an inferred melt index right through a grade change, and handing the operator's supervisory decisions to a machine, are the subjects of the Open challenge boxes in Section 8.9.

8.9 Limitations

The laboratory is not in the default cascaded loops. It is sampled on a 60 min interval with a 45 min turnaround, displayed, exported and discussed, but both cascaded quality controllers read the true bed-average states directly as described in Section 8.3.8. Under Cascades the simulator therefore demonstrates what a delayed and infrequent measurement looks like beside a soft sensor, and it does not demonstrate control through one. For Cascades the melt-index analyzer bias disturbance is the only path by which a quality measurement can be made wrong, and it applies a constant multiplicative error rather than the state-dependent error a real inferential sensor shows during a transition. Closing either cascaded quality loop on the laboratory value, with or without a bias update between samples, would be a straightforward extension and it would change the transition numbers in Table 8.9. Control through a slow analyzer of that kind is the subject of Volume 5, Chapter 3.

> **OPEN CHALLENGE** **A Melt Index Estimate That Survives the Grade Change**
>
> A soft sensor loses accuracy when the process changes, through catalyst deactivation or a change in the feed, so it has to be maintained. Recursive updating with a bias correction has predicted melt index through grade changes of high-density polyethylene, but recursive methods cannot cope with abrupt changes [29]. In a 2026 study of 425 industrial polypropylene runs, melt index models that were accurate within one product family lost accuracy when carried across families [25]. Progress would be an estimate that stays right through a transition, the moment at which this chapter's cascades read the true bed average and a plant cannot.

The MPC instead uses each delayed report for sample-time bias correction. Its nominal model omits poison, catalyst activity, changed bleed/header capacities, pressure interactions and cooler dynamics. The squared quality objective does not minimize the off-grade indicator, and soft output envelopes provide no invariance guarantee. In the prepared, drawdown and impurity runs of Table 8.10 the MPC loses to the cascades.

Only three loops are scored. Overshoot and settling time appear only after a setpoint step larger than the loop's band and read as a dash otherwise, so a regulatory run such as the lined-out plant reports integral absolute error, manipulated-variable travel and the saturated fraction alone. Each cascade loop is scored on its own output, the cooler outlet setpoint for temperature and the hydrogen ratio setpoint, between 4 and 80, for melt index. The temperature tile counts saturation from the water valve beneath it, because the external reset holds the setpoint near the outlet rather than at its own limit, so in the cooling-fault run it reports 27.6 %. The melt-index tile reports 48.9 % by $t = 360$ min in the suggested transition, the time its output sat at 80.

The modeling simplifications set out in the assumptions bound what the reactor can be used to teach. There is no transport delay, no bubble phase, no molecular-weight distribution, no rigorous flash, no inert accumulation and no lock-hopper discharge cycle, and the sticking limit is a linear correlation rather than a measured softening curve evaluated on the bed-average resin, so the constraint itself moves during a grade change. The six overrides cannot be switched off, which is deliberate but means a student cannot run the experiment of removing them to see what the failure looks like.

> **OPEN CHALLENGE** **Supervision Still Rests With the Operator**
>
> In condensed-mode polyethylene reactors the temperature is held by cascades of PID loops, and operators still assist the critical loops by hand. A 2026 industrial study finds their intervention indispensable under rapid, strongly nonlinear disturbances, as in deciding when to take over the inner temperature loop. A machine framework that learns online is not yet established, and extremes such as a sudden large depressurization were not stress-tested [12]. Progress would be supervision that a machine can carry through such events.

8.10 Conclusion

This chapter studied a gas-phase polyethylene reactor simulation built around a separation of time scales of two decades. Thirteen states carry four gas-phase species balances, a lumped catalyst activity, an integrating solids inventory, a bed energy balance with an effectiveness-NTU condensing cooler, and two bed-average quality inventories, all initialized by solving for the starting line-up for the scenario setpoints. The dominant time constants span 0.5 min on the cooler outlet, as measured, to 240 min on the resin property, and with the catalyst feed held the outer temperature loop is shown to see a lead-lag plant whose fast gain of 5.77 °C/°C decays to about 4.5 °C/°C over the 176 min catalyst time constant. Nine proportional-integral-derivative loops run in three tiers with three cascades, one feedforward path and six non-defeatable overrides, each loop on its own manual station so that any one of them can be opened for a step test. The grade transition from Film A to Molding C costs 179.1 t of off-specification resin on the shipped tuning, 94.5 t after the quality cascade is retuned, 80.9 t with the bed also started at 55 % and 77.5 t with it drawn down to that level before the change. Production rate cancels out of the leading-order transition tonnage, and the measurements agree, since every retuned run spends 0.77 to 0.84 t per tonne of bed in its first excursion. Cutting production to 20 t/h before the change recovers only 1.5 t, and holding the cut through the change costs 34.3 t more than the full-rate run, because the slower bed makes the retuned melt-index loop overshoot into a second excursion.

The simulator is a reduced-order teaching model and not a plant replica. Its coefficients are calibrated rather than measured, its default cascades bypass the laboratory, and its recycle loop carries no transport delay. A fuller model would add a recycle transport delay, a two-site kinetic model and direct optimization of transition tonnage. The optional predictive controller costs 93.8 t on the shipped case (107.0 t without preview), but loses to the prepared and drawn-down cascades and on the impurity run. On one plant the reactor shows cascade control, constrained operation and the economics of a grade change.

KEY POINTS

- The gas changes in minutes, but the resin that leaves averages a bed that holds four hours of production.
- Melt index and density are reached only through gas-ratio setpoints, so each quality loop is the outer half of a cascade.
- Production rate cancels from the off-grade tonnage of a transition. Bed mass and the outer loop's driving force decide it.
- Retuning cut the Film A to Molding C loss from 179.1 to 94.5 t, and a bed started at 55 % cut it to 80.9 t.
- The cooling-water valve warns of the heat-removal limit before the bed temperature does.

Where else this applies. Quality held through a gas ratio over a slower inventory is also the problem of Chapter 9, and control through a late measurement that of Volume 5, Chapter 3.

References

[1] 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.

[2] B. W. Bequette, *Process Control: Modeling, Design, and Simulation*. Upper Saddle River, NJ: Prentice Hall, 2003.

[3] K. J. Åström and R. M. Murray, *Feedback Systems: An Introduction for Scientists and Engineers*, 2nd ed. Princeton, NJ: Princeton University Press, 2021.

[4] M. Takeda and W. H. Ray, "Optimal-grade transition strategies for multistage polyolefin reactors," *AIChE Journal*, vol. 45, no. 8, pp. 1776–1793, 1999.

[5] T. Xie, K. B. McAuley, J. C. C. Hsu, and D. W. Bacon, "Gas phase ethylene polymerization: Production processes, polymer properties, and reactor modeling," *Industrial & Engineering Chemistry Research*, vol. 33, no. 3, pp. 449–479, 1994.

[6] K.-Y. Choi and W. H. Ray, "The dynamic behaviour of fluidized bed reactors for solid catalysed gas phase olefin polymerization," *Chemical Engineering Science*, vol. 40, no. 12, pp. 2261–2279, 1985.

[7] K. B. McAuley, J. F. MacGregor, and A. E. Hamielec, "A kinetic model for industrial gas-phase ethylene copolymerization," *AIChE Journal*, vol. 36, no. 6, pp. 837–850, 1990.

[8] K. B. McAuley, J. P. Talbot, and T. J. Harris, "A comparison of two-phase and well-mixed models for fluidized-bed polyethylene reactors," *Chemical Engineering Science*, vol. 49, no. 13, pp. 2035–2045, 1994.

[9] K. B. McAuley and J. F. MacGregor, "On-line inference of polymer properties in an industrial polyethylene reactor," *AIChE Journal*, vol. 37, no. 6, pp. 825–835, 1991.

[10] ——, "Nonlinear product property control in industrial gas-phase polyethylene reactors," *AIChE Journal*, vol. 39, no. 5, pp. 855–866, 1993.

[11] 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.

[12] Y. Liu, "Natural intelligence principle of supervisory-level control for condensed-mode polyethylene fluidized bed reactors: A proportional-integral-derivative perspective," *ACS Omega*, vol. 11, no. 39, pp. 60 064–60 072, 2026.

[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] C. Chatzidoukas, J. D. Perkins, E. N. Pistikopoulos, and C. Kiparissides, "Optimal grade transition and selection of closed-loop controllers in a gas-phase olefin polymerization fluidized bed reactor," *Chemical Engineering Science*, vol. 58, no. 16, pp. 3643–3658, 2003.

[15] S. BenAmor, F. J. Doyle, III, and R. McFarlane, "Polymer grade transition control using advanced real-time optimization software," *Journal of Process Control*, vol. 14, no. 4, pp. 349–364, 2004.

[16] A. Mirzaei, A. Kiashemshaki, and M. Emami, "Fluidized bed polyethylene reactor modeling in condensed mode operation," *Macromolecular Symposia*, vol. 259, no. 1, pp. 135–144, 2007.

[17] I. J. Levine and F. J. Karol, "Preparation of low and medium density ethylene polymer in fluid bed reactor," U.S. Patent 4,011,382, assigned to Union Carbide Corp., 1977, filed March 10, 1975, issued March 8, 1977.

[18] J. M. Jenkins, III, R. L. Jones, and T. M. Jones, "Fluidized bed reaction systems," U.S. Patent 4,543,399, assigned to Union Carbide Corp., 1985, filed April 3, 1984, issued September 24, 1985.

[19] S. Skogestad, "Simple analytic rules for model reduction and PID controller tuning," *Journal of Process Control*, vol. 13, no. 4, pp. 291–309, 2003.

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

[21] E. Bristol, "On a new measure of interaction for multivariable process control," *IEEE Transactions on Automatic Control*, vol. 11, no. 1, pp. 133–134, 1966.

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

[23] D. Q. Mayne, J. B. Rawlings, C. V. Rao, and P. O. M. Scokaert, "Constrained model predictive control: Stability and optimality," *Automatica*, vol. 36, no. 6, pp. 789–814, 2000.

[24] 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.

[25] J. Hernández-Fernández and J. Lopez-Martinez, "Reactor-grade non-additive polypropylene architecture defines the physicochemical limits of melt flow index model transferability: An industrial chemometric and machine learning study," *Polymers*, vol. 18, no. 15, p. 1880, 2026.

[26] M. A. Parvez and I. M. Mehedi, "An artificial intelligence-based melt flow rate prediction method for analyzing polymer properties," *Polymers*, vol. 17, no. 17, p. 2382, 2025.

[27] R. G. Aronson, "Fluidized bed discharge process," U.S. Patent 4,621,952, assigned to Union Carbide Corp., 1986, filed April 3, 1984, issued November 11, 1986.

[28] 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.

[29] M. Kano and K. Fujiwara, "Virtual sensing technology in process industries: Trends and challenges revealed by recent industrial applications," *Journal of Chemical Engineering of Japan*, vol. 46, no. 1, pp. 1–17, 2013.

8.11 Exercises

8.1 Concept check · 2 min

At the solved design point of Table 8.3, which statement about the bed energy balance of Equation (8.8) is right?

(a) The dry recycle gas alone carries the whole reaction heat, and the latent term is a spare margin

(b) The wall loss is the second largest removal term, ahead of the latent heat of the condensate

(c) The latent term removes 5.90 MW of 26.07 MW, and without it the dry gas falls short

(d) Most of the thermal inertia on the left side is the vessel steel rather than the resin in the bed

8.2 Concept check · 1 min

Under the default Cascades structure, how do the melt-index and density controllers act on the plant?

(a) They move the catalyst feeder, which sets how much resin of each kind is made

(b) They move the hydrogen and 1-hexene valves directly, one valve for each property

(c) They move the bed temperature setpoint, which shifts both correlations at once

(d) They write the H_2/C_2 and C_6/C_2 ratio setpoints, which inner loops hold with the valves

8.3 Concept check · 2 min

In the cooling-fault scenario the water warms, the cooler fouls and the compressor loses capacity, and none of the three is measured. Which reading warns first that the plant is approaching its heat-removal limit?

(a) The cooling-water valve position, together with the cooling utilization

(b) The bed temperature, because it is the variable the cascade is built to hold

(c) The bed-average melt index, because a hotter bed makes a different resin

(d) The reactor pressure, because the recycle compressor sets the gas inventory

8.4 Theory and calculation · 6 min

For the Film A to Molding C change, take $q_0 = 0$, the lower band edge $q_{spec} = \ln 7.2$, and a retuned cascade that holds the instantaneous property at $q_{inst} = 3.85$. Give each answer to three significant figures.

(a) Use Equation (8.20c) to estimate the off-grade tonnage with 120.1 t and with 98.6 t of bed at the change. *Checkpoint:* 86.3 t and 70.9 t.

(b) With 120.1 t of bed, find the off-specification time t_{off} at 28 t/h and at 20 t/h, and the tonnage in each case. *Checkpoint:* 185 min and 259 min, 86.3 t in both.

(c) Repeat (a) for 120.1 t if the cascade only drives the instantaneous melt index to the target, $q_{inst} = \ln 8$. *Checkpoint:* About 358 t.

8.5 Theory and calculation · 7 min

Use the constants of Table 8.2 at the design point, where $M_b = 119970\,\text{kg}$, $\dot{m}_R = 16382\,\text{kg/min}$ and $\dot{m}_{out}/M_b = 4.168 \times 10^{-3}/\text{min}$. Give each answer to three significant figures.

(a) Find the bed thermal lag $(M_b c_{p,s} + C_{metal})/(\dot{m}_R c_{p,g})$. *Checkpoint:* 11.3 min.

(b) The bed is held 5.5 K above 88 °C. Find k_d from Equation (8.6), the catalyst time constant, and the ratio of the new steady active inventory to the old at the same feeder position. *Checkpoint:* 1.97×10^{-3}/min, 163 min and 0.923.

(c) Find the factor by which the Arrhenius term of Equation (8.4) raises the propagation rate at the same temperature, and the product of the two factors. Explain what the product says about the temperature step test of Section 8.4. *Checkpoint:* 1.072 and 0.990.

8.6 Theory and calculation · 6 min

At the design point the recycle carries $\dot{m}_R = 16382\,\mathrm{kg/min}$ with $c_{p,g} = 1.515\,\mathrm{kJ/(kg\,K)}$ from 40.00 °C to the bed at 88.00 °C, 6.00 % of it condensed with $\Delta H_{vap} = 360\,\mathrm{kJ/kg}$, and the reaction runs at $r_p = 16550\,\mathrm{mol/min}$ with $-\Delta H_p = 94.5\,\mathrm{kJ/mol}$ while making 30 t/h. Give each answer to three significant figures, and the duties within 0.01 MW.

(a) Find the reaction heat, the sensible and latent duties and the wall loss $UA_{wall}(T_R - T_{amb})$ in MW. *Checkpoint:* 26.07, 19.85, 5.90 and 0.32 MW.

(b) Estimate the production the dry recycle could carry at the same temperatures. *Checkpoint:* About 23.2 t/h.

(c) Estimate the production each further percent of the recycle condensed would add, and compare it with the 0.525 t/h per percent of the running example in Section 1.4.4. *Checkpoint:* About 1.13 t/h.

8.7 App challenge · 8 min

Load scenario 2, "2 · Step test the inner cooler loop", at the default seed. The Cooler outlet temperature loop starts in Manual with the Cooling water valve at 50 %. Before Run, set the Cooling water valve to 60.0 %, so the step is applied at $t = 0$ to the plant lined out at the old position. Run at speed 1 (1 min per wall-clock second) until the clock passes 15 min, pause and export the CSV. Temperatures within 0.01 °C of the key (0.1 °C for the bed), the gain within 0.002 and the time within 0.05 min count as correct.

(a) Read `tc_C` in the rows at 0.0 and 2.0 min and find the process gain. *Checkpoint:* 40.00 °C and 38.54 °C, −0.146 °C per percent.

(b) Interpolate the `tc_C` rows to find when the outlet has made 63.2 % of the change it shows at 2.0 min, and compare it with $\tau_V + \tau_{HX}$. *Checkpoint:* About 0.51 min, against 0.65 min.

(c) Read `tc_C` and `temp_C` in the row at 15.0 min, and explain why the outlet is still moving. *Checkpoint:* 38.38 °C and 82.0 °C.

8.8 App challenge · 8 min

Load scenario 5, "5 · Fast gas, slow resin", at the default seed, with nothing changed. The Melt index loop starts in Manual, and the H_2/C_2 setpoint steps from 20 to 30 at 20 min. Run at speed 10 (10 min per wall-clock second) until the clock passes 360 min, pause and export the CSV. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from min. Values within 0.01 of the key (0.1 t for tonnages) count as correct.

(a) Read `h2c2` in the rows at 80.0 and 200.0 min, and `mi_inst` at 80.0 min. *Checkpoint:* 26.90, 30.02 and 2.02.

(b) Read `mi_bed` at 100.0, 200.0 and 360.0 min, `offgrade_t` and `produced_t` at 360.0 min, and the first row in which `on_spec` is 0. *Checkpoint:* 1.15, 1.50 and 1.99; 136.8 t of 177.0 t; 81.75 min.

(c) Use Equation (8.13) with $\tau_s = 240\,\mathrm{min}$ to estimate `mi_bed` at 360 min if the instantaneous melt index had jumped to its final 2.69 at 20 min. Explain the difference from (b). *Checkpoint:* About 2.12.

8.9 App challenge · 10 min

Load the graded challenge, "Challenge · Film A → Molding C", at the default seed. The grade target changes to Molding C at 90 min. Run at speed 10 (10 min per wall-clock second) throughout. A run longer than an hour exports its time column as Time (h), in hours, so convert each time below from min. Melt index within 0.01, density within 0.0001, tonnages and the margin within 0.1 and times within 0.5 min of the key count as correct.

(a) With nothing changed, run until the clock passes 360 min, pause and export the CSV. Read `mi_bed`, `density_bed` and `offgrade_t` in the row at 360.0 min, the largest `h2c2_sp` and its time, and say whether the challenge passes. *Checkpoint:* 6.59, 0.9321, 115.2 t; 73.8 at about 174 min; it fails on both properties.

(b) Continue to 900 min and export again. Read `offgrade_t` at 900.0 min and the last row in which `on_spec` is 0. *Checkpoint:* 179.1 t, at 489.5 min.

(c) Reload the case, press Reveal suggested tuning before Run, and repeat (a) and (b), reading also the smallest `stick_margin_C` up to 360 min. *Checkpoint:* 8.40, 0.9352, 80.9 t, margin 7.8 °C; 80.9 t at 900 min, last at 281.0 min.

8.10 Application area · 4 min

Use Equation (8.14) with the constants of Table 8.2, a gas with 12 mol% cyclohexane, and each bed at its grade's melt index and density (Table 8.4).

(a) Find the sticking temperature and margin of Film A at 88 °C, Molding C at 88 °C and HDPE D at 92 °C. *Checkpoint:* 8.0, 21.2 and 35.8 °C.

(b) A plant engineer proposes raising cyclohexane to 15 mol% on Film A to gain cooling. What does it cost in margin, and on which grades does the cost matter? *Checkpoint:* 1.05 °C, leaving 6.95 °C.

8.11 Application area · 3 min

In Scenario 5 the bed-average melt index leaves the band of 0.9 to 1.1 at 81.8 min. The laboratory draws a sample every 60 min from $t = 0$ and posts each result 45 min later. When does the first laboratory result outside the band arrive, how long after the bed left the band is that, and roughly how much off-grade resin has been discharged by then at 500 kg/min?

8.12 Review the agent · 5 min

An AI assistant asked how to cut the off-grade resin of the Film A to Molding C change writes: "Off-grade tonnage is the discharge rate times the time off specification. Keep the retuned cascade and the bed at 65 %, cut production from 28 to 20 t/h for the whole transition, and the loss falls by nearly a third, from about 94 to about 67 t." Find the flaw, and say how you would check it in the app.