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Full Papers

Decentralized control of the Tennessee Eastman Challenge Process

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A decentralized control system is developed for the Tennessee Eastman Challenge Process (TE problem). The design procedure begins with the selection of the method for production-rate control, to which inventory controls and other functions are then coordinated. Results show that production rate can be maximized at any of the three standard product compositions, even when the feed of reactant A is lost. All specifications of the challenge problem are satisfied despite large disturbances in feed composition and reaction kinetics. Variability in product rate and quality is less than that seen in previous studies. The process can operate on-spec for long periods without feedback from composition measurements. Setpoints for certain variables (such as reactor temperature and concentrations of A and C in the reactor feed) must be chosen *a priori*, and the effect on operating cost is estimated. The performance of the proposed decentralized control is compared to that of a nonlinear model predictive control (NMPC) developed previously. There appears to be little, if any, advantage to the use of NMPC in this application. In particular, the decentralized strategy does a better job of handling constraints – an area in which NMPC is reputed to excel. Reasons for this are discussed.

Keywords: multiloop control; predictive control; constrained control

The Tennessee Eastman Plant-wide Industrial Process Control Problem – hereafter called the 'TE problem' – was proposed as a test of alternative control and optimization strategies for continuous chemical processes[1]. As shown in *Figure 1*, it involves coordination of four unit operations: an exothermic two-phase reactor, a flash separator, a reboiled stripper, and a recycle compressor. There are 41 measured outputs (with added measurement noise). The 19 composition measurements (from gas chromatographs) are sampled at two different rates and include pure delay. There are 12 manipulated variables (11 valves and the reactor agitation speed). Downs and Vogel provide a steady-state material and energy balance, some physical property data, and qualitative information on the reaction kinetics. They also list specifications for regulation – setpoint tracking and rejection of 20 potential disturbances – and a cost function for steady-state optimization. The regulation problem is emphasized here, but implications for optimization are discussed.

One barrier to the use of model-based techniques (such as predictive control) is that no plant model is provided. Instead, a purposely-obscure FORTRAN code acts as the process. Another is that the plant is open-loop unstable and prone to rapid shutdown, so a stabilizing regulation strategy is a prerequisite to data-based empirical modelling. The development of such a strategy is challenging, as many can now attest.

The first was published by McAvoy and Ye[2], who used the steady-state relative gain array and other analysis techniques to study alternative decentralized configurations. Ye *et al.*[3] later showed how performance could be improved by modification of the level control strategy. Banerjee and Arkun[4] took a similar approach, but their screening tools included the dynamic characteristics of the process. Price *et al.*[5] emphasized plantwide aspects, advocating a tiered structure based on a choice of the production-rate and inventory- control loops. The remaining loops were coordinated with the production-rate control. Kanadibhotla and Riggs[6] proposed a combination of multiloop and model-based controllers. Their scheme neglects control of production, however. Desai and Rivera[7] used a decentralized control structure in which the loops were tuned using model-based techniques. They also discussed identification issues.

Several groups, including the author, have tried centralized, model-based control. Palavajjhala *et al.*[8] used linear model predictive control (MPC). Ricker and Lee[9] and Sriniwas *et al.*[10] claimed that nonlinearities prevented MPC from spanning the entire operating region, and suggested a nonlinear approach (NMPC). Performance was excellent, but the 'transparency' of the NMPC design was compromised by the need to include overrides for special cases.

The motivation for the present work was to compare

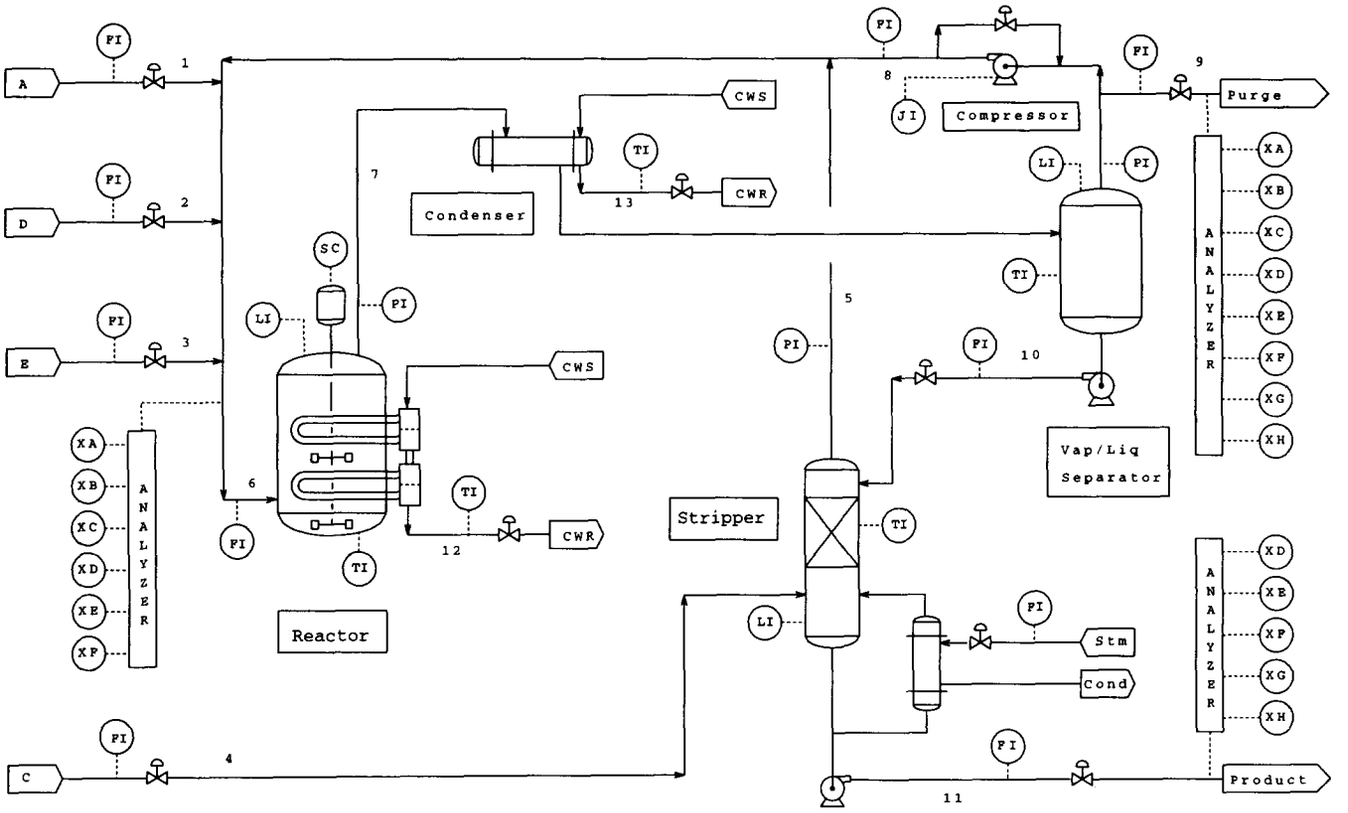


Figure 1 The Tennessee Eastman Challenge Process

the NMPC design to a more classical, decentralized approach. Decentralized designs had already been proposed, as noted above, but insufficient attention had been paid to the problems of constraint-handling and multiple operating modes. As will be shown later, the strategy developed here offers better performance, especially for maximization of production rate. Another motivation was to test the efficacy of proposed heuristic methods for control-system structure selection.

The remainder of the paper is organized as follows: the next section lists the goals for the TE problem. Following this is a description of the design procedure used here, which is contrasted with the centralized approach. Next, results are presented for several of the more demanding scenarios. The final discussion reflects on the lessons to be learned from the problem, especially with respect to centralized *vs.* decentralized design methods.

Design goals

Downs and Vogel[1] provide six specified operating modes, summarized in *Table 1*. Additional considerations are as follows:

1. *Product composition.* This must stay within ±5 mol % G of its setpoint, with no steady-state offset. The setpoint varies from 10 mass % to 90 mass % G, depending on the operating mode (see *Table 1*).
2. *Production rate.* The measurement is the volumetric rate of stream 11 (see *Figure 1*). This must stay within ±5 % of the setpoint, with no steady-state offset. The servo response must be 'good' for setpoint changes of ±15%.

Table 1 Operating modes for the TE process

Mode	G:H mass ratio	Production (kg/h)
1	50:50	14076
2	10:90	14076
3	90:10	11111
4	50:50	Maximum
5	10:90	Maximum
6	90:10	Maximum

The last three modes in *Table 1* require maximum of production rate. Thus, the system must push the process to one or more constraints without sacrificing other specifications or risking a shutdown.

3. *Liquid inventories.* There are specified bounds on all liquid inventories[1]. Optimal steady-state operation minimizes liquid inventory in the reactor[11]. Thus, one would like to have tight control near the lower alarm limit of 50%. Inventories in the separator and stripper have no influence on economics. They provide surge capacity to minimize fluctuations in production rate, and tight setpoint tracking is not desired.
4. *Reactor pressure.* If the reactor pressure exceeds 3 MPa, the process shuts down, but one can show *a priori* that optimal operation favours maximization of reactor pressure[11]. Thus, the system must be able to operate near the upper bound while avoiding a shutdown.
5. *Feed variability.* Feed streams 1, 2, and 4 have limited availability. The control strategy should minimize high-frequency variations in these flowrates[1].

6. *Chemical inventories.* The system must control the inventories of the eight chemical species. i.e., prevent excessive accumulation or depletion. For example, the inert, B, accumulates if the purge rate is too low, eventually causing a shutdown.
7. *Analysers.* The plant must be operable with one or more analysers temporarily out of service[2].
8. *Disturbance rejection.* Downs and Vogel provide 20 test disturbances. Some are step changes. Others have random character. Most are unmeasured, precluding feedforward compensation. They may occur individually or in combination.
9. *Optimal operation.* The design should allow optimal steady-state operation of the process – either minimization of operating costs at a given production rate, or maximization of production rate. Downs and Vogel[1] provide a formula for calculation of instantaneous operating costs.

Design procedure

Centralized design

One generic approach is to centralize decision-making. This has the appeal of generality, and has been advocated as the way to maximize economic benefits of advanced control (e.g., Cutler and Yokum[12]). For example, the use of a centralized model predictive control (MPC) involves the following steps[9]:

1. *Model definition.* As explained in the introduction, this is challenging for the TE problem. The resulting model will be inaccurate to an unknown degree.
2. *Configuration.* The design goals must be translated into a mathematical programming problem – typically a scalar objective function and associated constraints on the model states and manipulated variables. The objective function is a measure of setpoint tracking errors and control effort. One cannot define setpoints for all the model states, however*. Some must drift to accommodate unknown disturbances. Thus, the first MPC configuration problem is to select variables for which setpoints will be provided. In the MPC literature, the variables to be controlled are routinely 'given', but this is not the case in practice. For example, when there is recycle, one must control chemical inventories (goal 6), but where, and which chemicals? When the plant is nonlinear and there are many possibilities (here, eight chemicals, and at least four locations), these questions are difficult to resolve quantitatively.

The second configuration problem is to choose the manipulated variables: should a single centralized controller adjust them all, or should some be reserved for other purposes, e.g., commands from the operators? This decision is strongly coupled to the previous one.

Third is design of a state estimator (the feedback mechanism in the MPC framework). This can be routine, but if one is trying to estimate disturbances in feed compositions, parameter variations in a nonlinear model, etc., the structure of the model, estimator, and measurements must all be chosen with care.

Fourth is the choice of constraints. MPC treats constraints explicitly, and nominal stability of the constrained system can be guaranteed[13]. In practice, however, one faces two difficulties: (a) The constraints are unknown nonlinear functions of the states, which introduces additional model error and makes it impossible to guarantee constraint satisfaction in the real plant. (b) The inclusion of a particular constraint can *hurt* overall performance. This is explained more fully in the discussion at the end of the paper.

Finally one must select weights and horizons for the objective function, basis functions for the manipulated variables, and other details of implementation. These must compensate for shortcomings in the higher-level decisions. Their power to do so is limited, however, and reconfiguration may be required.

Since the real design goals are incorporated indirectly and the model error is unknown, there is no guarantee that the centralized design will achieve its objectives. Simulation studies are needed. If these are promising, the system is tested experimentally.

Decentralized control

The decentralized approach partitions the plant into sub-units, and designs a controller for each. In the limit, each sub-unit is a single feedback loop. The sub-unit controllers may either be conventional (e.g., PID) or some form of optimal/robust algorithm (e.g., MPC). The main difficulty is interactions between the sub-units, leading to violation of the design goals. There is no guarantee that a suitable partition exists. If one can be found, however, control is relatively robust because it does not rely on a model of the sub-unit interactions.

Before partitioning, one must choose the set of controlled and manipulated variables from among a large number of possibilities – just as in centralized control. Given such a set, one might use quantitative methods to analyse alternative partitioning strategies[2,4]. Unfortunately, there are serious shortcomings in the available methods. For example:

1. A model is required. It is usually restricted to be continuous, linear, and time-invariant. A quantitative model of the uncertainty (where needed) will be inaccurate and essentially arbitrary.
2. Numerical criteria used in the analysis are a limited and indirect reflection of the true design goals.
3. Constraints and abnormal conditions are not considered.

Consequently, both of the cited papers had to add

* We assume that the model states are observable from the available measurements.

heuristics to their analyses. Also, models were obtained by direct numerical linearization of the FORTRAN code, so base-case model accuracy was unrealistically good. Even so, performance was inferior to that obtained in the present work, especially with respect to constraints and large disturbances.

The present work explores the efficacy of the 'industrial' approach to such problems, which relies on heuristics and insight into the process dynamics to assign the available degrees of freedom. It most resembles that of Price *et al.*[5], who note that inventory management is crucial in plant-wide control, especially when there is recycle. Regulation (or maximization) of production rate is essential, and interacts strongly with the inventory control, so the production-rate mechanism is a good focal point for the overall design[14]. One identifies several reasonable candidates. For each, the inventory control strategy follows logically, reducing the number of possibilities for the remaining loops. In each candidate strategy, all degrees of freedom are assigned. The most promising candidates are tested to determine whether one satisfies the system requirements. Price *et al.*, however, also failed to consider fully the effect of constraints and abnormal conditions.

Summary of recommended strategy

The TE process has 12 degrees of freedom: 11 valves, one agitation rate. From the goals listed previously, one can see that at least six measured variables must be controlled at setpoints. These are:

1. Production rate.
2. Mole % G in product.
3. Reactor pressure.
4. Reactor liquid level.
5. Separator liquid level.
6. Stripper liquid level.

At least six degrees of freedom must be assigned to these tasks.

In addition, the agitation rate influences heat transfer in the reactor only[1], i.e., it has the same effect as a change in coolant rate[2]. The present work sets the agitation at 100%, which maximizes cooling potential. This leaves a maximum of five degrees of freedom. One must identify appropriate uses for these as part of the design procedure.

Figure 2 shows the primary loops recommended here. Override logic is discussed in a later section and is not shown. *Table 2* lists the characteristics of each loop, including the PI controller constants. Note that Loops 1–7 are a combination of a ratio controller and a flow controller (see *Figure 3*); the constants are for the flow controller. The following sections explain how the design was structured around the choice of a production-rate control mechanism.

Production rate

Overview. There are three basic options[5]:

1. manipulation of one or more feed rates.
2. manipulation of an internal variable along the main path from feed to product (Price *et al.*[5] recommended use of the condenser coolant rate for the TE problem).
3. direct manipulation of the product rate.

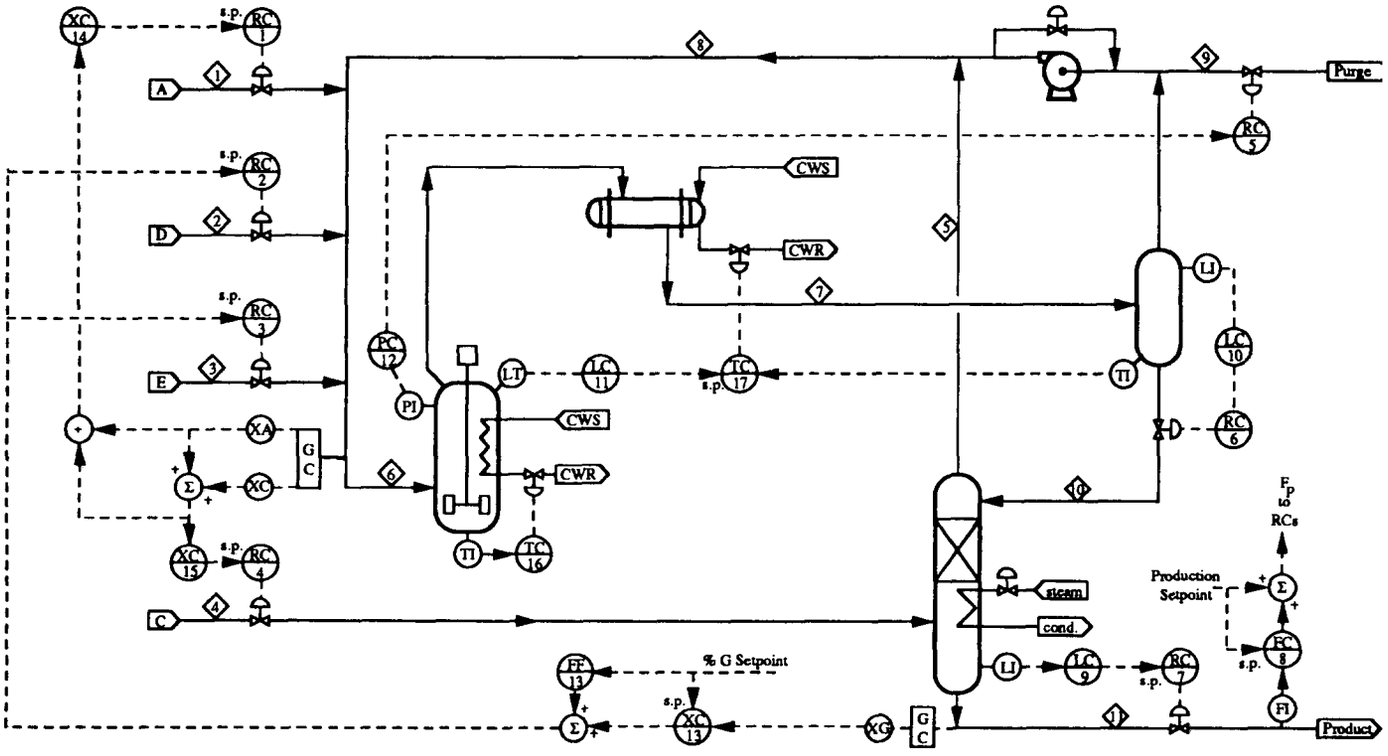
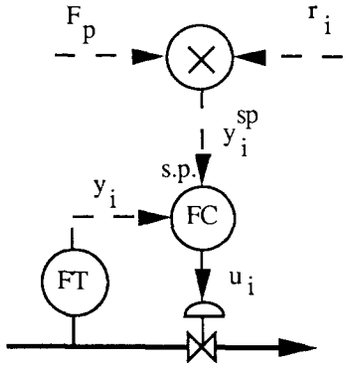


Figure 2 Schematic of proposed control strategy. Override loops are not shown

Table 2 Loop characteristics fo the strategy of *Figure 2*. *xmv*(i) is the *i*th manipulated variable in *Table 3* of Downs and Vogel[1]

Loop	Controlled variable	Manipulated variable	Gain	Integral time (min)
1	A feed rate (stream 1)	*xmv*(3)	0.01	0.001
2	D feed rate (stream 2)	*xmv*(1)	1.6×10^{-6}	0.001
3	E feed rate (stream 3)	*xmv*(2)	1.8×10^{-6}	0.001
4	C feed rate (stream 4)	*xmv*(4)	0.003	0.001
5	Purge rate (stream 9)	*xmv*(6)	0.01	0.001
6	Sep. liq. rate (stream 10)	*xmv*(7)	4.0×10^{-4}	0.001
7	Strip. liq. rate (stream 11)	*xmv*(8)	4.0×10^{-4}	0.001
8	Production rate	F_p	2.0	400
9	Stripper liquid level	Ratio in loop 7	-2.0×10^{-4}	200
10	Separator liquid level	Ratio in loop 6	-1.0×10^{-3}	200
11	Reactor liquid level	Sepoint of loop 17	0.8	60
12	Reactor pressure	Ratio in loop 5	-1.0×10^{-4}	20
13	Mol % G in stream 11	E_{adj} (See Equations (5) & (6))	−0.4	100
14	y_A (see Equation (7))	Ratio in loop 1, r_1	2.0×10^{-4}	60
15	y_{AC} (see Equation (8))	Sum of $r_1 + r'_4$	3.0×10^{-4}	120
16	Reactor temperature	Reactor coolant valve	−8.0	7.5
17	Separator temperature	Cond. coolant valve	−4.0	15
18	Maximum reactor press.	Production index, F_p	2.0×10^{-6}	0.001
19	Reactor level override	Recycle valve, *xmv*(5)	1.0×10^{-6}	1.0×10^{5}



Figre 3 Ratio control structure for stream *i*

Price *et al.*[5] discuss advantages and disadvantages of each, and give useful heuristics for designing a consistent system of inventory controls.

An additional heuristic was a key factor in the present work:

The variable most likely to constrain steady-state production is a good candidate for the production rate control. Such variables are poor candidates for key low-level loops.

In practice, plants are often run at full capacity, corresponding to a constraint on one or more variables. Suppose the bottleneck is saturation of a manipulated variable. If the control strategy uses this manipulated variable for some other critical purpose, such as inventory control, a degree of freedom will be lost at maximum production. One must then modify the loop structure to maintain control. This is also discussed by McAvoy and Ye[2].

Consider the simple example shown in *Figure 4*. All three stream rates can be manipulated, and we require

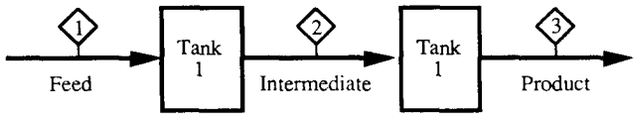


Figure 4 Example of production rate control alternatives

inventory (i.e., level) control in both tanks. Following Price *et al.*[5], we identify the following candidates:

a. Control production with stream 1. Use stream 2 to control inventory in Tank 1, and stream 3 to control inventory in Tank 2. This corresponds to option 1, above.
b. Control production with stream 2. Use stream 1 to control inventory in Tank 1, and stream 3 to control inventory in Tank 2 (option 2).
c. Control production with stream 3. Use stream 1 to control inventory in Tank 1 and stream 2 to control inventory in Tank 2 (option 3).

Suppose we choose scheme b, but it turns out that stream 1 limits maximum production. Then as we increase the production setpoint (stream 2), stream 1 eventually saturates, and we lose control of the inventory in Tank 1 unless there is an automatic override mechanism or the operators switch to manual control.

In the TE problem, the D and E feed rates are most likely to constrain production[11]. The rates of liquid streams 10 and 11 are never constraining at steady-state. Thus, the present work recommends a ratio control which, in effect, uses a combination of the D and E feeds to control production rate. Ratios are adjusted by feedback to eliminate offset. The following section describes the ratio control in more detail.

Ratio control of feed rates (Loops 1–7). The material balance provided by Downs and Vogel shows that reactant losses are small relative to the production rate[1]. Overall conversions are 96.5% A, 96.8 C, 99.1% D, and 94.5% E. Optimization can increase conversions further, mainly by reducing purge losses[11]. Thus, knowledge of the steady-state feed rates allows accurate prediction of the production rate and product composition. This suggests that a simple ratio control should be effective. We define a production index, F_p, which

has a value of 100 at the base-case rate of 23.0 m³/h (stream 11). We then calculate the setpoint for the flow controllers in loops 1–7 as follows:

$$y_i^{sp}(t) = r_i(t)F_p(t) \quad (1)$$

where y_i^{sp} is the setpoint for stream i, and r_i is the current ratio for stream i (see *Figure 3*). In all cases, these ratios are adjusted by feedback from other loops (see *Figure 2*).

Potential problems with the above strategy are:

1. A sudden change in F_p would cause step changes in all the streams under ratio control. Large step changes are unacceptable, and three of the feeds have limited availability (see Goals). Also, a step in the rates of streams 10 and 11 may cause the separator or stripper liquid levels to exceed their bounds.
2. *A priori* upper bounds on the stream flowrates are unknown because flowrates are not always proportional to the valve positions[1]. If F_p or r_i is too large, Equation (1) may yield a setpoint that is above the maximum possible flow for stream i, causing deviations from the desired ratios. Maintenance of the proper ratios is especially critical for the feeds.
3. Poor component inventory control. The proposed strategy assumes that an increase in the reactant feed rates will increase the reaction rates. This may not be the case if the individual feed rates or the purge are out of balance. See Component Inventory Control.

To minimize problem 1, we arbitrarily limit the rate-of-change of production. Thus, if the operator makes a step change in the desired production, F_p ramps from the current value to the new value. All simulations in the present work limited the ramp rate to ±30% in 24 h.

To handle problem 2, we estimate the maximum flow of each feed stream using a linear extrapolation, as follows:

$$y_i^{max}(t) = 100\frac{y_i(t)}{u_i(t)} \quad (2)$$

where y_i is the measured rate of stream i, and $u_i(t)$ is the current setting of the valve controlling this stream (%). To prevent inaccurate extrapolations, Equation (2) applies when $u_i > 50$; otherwise $y_i^{max}(t) = y_i^{max}(t-\Delta t)$. We then compare y_i^{max} to the desired flow, $y_i^{sp}(t)$. If any setpoints exceed the estimated maximums, we compute:

$$F_i^{max}(t) = \frac{y_i^{max}(t)}{r_i(t)} \quad (3)$$

The stream for which $F_{max,i}(t)$ is the smallest is the limiting flow. Suppose it is stream j. The production rate index is then set to:

$$F_p(t) = F_j^{max}(t) \quad (4)$$

and we recalculate the flow setpoints (Equation (1). An important advantage is that the feed rates can be pushed to a constraint (to maximize production) while maintaining the desired feed ratios automatically.

Feedback adjustment of production (Loop 8). As shown in *Figure 2*, Loop 8 trims the value of F_p to eliminate steady-state offset in the rate of stream 11. If production is constrained, however, this feedback is disabled to prevent windup. In any case, the feedback adjustment is limited to ±10 units of F_p (i.e., 10% of nominal production), because the ratio control should be accurate; a large feedback adjustment is an alarm condition.

Inventory Control (Loops 9–12)

The next step in the design is to coordinate inventory control with the chosen production rate control. Inventories to be controlled are the liquid levels in the reactor, separator, and stripper, and one or more system pressures.

Stripper bottoms liquid level (Loop 9). Possible manipulated variables are the steam rate, and the flows of streams 4, 10 and 11. The gains for the first two choices are very small, however (see Loop 13), so the only realistic options are the streams 10 and 11. Stream 11 is chosen because – given the choice of production rate control – it cannot be used to advantage in another loop.

Separator liquid level (Loop 10). Similarly, the best remaining use of stream 10 is to control the liquid level in the separator.

Note: the setpoint of this loop is the current level in the stripper bottoms (see *Figure 2*). Coordination of the levels in the separator and stripper helps to reduce fluctuations in the product flow. Variations in F_{10} cause only minor upsets in the stripper, otherwise this would not be attractive.

Reactor liquid level (Loop 11). Since there is no flow of liquid entering or leaving the reactor, the only ways to control liquid level in the reactor are:

a. Adjust the rate of liquid production by reaction.
b. Adjust the rate at which liquid components are carried off in the gaseous reactor effluent (stream 7).

Option (a) would conflict with the chosen production-rate control, so (b) is the logical choice. There are at least three ways it could be done with the remaining manipulated variables:

1. Use the reactor coolant to control the reactor temperature, and thus the vapour pressures of the liquid components (D–H).

2. Use the condenser coolant to control the concentrations of G and H in the recycled gas. For example, to reduce the liquid level in the reactor, lower the temperature in the separator to reduce the amount of G and H recycled. This increases the driving force for vaporization of G and H in the reactor.
3. Use the compressor recycle valve to adjust the recycle rate. For example, to reduce the reactor level, close the valve, which *increases* the recycle rate.

Option (1) is a poor choice because the reactor temperature has a strong effect on reaction rate, which acts in the opposite direction.

Options (2) and (3) are both effective. However, optimization studies suggest that the recycle valve should usually be at its lower bound[11] (maximizing the recycle rate as advocated by Fisher *et al.*[15]). Thus, the present work uses the condenser valve as the primary manipulated variable for reactor liquid level. If it approaches saturation, an override (described later) adjusts the recycle valve instead.

The recommended setpoint for Loop 11 is 55%. Typical disturbances cause deviations of ± 5%.

Pressure (Loop 12). Several authors have pointed out that independent control of the three measured pressures is impossible (e.g., McAvoy and Ye[2]). It is better to control a single pressure, letting the others float. The reactor pressure is an obvious choice because (a) it has a specified upper limit that must not be violated; (b) minimization of operating cost requires operation near this limit, as discussed previously.

Control of reactor pressure requires that we balance the rate at which gas enters and leaves the reactor. The only entry point is the feed, which we have allocated to production rate control. Of the remaining variables, the most effective are those controlling reaction rate, i.e, the conversion of gas to liquid. These include:

1. The reactor temperature. An increase in reactor temperature increases all the reaction rates, which decreases the pressure[4,11].
2. The partial pressure of a limiting reactant, which regulates one or more reaction rates.
3. The partial pressure of inerts, which influences the partial pressures of the reactants. For example, an increase in the purge rate tends to decrease the inert's partial pressure, which increases reaction rates and decreases the reactor pressure.

This decision is probably the most controversial; all of the above have been advocated by at least one author.

Option 1 provides excellent servo and regulatory responses. Its main drawback is a gradual upward drift in temperature. Suppose that a sustained disturbance causes pressure to increase. The pressure controller increases the reactor temperature. The short-term effect is to decrease the pressure, but in the long term, production of F is favored at high temperature. As F builds up in the recycle loop, it dilutes the reactants and increases the pressure, leading to a further increase in temperature, etc.

Option 2 has the following disadvantages:

1. The sign of the gain can change as a reactant goes from a limiting partial pressure to one in excess. This can happen with reactant A in the vicinity of the minimum-cost operating conditions.
2. If the reactant is limiting for only one of the major reactions, its adjustment will upset the product composition. This eliminates D and E from consideration.

Option 3 suffers from a relatively slow response, and the maximum purge rate is limited, i.e., the valve may saturate. On the other hand, the use of the purge (in combination with a constant reactor temperature) has an important advantage: the optimal setpoint for the pressure is known, whereas the optimal purge rate is not. Since the purge rate has a dominant effect on operating costs, its use as the manipulated variable in Loop 12 tends to minimize operating costs automatically. Most previous work has used the purge rate to control % B in the purge[2,5], but the optimal setpoint for %B depends strongly on operating conditions[11]. A poor choice increases costs dramatically.

On balance, simulation results suggest that Option 3 is best. (It should be noted that McAvoy and Ye found favourable RGAs for this option but chose option 2 instead[2].) An override must be provided, however, to maintain pressure control when the purge valve saturates (see Loop 18).

The recommended setpoint for Loop 12 is 2850 kPa. The control strategy will normally keep the pressure within ±40 kPa of this value, so high alarm violations will be infrequent. The override loop (see below) keeps the pressure less than the shutdown limit of 3000 kPa under all conditions.

Overall, the structure of the liquid inventory loop follows the main process path in a consistent downstream direction, as recommended by Price *et al.*[5]. The same cannot be said of the pressure control, however.

Product composition (Loop 13)

Now that production-rate and inventory controls have been chosen, we consider product quality – the composition of stream 11. There are two aspects to this problem:

1. Control proportions of G and H, as stipulated in the Goals.
2. Control of 'product losses', i.e, amount of D and E in stream 11. This is primarily an economic issue, as variation in these components rarely exceeds 1 mol %, i.e, it has little impact on the primary objective: variability of % G.

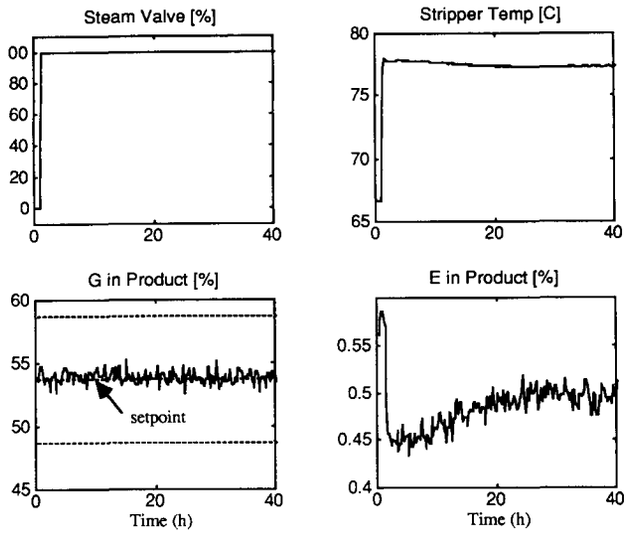


Figure 5 Effect of step in steam valve, with feed rates held constant

We now consider each of these points in detail.

Effects of stripper stream on % G in product. *Figure 5* shows the effect of a full-range step in the stripper steam valve position. The plant is initially at the Mode 1 (50:50) operating point described by Ricker[11]. The inventory control loops are active, but production-rate control is off, and the feed rates (streams 1–4) are constant. The reactor pressure is controlled at 2800 ± 4 kPa, reactor temperature is 123 ± 0.05°C, and reactor liquid level is 65 ± 2%.

The stripper temperature increases rapidly by about 10°C (*Figure 5*). There is no discernible effect on the % G in the product, however, i.e., the stripper is a poor manipulated variable for control of % G in the product.

Choice of manipulated variable for % G control. In contrast, the relative rates of reactions 1 and 2 have a major effect on product composition. The plant normally operates with D and E as limiting reactants, so their feed rates affect the reaction rates. The problem is to adjust composition without upsetting the production rate. We thus combine % G control with the production-rate control using feedforward/feedback.

The feedforward component is a table look-up, which linearly interpolates *Table 3* with respect to the % G target to determine r_{2FF} and r_{3FF}. *Table 3* was derived through experiments in which the plant was operated at three different product compositions – Modes 1–3 of *Table 1*.

The feedback adjustment uses a discrete-time PI algorithm with a sampling period of 0.25 h, (synchronized with the product analyser). The loop setpoint is the same as for the feedforward component, and the measurement is % G from the product analyser. If the measured % G is too high, it decreases the feed rate of D. To minimize production-rate upsets, it simultaneously increases the feed rate of E. According to the stoichiometry, one should keep the total feed of D + E constant (on a molar basis). Thus, the combined feedforward-feedback strategy is:

$$r_2(t) = r_{2FF}(t) - \frac{32E_{adj}(t)}{F_p(t)} \quad (5)$$

$$r_3(t) = r_{3FF}(t) - \frac{46E_{adj}(t)}{F_p(t)} \quad (6)$$

where E_{adj} is the signal from the feedback controller, and may be interpreted as an adjustment to the molar feed rate of E. The constants 32 and 46 are the molecular weights of D and E, respectively.

In practice, the feedforward mode provides excellent control, and the feedback adjustment mainly eliminates small offsets (see Results). Feedback is de-tuned to minimize interactions with other loops.

Table 3 Ratios for feedforward control of % G in product

Setpoint mol % G	11.7	53.7	90.1
Feedforward r_{2FF}	7.44	36.58	66.17
Feedforward r_{3FF}	81.44	44.34	8.94

Limit on rate of change in % G setpoint. Since the allowed rate of change of D is limited, changes in the setpoint of % G must be gradual. We therefore impose a maximum rate-of-change on the % G setpoint. Thus, if the operator makes a step change in the % G target, this is converted automatically to a ramp. Here, the maximum ramp rate was ± 50% G in 24 h.

Control of product losses. Nearly all previous authors have recommended a loop to control % E in the product via adjustment of steam rate (or stripper temperature). These have a limited impact on the % E, however (see *Figure 5*). It is difficult to specify a feasible setpoint, so the loop has little benefit, often saturating during disturbances or changes in production targets. The recommended strategy is no direct control of product losses. The steam valve position is held constant. Ricker[11] shows that the valve should usually be fully closed.

Control of chemical inventories

We now consider control of inventories of the eight chemicals, A–H. Chemicals that tend to accumulate (or disappear) in an uncontrolled manner are termed 'non-self-regulating' and can cause oscillations or stability problems[16].

Inert (B). The recommended strategy uses the purge rate to control the reactor pressure (Loop 12). The following is the typical sequence of events following a doubling of the % B in stream 4:

a. B accumulates in the process. % B in the purge increases, as does that in the feed to the reactor.
b. Partial pressures of the reactants decrease, causing both main reaction rates to decrease.

c. The imbalance between the reactant feed rates (streams 1–4) and liquid production increases the reactor pressure.
d. The purge rate increases, eventually compensating for the disturbance.

Thus, the concentration of B in the system varies with disturbances, but is self-regulating via the reactor-pressure control loop. As discussed previously, this has important economic advantages over strategies that use the purge rate to hold either the %B or %F at a setpoint.

Byproduct (F). The main control on selectivity is the reactor temperature; reactions 3 and 4 are relatively temperature-sensitive[17]. Thus, it is recommended that reactor temperature be kept in the range of 120–130°C. The optimal value depends on the control objectives – especially the production rate and % G targets – and the constraints, but a deviation of ± 2°C from optimum will usually increase costs by only a few percent, as will be demonstrated below. As long as the temperature is 120–130°C, F will be self-regulating. It escapes in the purge and the product. The suggested pressure-control strategy automatically controls the buildup of F, should it become the dominant inert.

Products (G and H). The products G and H are self-regulating through the liquid inventory control loops (reactor, separator, and stripper).

Reactants (A, C, D, and E). Reactants D and E are manipulated to control product rate and composition (Loop 13). The recommended strategy keeps A and C in excess, so that D is rate-limiting for reaction 1, and E is rate-limiting for reaction 2. Thus, D and E are self-regulating as long as the partial pressures of A and C are above some minimum value. For example, if the partial pressure of E increases due to a disturbance, the rate of reaction 2 will increase, reducing the partial pressure of E.

One way to ensure that A and C are in excess is to set the r_1 and r_4 values (equivalent to the flows of streams 1 and 4) sufficiently high, and hold them constant. Under normal conditions, the plant can run for long periods in this manner, even during disturbances in feed composition (see 'Loss of the analysers'). The pressure control loop prevents excess accumulation of A and C by increasing the purge rate.

Of course, this is unlikely to be optimal, as it wastes reactants. The recommended strategy is therefore to use r_1 and r_4 to keep partial pressures of A and C in a 'good operating range'. There are many ways this could be done (see, e.g., Banerjee and Arkun[4], who also recommend control of A and C). Here, we choose the following approach:

Loop 14 uses r_1 to control the amount of A in stream 6 (reactor feed), relative to the amount of A + C (as a percent). In terms of the measured variables, this is:

$$y_A = 100 \frac{xmeas(23)}{xmeas(23) + xmeas(25)} \quad [\%] \tag{7}$$

Loop 15 uses $r_1 + r_4$ control the amount of A + C in stream 6, i.e.

$$y_{AC} = xmeas(23) + xmeas(25) \quad [\%] \tag{8}$$

The rationale is that stream 1 is pure A, so it mainly influences the relative amount of A in the feed. The sum of streams 1 and 4 determines the amount of A + C relative to the other components. Let the change in the output of Loops 14 and 15 be $\Delta r_1(t)$ and $\Delta r_{14}(t)$, respectively. Then the adjustments to the ratios are:

$$r_1(t) = r_1(t-\Delta t) + \Delta r_1(t) \tag{9}$$

$$r_4(t) = r_4(t-\Delta t) + \Delta r_{14}(t) - \Delta r_1(t) \tag{10}$$

Both loops are discrete-PI controllers (velocity form) with a sampling period synchronized to the reactor feed analyser (0.1 h). Loop 14 executes first. The $r_4(t)$ signal has a specified lower limit of 0.084, designed to prevent overshoot during large upsets, as when there is a sudden change in availability of stream 1 (Disturbance 6 of Downs and Vogel[1]).

Temperature control (reactor and separator – Loops 16–17)

The reactor temperature determines selectivity (relative rates of reactions 3–4). Also, there is potential for a thermal runaway. Although there is no defined setpoint, reactor temperature should be controlled. The obvious manipulated variable is the reactor coolant valve. A PI controller (Loop 16) keeps reactor temperature within 0.1°C of its setpoint under all but the most extreme conditions. Deviations of more than 1°C have never been observed. The more complex nonlinear model-based scheme used by Kanadibhotla and Riggs[6] is not required for high performance.

Separator temperature control (Loop 17) is the inner (slave) loop of a cascade structure that regulates reactor level (Loop 11). The slave loop rejects disturbances in the condenser coolant temperature. The results of Price *et al.*[5] suggests that the omission of this loop increases production-rate variability.

Summary – degrees of freedom

As discussed previously, six process variables have *a priori* setpoints and must be controlled, and reactor agitation rate is to be fixed. The above strategy uses seven of the 12 available degrees of freedom for these tasks. The remaining five degrees of freedom are assigned to the following variables, given in rough order of importance, with the most important first:

1. Reactor temperature, T_r.
2. y_{AC} – the combined % A + % C in the reactor feed.
3. y_A – the amount of A in the reactor feed relative to the amount of A + C (as a percent).
4. Recycle valve position.
5. Steam valve position.

The first three have a major impact on process stability and operating costs. Appropriate setpoints must be determined, as none of the five have *a priori* optimal values.

Overrides

Certain abnormal conditions require a change in operating strategy. The philosophy of this paper has been to automate these changes where possible, realizing that operator intervention might be needed in extreme cases. Two proposed overrides are considered below. The first is the more important.

Maximum reactor pressure (Loop 18)

Suppose the reactor pressure, P_r, has a setpoint of 2850 kPa, as recommended previously. If there is a large disturbance, the pressure may approach the high-alarm limit of 2895 kPa. A sustained disturbance will cause the purge valve to saturate (see Loop 12). A poor choice of one of the 'free' setpoints – T_r, y_{AC} and Y_A – could also cause the pressure control to saturate.

If Loop 12 saturates, the safest policy is to reduce the production rate target, F_p. This decreases the rate of all the feeds (in proportion), which reduces the reactor pressure. In fact, the need for such an override was another important driving force in the choice of F_p as the production-rate control, i.e., this variable has an immediate and relatively large effect on the pressure.

In the present work, the production rate decreases automatically whenever the reactor pressure exceeds 2950 kPa. The strategy uses a PI loop for which P_r is the measured variable. The setpoint is 2950. Let the output of this controller be $F_{p,OR}$, which is restricted such that:

$$F_{p,OR}(t) \leq 0 \tag{11}$$

The $F_{p,OR}(t)$ signal adds to $F_p(t)$. The modified F_p is used in Eq. (1) for ratio control. As will be demonstrated in simulations, this strategy allows the plant to operate in a stable manner during severe disturbances (such as #6) while maintaining a near-maximum production rate.

This override is independent of the reduction in production rate target that occurs when a feed stream saturates (see discussion related to Loops 1–8).

Separator temperature saturation (Loop 19)

Control of reactor liquid level relies on control of the temperature in the separator. If the condenser coolant valve saturates – at either 0% or 100% – another variable must be used to maintain reactor level control. The present work uses the recycle valve as the backup.

Normally, the recycle valve is held at a specified setpoint. Let this be u_{5sp}. We define two override loops:

a. High override. If a high reactor liquid level persists, the separator temperature setpoint decreases, and the condenser valve approaches 100% open. We then need to close the recycle valve (increasing the recycle flow). This tends to decrease the reactor liquid level. The override is a PI controller for which the measured variable is the condenser valve position, and the setpoint is (arbitrarily) chosen as 95%. Let the output of this controller be u_{5Hi}, with the restriction that $u_{5hi} \leq 0$.

b. Low override. As for the high override, except the setpoint is 5%, and the controller output is $u_{5,Lo}$, with the restriction that $u_{5,Lo} \geq 0$.

The recycle valve position is then the sum of the operator setpoint and the two override signals:

$$xmv(5) = u_{5sp} + u_{5Hi} + u_{5Lo} \tag{12}$$

Normally, both override signals are zero, and the recycle valve is at its setpoint.

Other possible overrides

The reactor temperature and liquid level both have shutdown limits. If the reactor cooling capacity were limited, a high-temperature override might be justified. It could be done by reducing production, as for the maximum pressure override. However, experience has shown that the reactor cooling valve is always far from saturation, even during transients at maximum production (as it should be for safety). Thus, an override for reactor temperature was not included. Similarly, the proposed strategy provides tight control of the reactor liquid level under all conditions tested.

The other potential problems are the liquid levels in the separator and stripper. The level control loops have been tuned loosely to minimize variations in product flow, i.e., they act as surge tanks. Under extreme conditions, the levels can exceed their alarm limits, and it is possible that they could cause a shutdown (though it has never happened in simulations). The rate-of-change in level is slow, however, and could be handled by operator intervention.

Results

Downs and Vogel suggest specific setpoint changes and disturbances to test performance[1]. All of their tests were carried out in the present work. In contrast to previous studies, which focus on the base case, performance was evaluated for all six modes in *Table 1*. The control system always satisfied the performance specifications. In particular, most disturbances in *Table 8* of Downs and Vogel[1] are handled easily and are not considered in detail here. For example, disturbances caused by sticking valves and coolant temperature variations (#3, #4,

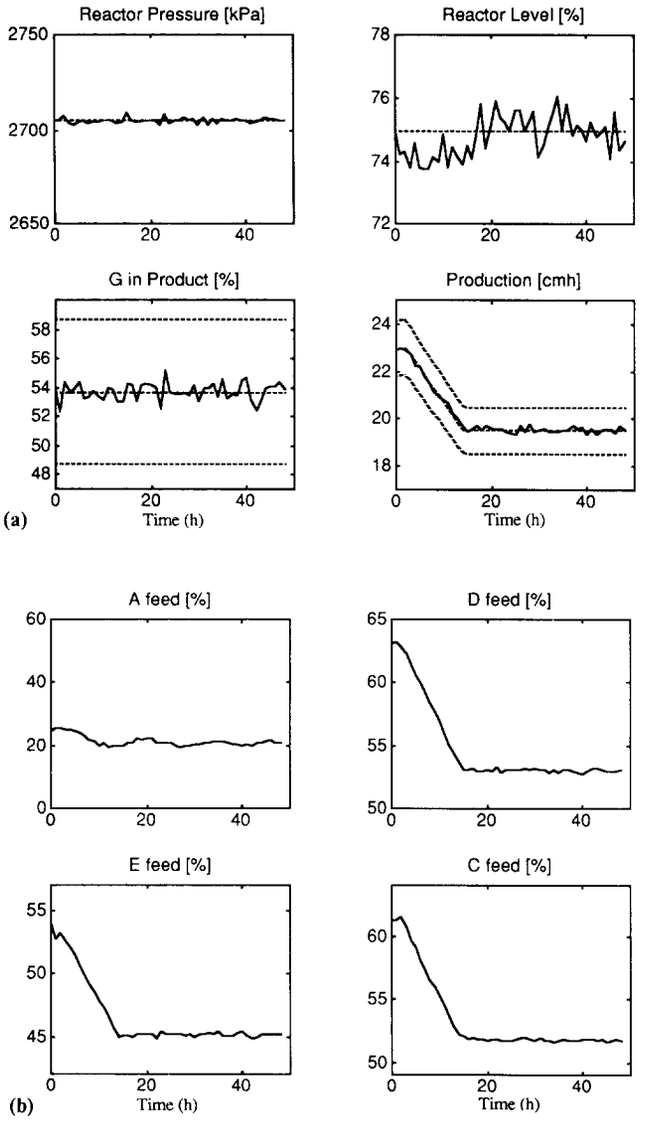


Figure 6 a Key controlled variables during 15% step decrease in production-rate setpoint at t = 2. Dashed lines are setpoints or specified bounds; **b** valve positions (feed streams) during 15% step decrease in production rate setpoint at t = 2 h

#5, #9–#12, #14, and #15) are rejected by the slave temperature-control loops before they affect more important variables. Similarly, the disturbance in C header pressure (#7) is rejected by the slave flow controller on stream 4. Results of the more difficult tests are presented in the remainder of this section.

Change in production at the base case

Figure 6 shows the servo-response for a 15% decrease in production. The initial condition is the steady-state base-case provided by Downs and Vogel[1]. The setpoint changes step-wise at t = 2 h. As explained previously, the step is converted automatically to a ramp, which is tracked almost perfectly (see *Figure 6a*). The other important controlled variables are nearly constant. *Figure 6b* shows that the feeds vary smoothly during the transient. Reactor temperature was controlled at 120.4 ± 0.1°C (not shown).

Change in reactor pressure at the base case

Figure 7 shows the servo-response for the reactor pressure setpoint. Initial conditions are the base case, and the setpoint changes step-wise at t = 2 h from 2705 to 2645 kPa. Although there is a slight delay followed by an overshoot, the pressure transient is satisfactory, and disturbances in the other loops are small (*Figure 7a*). Reactor temperature is 120.4 ± 0.1°C (not shown). The averaging level control strategy prevents production upsets by allowing significant variations in the separator and stripper liquid levels (*Figure 7b*). The concentration of inert, B, decreases about 2 mol % (*Figure 7b*), which increases costs by about 5%. As noted earlier, economics favour an *increase* in P_r rather than a decrease.

Change in product composition at the base case

Figure 8 shows the servo-response for a step in product concentration. The step magnitude is −10%, as sug-

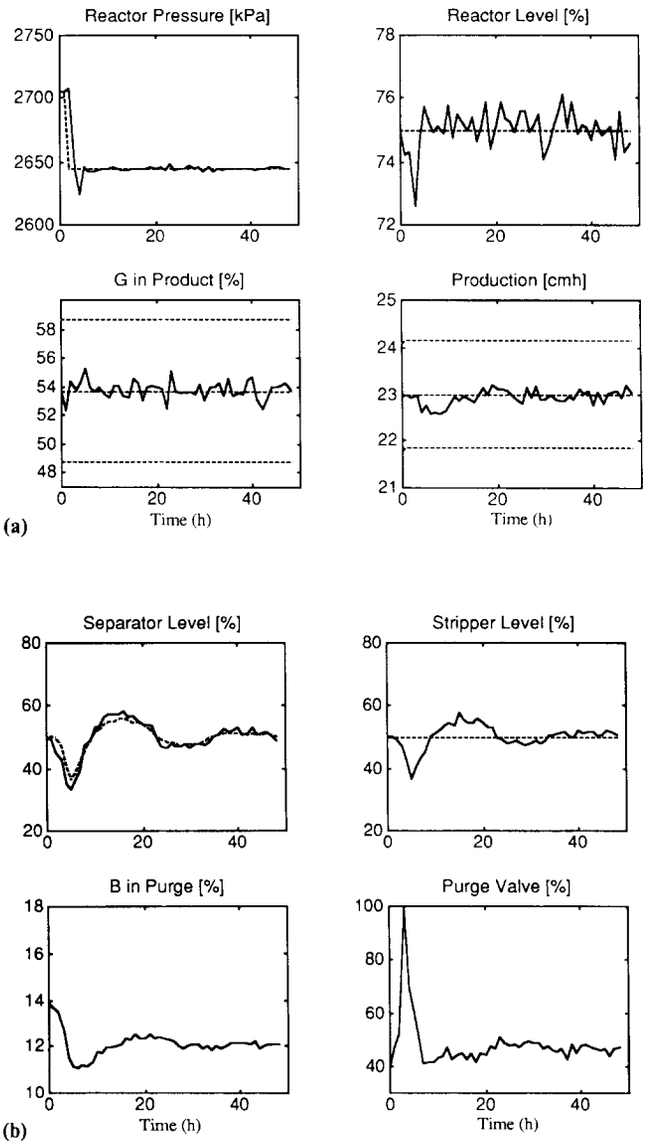


Figure 7 a Key controlled variables following step decrease in reactor pressure setpoint at t = 2. Dashed lines are setpoints or specified bounds; **b** auxiliary variables following step decrease in reactor pressure setpoint at t = 2 h. Dashed lines are setpoints or specified bounds

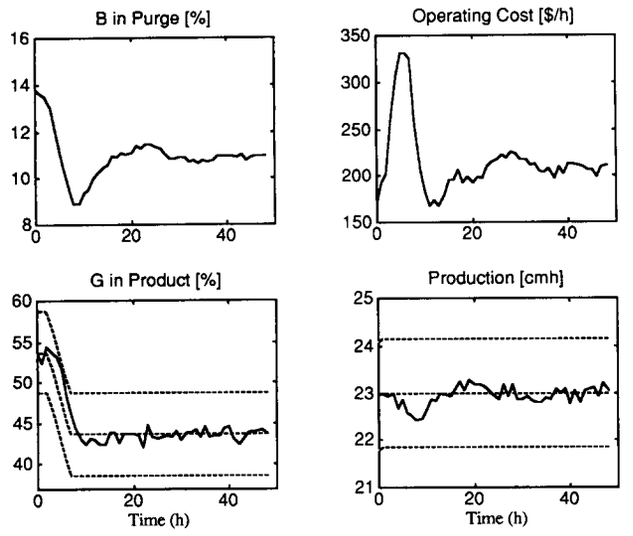


Figure 8 Result of step in % G setpoint for base case. Dashed lines are setpoints or specified bounds

gested by Downs and Vogel[1]. Reactor pressure, temperature, and other key variables are held constant at the base-case conditions. As in the previous examples, upsets in other loops are negligible. Reaction 2 is relatively slow[17], so isobaric and isothermal operation requires a decrease in inerts concentration. Again, this is done automatically by the pressure control system. There is a large transient in the operating cost (*Figure 8*), caused by the increased purge rate (not shown). The plant settles at the new condition after about 24 h, however.

Random disturbances in feed composition at the base case

One of the more interesting cases is the random disturbance in feed composition (#8 in *Table 8* of Downs and Vogel[1]), which was active for the entire 70-hour simulation shown in *Figure 9*. The initial condition was the base case. Large step changes in reactor pressure, level and temperature setpoints were made at t = 20 h; additional steps occurred at t = 30 (*Figure 9a, b*). Servo and regulatory response of the reactor temperature controller is excellent, despite the disturbances.

The sudden increase in the reactor temperature increases reaction rates substantially, which causes a temporary drop in pressure (during which the purge valve is closed), but this causes no problems in the more critical loops. Product rate and composition are always well within tolerances (*Figure 9a*). The rate of stream 1 varies significantly, but at low frequency (*Figure 9c*).

These results show that the plant can be moved smoothly to a more economical operating point (higher pressure, lower liquid level in the reactor) during a large disturbance without a sacrifice in product quality.

Maximization of 10:90 production with random disturbances

We now consider maximization of production rate for the 10:90 (G:H) product, which is difficult because

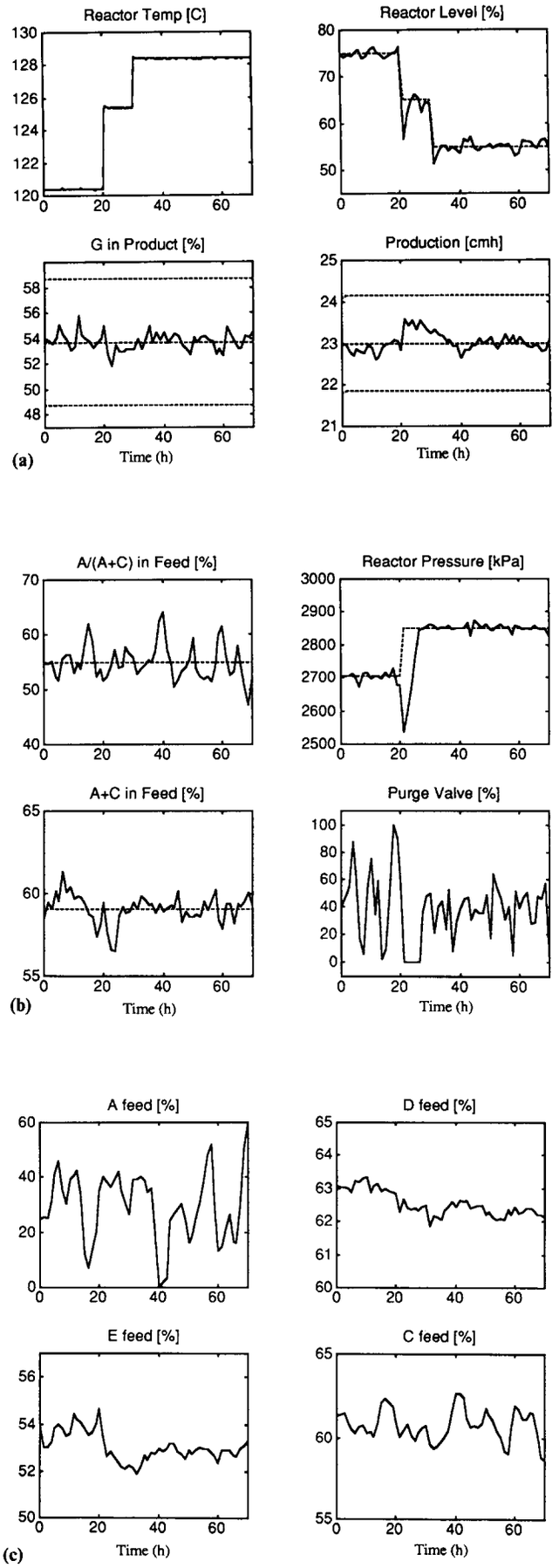


Figure 9 a Key controlled variables during random disturbances in composition of stream 4 (IDV_8). Dashed lines are setpoints or specified bounds; **b** key controlled variables during random disturbances in composition of stream 4 (IDV_8). Dashed lines are setpoints or specified bounds; **c** valve positions for feeds during random disturbances in composition of stream 4 (IDV_8)

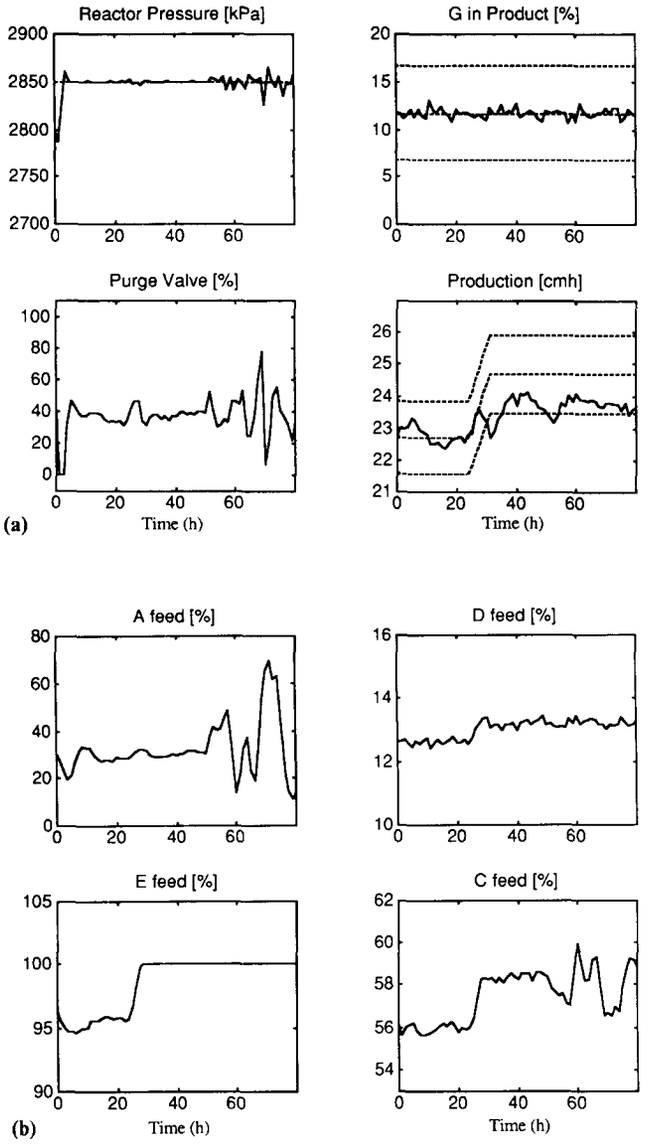


Figure 10 a Variation of key controlled variables as production rate is maximized for 10:90 product (Mode 5). Random variation in stream 4 composition (IDV_8) begins at $t = 50$. Dashed lines are setpoints or specified bounds; **b** variation of feed-value positions as production rate is maximized for 10:90 product (Mode 5). Random variation in stream 4 composition begins at $t = 50$

reaction 2 is relatively slow. In *Figure 10*, the plant is initially at the Mode 2 operating point described by Ricker[11]. Unless noted otherwise, all controlled variables are held constant at this initial condition.

At $t = 0$, we increase the reactor pressure to 2850 kPa and decrease the reactor level to 55% as recommended previously. At $t = 20$ we attempt to increase the production setpoint by about 10%. As shown in *Figure 10a*, production can only increase about 5%, because the E feed saturates (*Figure 10b*). Thus, there is an offset in the production rate (*Figure 10a*). The constraint-control strategy proposed here prevents offsets in the other controlled variables, however.

Beginning at $t = 50$, there are also random disturbances in feed composition, (disturbance #8). This causes higher variability in the manipulated variables – especially the A feed and the purge – but product composition and rate show the same variability as before, even though we have lost a degree of freedom.

Maximization of 10:90 production with loss of A feed

Another interesting case is the loss of the A feed (disturbance #6). Other researchers have advocated control strategies that lead to large production losses during this disturbance. The strategy proposed here can maintain the base-case production (not shown).

Figure 11 shows the more challenging situation when the plant is operating at maximum production for the 10:90 product. The first 50 h are as for the previous case. Again, the E feed saturates as we attempt to maximize production. When the A feed is subsequently lost at $t = 50$, the imbalance of reactants causes a rapid pressure increase, and the purge valve saturates. The pressure continues to increase. When it reaches the pre-specified value of 2950 kPa, the high-pressure override loop gradually reduces the production rate, which quickly stabilizes the pressure. There is no discernible effect on product composition. Thus, the proposed strategy provides safe operation with only a 15%

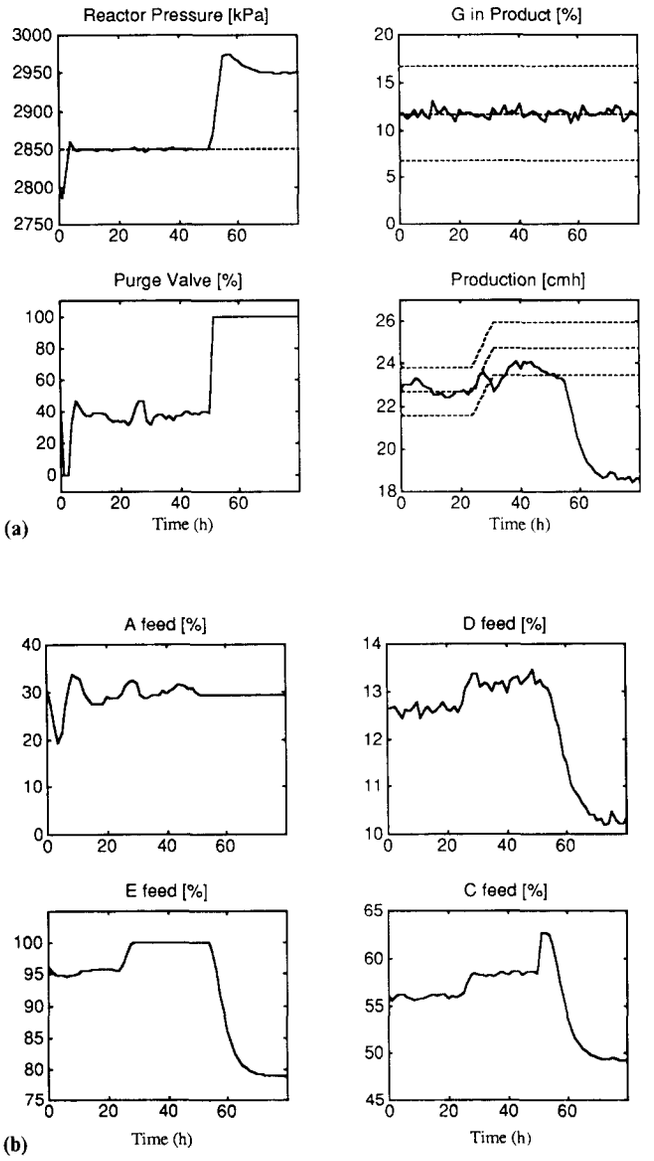


Figure 11 a Variation of key controlled variables as production rate is maximized for 10:90 product (Mode 5). Dashed lines are setpoints or specified bounds; **b** variation of feed-value positions as production rate is maximized for 10:90 product (Mode 5). Feed 1 is lost at $t = 50$

decrease in production, which is near-optimal for this case. No operator intervention is required.

Maximization of 90:10 production with step disturbances

We now consider the other extreme of product composition, 90 mass % G. The initial condition is Mode 3 of Ricker[11]. As in the previous cases, we change reactor pressure and liquid level to the recommended values of 2850 kPa and 55%. Then at t = 20 we attempt to increase production (*Figure 12a*). This time, the D feed saturates (*Figure 12c*), limiting the increase to about 10%, as expected from steady-state analysis[11].

At t = 40, disturbance #1 occurs (step in A/C ratio in stream 4). The rates of feeds 1 and 4 vary to compensate (*Figure 12c*). At t = 60, disturbance #2 occurs (step in B concentration in stream 4), and the purge rate compensates (to hold the pressure constant). Note that the B concentration automatically increases by about 2 mol %, reducing operating costs relative to strategies that hold % B constant. As in the previous example, the system controls product composition in the face of sustained disturbances, even though one of the limiting reactants is constrained.

Loss of the analysers

Two gas chromatographs provide feedback on % G in the product, and % A and % C in the reactor feed. Such analysers are relatively unreliable, so it is important that the plant be operable while they are out of service. This section demonstrates that control can be maintained even in the event of serious disturbances.

The proposed static feedforward control is accurate, especially for control of product composition. If the product were on-spec. and the product analyser were lost, one could hold the r_2 and r_3 ratios constant, and the product would usually stay within ± 5% of the setpoint. One could also start up the plant on feedforward only, and be likely to satisfy the product specifications. Similarly, it is easy to choose r_1 and r_4 values that will at least allow the plant to run.

Figure 13 compares the control strategy of *Figure 2* (with all loops operating – solid lines in plots) to one in which both analysers are off, and all feed ratios are held constant (dot-dash lines). The initial condition is the base case of Downs and Vogel. Disturbances #8 (random feed composition variations) and #13 (drift in reaction kinetics) are both active for the duration of the simulation.

This combination of disturbances is challenging, especially when the plant is operating at extreme conditions. In the present work, for example, specifications on production rate variability were nearly violated when the plant was operating in Mode 2 (not shown). In the present case, regardless of analyser availability, there are large disturbances in the reactor pressure and the purge valve saturates frequently (*Figures 13a, b*). Although Downs and Vogel[1] characterize disturbance

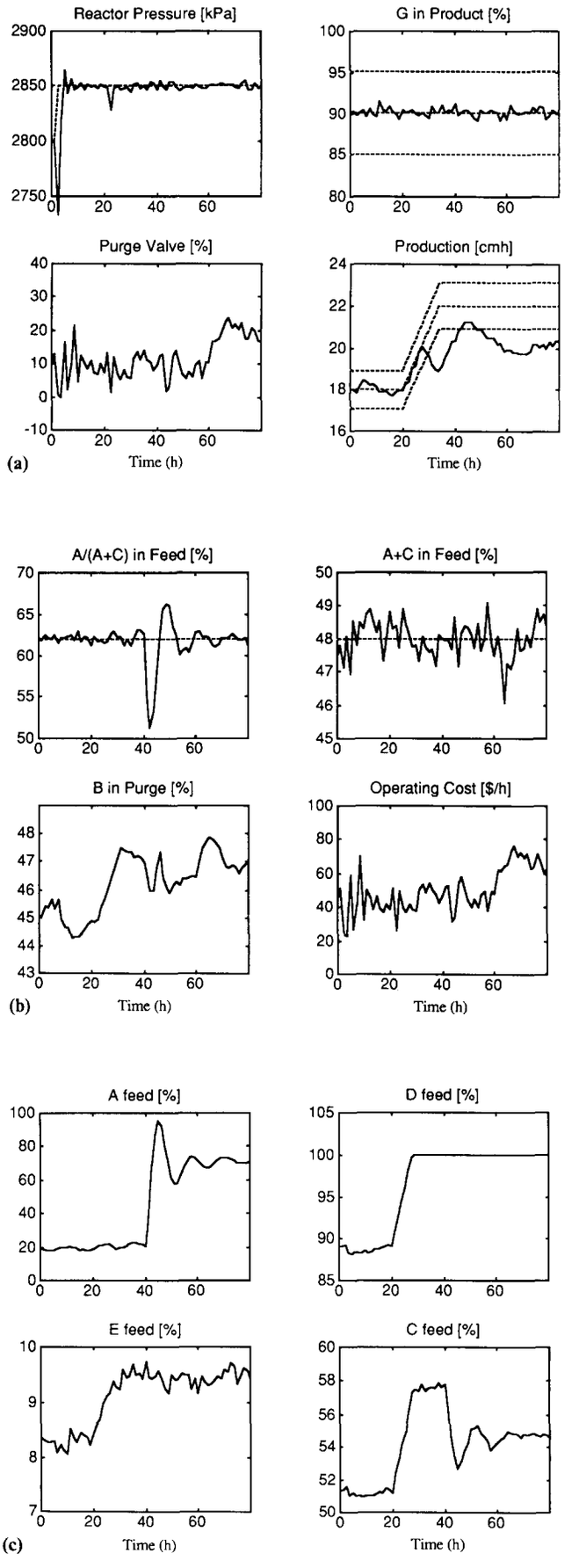


Figure 12 a Variation of key controlled variables as production is maximized for 10:90 product (Mode 6). Dashed lines are setpoints or specified bounds; **b** variation in auxiliary variables as production is maximized for 90:10 product (Mode 6). Dashed lines are setpoints or specified bounds **c** variation of feed-value position as production is maximized for 10:90 product (Mode 6)

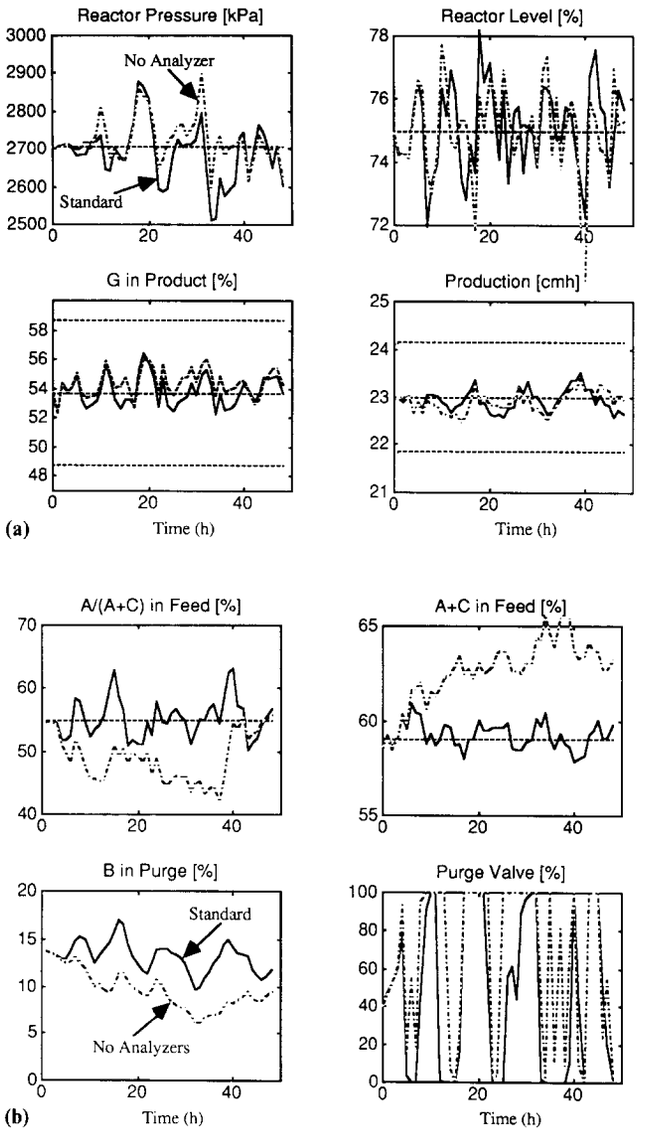


Figure 13 a Test of analysers feedback during two random disturbances (IDV_8 and IDV_{13}) at the base-case point. Dot-dash lines show effect of loss of analysers at $t = 0$. Dashed lines are setpoints or specified bounds; **b** test of analysers feedback during two random disturbances (IDV_8 and IDV_{13}) at the base-case point. Dot-dash lines show effect of loss of analysers at $t = 0$. Dashed lines are setpoints or specified bounds

#13 as 'drift', there are sudden and rather large changes in kinetics, causing rapid accumulation or depletion of gas. As shown in *Figure 13a*, however, product rate and composition are essentially constant, with or without the analysers. In the latter case, there is a drift of about 0.5% in the mean value of % G, but that is well within specifications.

More serious is the drift in reactor feed composition (*Figure 13b*, dot-dash lines). To compensate for this, the pressure controller gradually reduces the inerts content of the purge, which significantly increases operating costs. With the feed-gas analyser on-line, the average operating cost for the run was \$188/h. Compare this to \$171/h at the steady-state of Downs and Vogel[1], i.e., the disturbances are costly. Without the analyser, the drift in recycle gas composition increases average costs by more than 30% to \$249 per hour! This demonstrates that control of reactant inventories is important from an economic point of view, at least.

Effect of non-optimal setpoints

The proposed strategy requires one to specify setpoints for certain variables (e.g., reactor temperature) that influence operability and economics. In practice, one would like to optimize these variables, but that may be difficult on-line. In this section we consider the sensitivity of the plant to these choices.

Reactor temperature. There is an optimal value between the bounds specified by Downs and Vogel. If the setpoint is too low, one must increase reactant partial pressures in order to achieve the desired production, which increases purge losses. If the setpoint is too high, selectivity suffers. Ricker showed that the optimal operating temperature varies with product rate and composition, but at the nominal production rate, the variation is small: 122, 123, and 124°C in Modes 3, 1, and 2, respectively[11]. To test the effect of a non-optimal choice, the plant was run in Mode 1 for 72 h at three different temperatures. In each case, the strategy of *Figure 2* controlled the plant, and disturbance #8 (random feed composition variations) was active. At the optimal temperature of 123°C, the operating cost was \$114.2/h, essentially the same as determined by Ricker[11], which, however, was for steady-state with no disturbances. At the non- optimal temperatures of 121 and 125°C, costs were \$117.5 and \$116.2, respectively, i.e., an increase of less than 3%. Thus, it should be easy to choose a near-optimal setpoint for the reactor temperature.

Reactor feed composition. The effect of setpoints for y_A and y_{AC} were evaluated in the same way (see definitions, Eqs. (7) and (8). For Modes 1–3, the optimal y_A is 63 ± 1%, and y_{AC} ranges from 48% (Mode 3) to 54% (Mode 2). Values 5% above and below optimal were tested. For y_A, these variations increased costs by less than 4%. For y_{AC}, however, the increase was as much as 11% (in the case of a value 5% too high). This is not surprising, as an excess of A + C requires that one decrease the inerts concentration, increasing purge losses.

Recycle valve. Ricker determined that the recycle valve should usually be closed[11]. For Mode 1, if the valve is instead 30% open, operating costs only increase by about 5%. The control system compensates by reducing the separator temperature (to hold reactor level), which increases product losses, but reduces purge losses.

Discussion and conclusions

It is essential that the control system be structured to accommodate the likely constraints, i.e., to operate in the desired manner as the process loses degrees of freedom. In the TE problem, steady-state analysis showed that one of three feed rates normally limits production

capacity. This was a primary motivation for the production-rate control strategy used here. In the maximum-production modes, a simple algorithm identifies the active constraint, then holds the plant there while maintaining the specified product composition. The strategy recommended by Price *et al.*[5], for example, would have to be modified in order to operate at maximum production. McAvoy and Ye[2] were similarly forced to restrict production to 90% of maximum to prevent saturation of a feed valve that was being used for level control in the reactor.

A second motivation was the need to handle large disturbances in the reactor pressure. Purge adjustments can compensate for small disturbances – especially pressure increases. A purge-rate increase counteracts a buildup in any of the gaseous components, whereas other adjustments are more selective and, hence, will not work in all cases. Use of the purge for pressure control also has clear economic advantages. The problem is that the purge rate is limited, so large disturbances require an override. It is argued here that the correct response to a sustained increase in pressure (causing purge-valve saturation) is a reduction in production rate. Again, the recommended production-rate control is advantageous because it has a direct and rapid effect on reactor pressure. Therefore, one can design an override that smoothly reduces production to the maximum possible value that keeps the pressure in the safe operating range. This was demonstrated in several simulations.

A third motivation was the ease with which simple static feedforward control could be included. The present work demonstrates that feedforward provides excellent control of product composition and production rate. The main role of feedback in those loops is to eliminate small offsets.

A more systematic approach to the design and tuning of decentralized controllers for constrained systems is the MMC method developed by Brosilow and co-workers[18], which encourages the use of hierarchical structures. Given the required process insight, MMC performance would probably be equivalent to that demonstrated in the present work, but this was not verified.

A centralized, model-predictive controller (MPC) is another possibility. The author has had 15 years of experience with MPC, including a successful application to a real, large-scale system[19]. In an earlier paper he applied nonlinear MPC to the TE problem[9]. The following observations are based on more than three years of experience, during which both the NMPC and decentralized approaches were tested exhaustively:

1. *Structure selection.* Both MPC and decentralized methods require one to make critical decisions without quantitative justification. Foremost among these is the selection of the controlled-variable set. A naive MPC designer might be tempted to control only variables having defined setpoints, relying on optimization to make appropriate use of the remaining degrees of freedom. This fails in the TE problem. As discussed previously, all chemical inventories must be regulated; it cannot be left to chance. Unless setpoints for key internal concentrations are provided, MPC allows reactant partial pressures to drift to unfavourable values[9].

   It is difficult to decide how many internal concentrations to control, which chemicals, which locations, *etc.* Existing quantitative methods for structure selection are inadequate for this purpose. The most thorough attempt could only configure four of the more obvious temperature, pressure, and flow loops quantitatively[4]. Their composition control structure was based on overall stoichiometry and physical arguments, as in the present work. Further research is needed on plantwide structure-selection tools. Meanwhile, the more qualitative approach of Downs[16] is recommended.
2. *Nominal, unconstrained performance.* Ricker and Lee[9] and others have demonstrated excellent MPC setpoint tracking in the absence of constraints. Selection of horizons and penalty weights is easy (once the right set of controlled and manipulated variables has been chosen). Tuning of individual PI loops is more tedious, but performance is nearly as good.
3. *Constraints.* One might expect MPC to do better than decentralized control when constraints are active. For the TE problem, the opposite was observed. This was the case not only for constraints on outputs, which are known to be problematic[20], but also for constraints on manipulated variables. The reason is that the TE problem has too many competing goals and special cases to be dealt with in a conventional MPC formulation.

   Consider, for example, the design of Ricker and Lee[9], in which there are eight manipulated and eight controlled variables. Suppose one of the manipulated variables becomes constrained. It is physically impossible to maintain all eight setpoints. MPC instead minimizes the sum of weighted, squared, setpoint-tracking errors. If the constraint remains active, MPC allows steady-state offset in all eight controlled variables. This is rarely the desired response. One would rather sacrifice a less-critical variable in order to control the others.

   In simple applications, the choice of the MPC setpoint-tracking weights provides a solution: high-priority variables are given higher weights. In the TE problem, however, the importance of a given variable depends on the situation. For example, when reactor pressure is far from its upper bound, product rate and composition have higher priority, but the order reverses during certain disturbances. Ricker and Lee found that no single set of weights and constraints could provide the desired performance in all cases[9]. Thus, they were forced to add SISO override loops to their MPC design.

   The classical approach required an equal number

of overrides. Coordination of the many system elements was non-trivial. In addition to experience and judgment, the availability of a dynamic simulation was essential. It allowed tuning of the override loops and testing over a range of conditions that would be difficult and/or too risky in a real plant. Trial-and-error tuning for constraint handling was equally important and time-consuming in the MPC design.

4. *Overall.* Both the MPC and classical designs satisfied the specifications of Downs and Vogel[1]. Differences in performance were small. The usual transparency of MPC was tarnished in the TE problem by the need to include extra override loops for constraint handling. More research is needed on easily-configured, plantwide, model-based controllers.

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