Pergamon

Computers chem. Engng Vol. 19, No. 9, pp. 949–959, 1995

0098-1354(94)00043-3

0098-1354/95 $9.50 + 0.00

OPTIMAL STEADY-STATE OPERATION OF THE TENNESSEE EASTMAN CHALLENGE PROCESS

N. L. RICKER

Department of Chemical Engineering, BF-10, University of Washington, Seattle, WA 98195, U.S.A.

(Received 15 March 1993; final revision received 31 March 1994; received for publication 27 April 1994)

Abstract—Optimal steady-state conditions are determined for the six operating modes of the industrial challenge problem proposed by Downs and Vogel. The problem is formulated as a nonlinear program with 50 variables and 44 nonlinear constraints. It uses the full state vector from the Downs and Vogel FORTRAN code, and thus is *not* a demonstration of optimization in a plant environment. Solutions are obtained using MINOS 5.1. The results show that the base case provided by Downs and Vogel is far from optimal. The operating cost (primarily purge losses) is easily reduced by more than 30%. In general, reactor pressure and liquid level should be held at their upper and lower bounds, respectively. Steam use can be eliminated, and the agitator speed can be fixed at its upper bound. The compressor recycle valve is closed in four of the six cases (the exceptions being the two cases requiring production of 90/10 G/H). Production can be increased by 59% for the 50/50 G/H product, but only by 4% and 12% in the 10/90 and 90/10 cases, respectively (relative to the nominal rates). Product rates are limited by reactant E for the 10/90 case, and by D otherwise. Most process variables change significantly with operating mode, and should not be held at constant setpoints. Other factors related to process control are discussed.

1. INTRODUCTION

Downs and Vogel (1993) have proposed an "industrial challenge problem" for researchers in process control and related fields. The problem is based on a Tennessee Eastman Company (TEC) process; Fig. 1 is a schematic. Unit operations include a reactor, a partial condenser, a recycle compressor and a stripper. The reactor is a two-phase CSTR in which the exothermic, irreversible reactions (shown below) occur.

A nonvolatile catalyst is dissolved in the liquid phase. The products have moderate volatility, and flow out of the reactor with the unreacted gases. The partial condenser recovers them from the recycle gas. The stripper minimizes losses of D and E from the liquid product. Overhead from the stripper combines with the off-gas from the partial condenser for recycle to the reactor. An inert component B makes up about 0.5% of feed stream 4. It is noncondensable and must exit in the purge (stream 9 in Fig. 1). The purge can also be used to prevent buildup of excess reactants (if any), and the byproduct F.

Downs and Vogel omit details of the kinetics, noting only that reaction rates are "approximately first-order" with respect to reactant partial pressures, and production of G is relatively sensitive to temperature. The kinetics, phase equilibria and process dynamics are provided in a FORTRAN code, which is purposely obscure.

Table 1 summarizes the six different operating modes proposed by Downs and Vogel. The plant must operate over a wide range of product composition (from a G:H ratio of 9:1, to 1:9). The product rate is either specified or to be maximized. The present work determines optimal steady-state conditions for these six modes. *It is not a demonstration of realistic on-line optimization, however.* The formulation described in the next section assumes noise-free measurements and full knowledge of the plant states—conditions that are never satisfied in practice. Thus, the results serve primarily as benchmarks for future on-line optimization studies. They also shed light on process steady-state characteristics that should be considered when designing a control system.

$$\begin{array}{lll} A\,(g) + C\,(g) + D\,(g) \rightarrow G\,(liq) & & \text{Product 1} \\ A\,(g) + C\,(g) + E\,(g) \rightarrow H\,(liq) & & \text{Product 2} \\ A\,(g) + E\,(g) \rightarrow F\,(liq) & & \text{By-product} \\ 3\,D\,(g) \rightarrow 2\,F\,(liq) & & \text{By-product} \end{array}$$

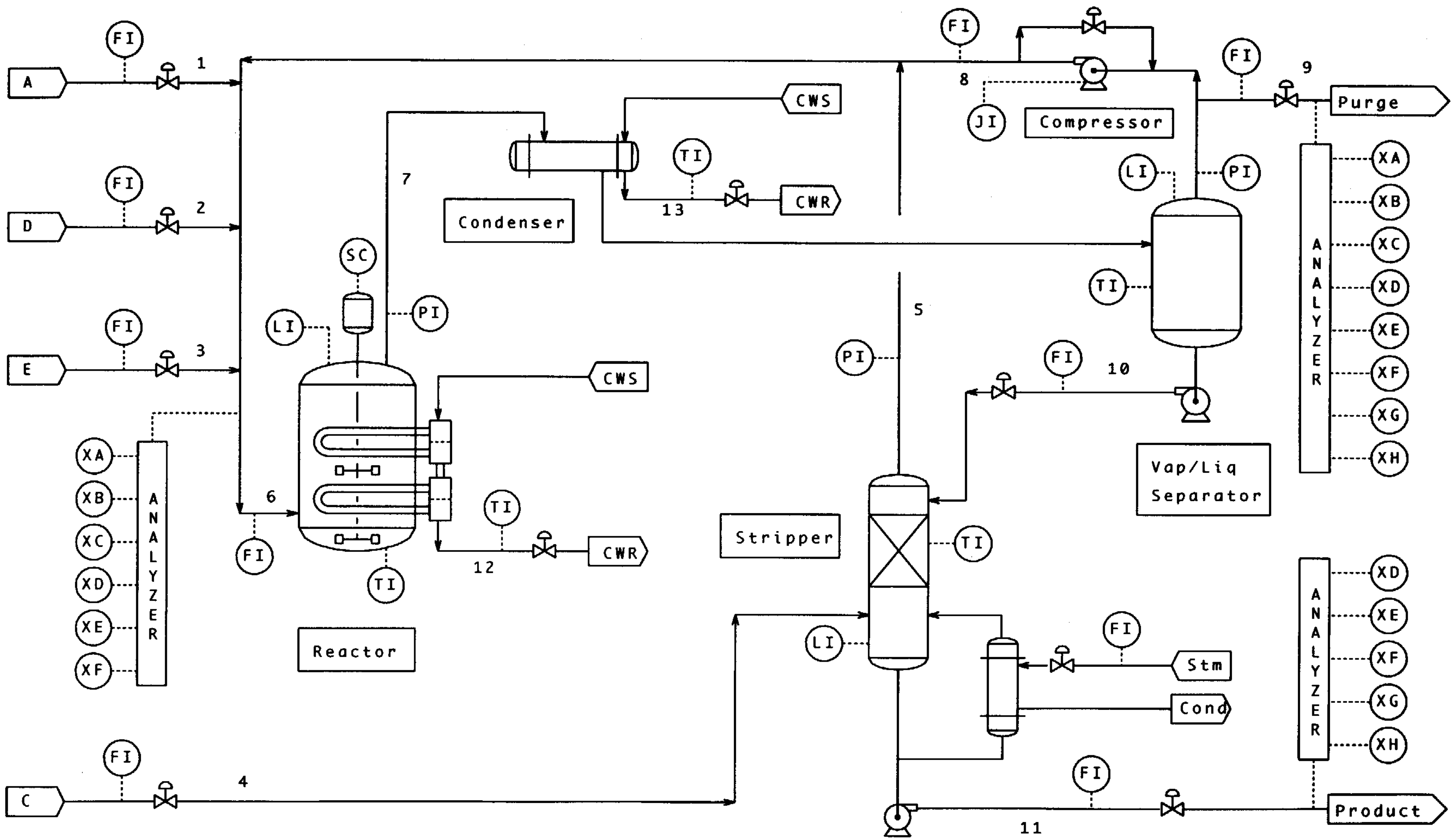

Fig. 1. Schematic of the TEC process, from Downs and Vogel (1993).

Table 1. Operating modes proposed by Downs and Vogel (1993)

Mode	Desired G/H mass ratio	Desired production (kg/h)
1	50/50	14076
2	10/90	14077
3	90/10	11111
4	50/50	Maximum
5	10/90	Maximum
6	90/10	Maximum

2. FORMULATION OF OPTIMIZATION PROBLEM

Downs and Vogel (1993) distribute the TEC problem as a FORTRAN code in the following form:

$$\frac{d\mathbf{x}}{dt}=\dot{\mathbf{x}}(t)=\mathbf{f}(\mathbf{x},\mathbf{u},t), \tag{1}$$

$$\mathbf{y}(t)=\mathbf{h}(\mathbf{x},t), \tag{2}$$

where

$\mathbf{x}(t)\in\Re^{n}$ = vector of $n=50$ state variables,
$\mathbf{u}(t)\in\Re^{n_u}$ = vector of $n_u=12$ manipulated variables,
$\mathbf{y}(t)\in\Re^{n_y}$ = vector of $n_y=41$ measured outputs,
$\mathbf{f}\in\Re^{n}, \mathbf{h}\in\Re^{n_y}$ = nonlinear vector functions.

The function **f** is implicit; it models multicomponent equilibria in the reactor, product separator and stripper (under conditions of varying temperature, pressure and composition). It depends on t because the code includes disturbances, which are functions of time. These can be turned "on" and "off" by setting switches in the interface subroutine. The function **h** is also implicit, and includes random measurement noise, which depends on t. When $t=0$, however, the measurement noise is zero, and one sees the "true" values of the measured variables for the given states **x**.

Downs and Vogel also provide an expression for the operating costs. The present work uses it in the following form:

$$\begin{aligned}c(t)&=0.0536y_{20}(t)+0.0318y_{19}(t)\\&+0.44791y_{10}(t)[2.209y_{29}(t)+6.177y_{31}(t)\\&+22.06y_{32}(t)+14.56y_{33}(t)+17.89y_{34}(t)\\&+30.44y_{35}(t)+22.94y_{36}(t)]\\&+4.541x_{46}(t)[0.2206y_{37}(t)+0.1456y_{38}(t)\\&+0.1789y_{39}(t)],\end{aligned} \tag{3}$$

where $c(t)$ is in \$/h. The term $4.541x_{46}(t)$ in equation (3) is the product rate in kmol/h. Table 2 gives the significance of the output variables appearing in equation (3).

The *minimum cost* problem is to determine *steady-state* values, $\mathbf{x}(0)$ and $\mathbf{u}(0)$, that minimize the operating cost while satisfying certain additional constraints, i.e.:

$$\min_{\mathbf{x},\mathbf{u}} c(\mathbf{x},\mathbf{u},0), \tag{4}$$

subject to

$$\mathbf{f}(\mathbf{x},\mathbf{u},0)=\mathbf{0}, \tag{5}$$

$$\mathbf{g}(\mathbf{x},\mathbf{u},0)\leq\mathbf{0}, \tag{6}$$

$$0\leq u_i(0)\leq 100\,\forall i=1,n_u, \tag{7}$$

$$0\leq x_i\,\forall i=1,n, \tag{8}$$

where **g** is a nonlinear vector function specified below. Equations (7) and (8) represent specified bounds on the manipulated and state variables. The choice of $t=0$ as the steady-state point eliminates measurement noise, as discussed previously. All disturbances were turned "off", except for the case described in Section 3.8.

A brief experience with the code showed that the last 12 states represent the *actual* settings of the n_u final control elements. A change in **u** causes these states to vary at a certain rate. At steady state, however:

$$x_{38+i}(0)=u_i(0)\,\forall i=1,12. \tag{9}$$

Thus, **u** can be eliminated from equations (4–7) and the problem reduces to the determination of the optimal steady-state values of the 50 state variables. Also, only the first 38 elements of **f** in equation (5) need to be considered, as the remaining 12 are satisfied automatically by the choice of u_i in equation (9).

The elements of $\mathbf{g}(\mathbf{x},0)$ were as follows:

$$g_1=1-\frac{y_{12}}{50}=0, \tag{10}$$

$$g_2=1-\frac{y_{15}}{50}=0, \tag{11}$$

$$g_3=1-\frac{2.8153x_{46}y_{40}}{p_G}=0, \tag{12}$$

$$g_4=1-\frac{3.4510x_{46}y_{41}}{p_H}=0, \tag{13}$$

$$g_5=\frac{y_7}{P_{max}}-1\leq 0, \tag{14}$$

$$g_6=1-\frac{y_8}{L_{min}}\leq 0. \tag{15}$$

Equations (10) and (11) specify target values for the liquid levels in the product separator and stripper, respectively. These have no effect on the operating cost, and were arbitrarily chosen to be half-full (as in the base case provided by TEC). Equations (12) and (13) specify targets for production of chemicals G and H, respectively. The constant p_G is the desired rate of G(kg/h), and p_H is the desired rate of H (kg/h).

In equation (14), P_{max} is the maximum allowed reactor pressure. As shown in Section 3.1, optimal operation maximizes the reactor pressure, so the choice of P_{max} affects profitability. This pressure has a high alarm at 2895 kPa, and a shutdown limit at 3000 kPa. Since the process is subject to disturbances, however, one must keep a safe distance from the shutdown limit. The effect of various safety margins in P_{max} were thus investigated (see Section 3.1).

Similarly, L_{min} is the minimum liquid level in the reactor [equation (15)]. Optimal operation also activates this constraint. The low alarm is at 50% full, and the shutdown limit is at 8.5%. The effect of varying safety margins in L_{min} were also evaluated (Section 3.2). Downs and Vogel provide additional inequality constraints that could be included in the above formulation. It was determined that these have no influence on optimal steady-state operation, however, so they are not considered here.

The *maximum production* problem is to maximize the steady-state production of G and H while maintaining a specified G/H ratio in the product. One could re-formulate the above problem to handle this case by replacing equation (3) with $c = -x_{46}y_{41}$, replacing equation (11) with a specification on the G/H product ratio, and eliminating equation (12). This was tested, but convergence was unreliable. The following two-step approach was used instead:

Table 2. Measured output variables (y) for the base case (from Downs and Vogel, 1993), and corresponding optimal steady-state values for six operating modes. Values in italics are either upper bounds, lower bounds, or specified values (equality constraints)

	Measurements	Base case	Mode 1 (50/50)	Mode 2 (10/90)	Mode 3 (90/10)	Mode 4 (50/50)	Mode 5 (10/90)	Mode 6 (90/10)
1	A Feed, kscmh	0.251	0.267	0.309	0.194	0.503	0.325	0.219
2	D Feed, kg/h	3664	3657	734	5179	5811	761	5811
3	E Feed, kg/h	4509	4440	8038	700	7244	8354	788
4	A + C Feed, kscmh	9.35	9.24	8.55	7.83	14.73	8.87	8.79
5	Recycle flow, kscmh	26.90	32.18	31.69	19.67	29.22	31.27	20.08
6	Reactor feed, kscmh	42.34	47.36	46.08	32.09	53.76	46.24	34.02
7	Reactor pressure, kPa	2705	*2800*	*2800*	*2800*	*2800*	*2800*	*2800*
8	Reactor level, %	75	*65.0*	*65.0*	*65.0*	*65.0*	*65.0*	*65.0*
9	Reactor temperature, °C	120.4	122.9	124.2	121.9	128.2	124.6	123.0
10	Purge rate, kscmh	0.337	0.211	0.361	0.087	0.462	0.384	0.099
11	Sep temperature, °C	80.1	91.7	90.3	83.4	74.1	88.9	80.9
12	Sep level, %	50	*50.0*	*50.0*	*50.0*	*50.0*	*50.0*	*50.0*
13	Sep pressure, kPa	2634	2706	2705	2765	2699	2705	2761
14	Sep underflow, m³/h	25.16	25.28	26.31	17.55	40.06	27.45	19.60
15	Stripper level, %	50	*50.0*	*50.0*	*50.0*	*50.0*	*50.0*	*50.0*
16	Stripper pressure, kPa	3102	3326	3327	2996	3365	3330	3015
17	Stripper underfow, m³/h	22.95	22.89	22.73	18.04	36.04	23.55	20.20
18	Stripper temperature, °C	65.73	66.5	65.4	62.3	51.5	63.9	60.5
19	Steam flow, kg/h	230	4.74	4.90	5.34	6.87	5.11	5.59
20	Compressor work, kW	341	278.9	274.7	272.6	263.2	271.7	293.2
21	React. cool temperature, °C	94.6	102.4	108.6	101.9	96.6	108.5	100.6
22	Cond. cool. temperature, °C	77.3	92.0	91.6	45.0	73.5	89.8	45.7
23	Feed %A, mol%	32.19	32.21	34.82	29.46	36.40	34.78	29.99
24	%B, mol%	8.89	14.93	8.18	27.74	8.78	7.85	26.34
25	%C, mol%	26.38	18.75	19.43	17.97	22.36	19.54	18.80
26	%D, mol%	6.88	6.03	1.20	12.68	7.95	1.24	13.23
27	%E, mol%	18.78	16.71	25.47	3.86	17.01	26.03	3.91
28	%F, mol%	1.66	4.04	5.60	1.29	3.88	5.60	1.33
29	Purge %A, mol%	32.96	32.73	36.63	27.86	40.94	36.71	28.61
30	%B, mol%	13.82	21.83	11.77	45.07	15.90	11.47	44.41
31	%C, mol%	23.98	13,11	14.63	9.22	15.68	14.57	9.76
32	%D, mol%	1.26	0.90	0.13	2.18	0.68	0.13	2.09
33	%E, mol%	18.58	16.19	22.37	3.94	15.41	22.92	4.00
34	%F, mol%	2.26	5.39	7.37	1.82	5.72	7.44	1.91
35	%G, mol%	4.84	6.62	1.32	9.40	3.85	1.26	8.76
36	%H, mol%	2.30	3.23	5.79	0.50	1.82	5.51	0.46
37	Product %D, mol%	0.02	0.01	0.00	0.03	0.02	0.00	0.03
38	%E, mol%	0.84	0.58	0.92	0.16	1.21	1.01	0.18
39	%F, mol%	0.10	0.19	0.29	0.07	0.04	0.32	0.08
40	%G, mol%	53.72	53.83	11.66	90.09	53.35	11.65	90.07
41	%H, mol%	43.83	43.91	85.64	8.17	43.52	85.53	8.16

1. Using the minimum cost formulation given above, the production rates (p_G and p_H) were increased in a series of runs until a reactant feed was nearly at a constraint. For all cases studied, either the D feed (stream 2) or the E feed (stream 3) was the limiting reactant.
2. The minimum-cost problem was modified to constrain this limiting reactant at 100% utilization. Solution of this modified problem is essentially the same as the true maximum production solution; once the limiting reactant is constrained, minimization of operating costs promotes maximum (and economical) production of G and H.

2.1. Solution method

MINOS 5.1 (Murtagh and Saunders, 1987) was combined wth the TEC code to solve the nonlinear programming problem (NLP) posed in Section 2. MINOS uses a projected augmented Lagrangian strategy that allows the constraints to be violated as it searches for the optimum. It penalizes constraint violations in the objective function as an aid to convergence. In most cases, the default MINOS penalty strategy was used.† MINOS also evaluated all gradients numerically, assuming a dense Jacobian. Double-precision floating-point operations were used throughout. At the solution, the maximum constraint violation was typically less than 10^{-10}. The minimum cost was influenced by numerical errors; the reported values estimated to be within ±1% of the true value in all cases.

Similar applications are discussed in standard texts (e.g. Edgar and Himmelblau, 1988). Bailey *et al.* (1993) give a recent example, which is a fractionation process described by 2891 variables with 10 df (solved using MINOS). On the surface, this might appear to be much more challenging than the TEC process, which has 50 variables, 42 nonlinear equality constraints, 2 nonlinear inequality constraints, and $50-42=8$ degrees of freedom. The number of implicit equations and variables used to develop the TEC code is unknown, but is probably of the order of hundreds. On the other hand, the fractionation system of Bailey *et al.* contains no recycle. The resulting optimization problem is relatively sparse, and interaction between the design variables is limited to the downstream direction. Thus, while each iteration of the problem of Bailey *et al.* was time-consuming, their discussion indicates that convergence was more reliable than in the present work.

† Increasing the penalty weight by a factor of 10 sometimes improved convergence of difficult cases.

The choice of a reasonable initial estimate of **x** was essential for the TEC application. The problem was first solved with **x** initialized to the base case values given by Downs and Vogel (1993). Additional problems were solved in a progression that allowed the solution of one to act as the starting point for the next. Other starting points were used occasionally to check for the existence of a local minimum, which did occur in several instances (see Section 3.3). It is believed that the results given here are correct, but there is no practical way to guarantee global optimality for a NLP of this complexity.

The TEC code imposes hard limits on the manipulated variables as defined in equation (7). This can cause numerical problems if MINOS tries to evaluate the constraints (or their gradients) for values of **x** slightly outside the bounds. When this happened, bounds on the variable(s) in question were arbitrarily set at 1 and 99 (rather than 0 and 100).

The states were scaled so that the first 38 were unity at the starting condition. The remaining 12 were divided by 100, so their allowed range was the interval 0 to 1. The function values in equation (5) (the time derivatives) were scaled such that they were 10^{-6} at the base case provided by Downs and Vogel.

Most solutions required less than 10 min on a Macintosh IIfx, and often took less than 2 min. Convergence was fairly reliable, but there were cases that differed only slightly from a previous case (used as the starting point), yet the algorithm diverged. Those approaching the maximum production rate were especially prone to this behavior, as might be expected—such problems are "nearly infeasible". It is possible that a more clever definition of the problem—or better scaling of the states and function values—would improve convergence in these cases. Another likely cause of difficulties is the occasional need to make radical changes in operating strategy in order to reduce costs by a small amount. This is illustrated in Section 3.3.

3. RESULTS AND DISCUSSION

Tables 2–4 summarize the optimal conditions for the six operating modes. The Downs and Vogel base case is included for perspective. Tables 2 and 3 contain the measured outputs **y** and the manipulated variables **u**. Italicized values are specified upper or lower bounds, or variables fixed by equality constraints. Table 4 gives the operating costs broken down by major categories. Optimal values of the states **x** are available in electronic form (see Conclusions).

Table 3. Manipulated variables (**u**) for the base case (from Downs and Vogel, 1993) and corresponding optimal steady-state values for six operating modes. Values in italics are either lower or upper bounds

	Man. vars. (u_i)	Base case	Mode 1 (50/50)	Mode 2 (10/90)	Mode 3 (90/10)	Mode 4 (50/50)	Mode 5 (10/90)	Mode 6 (90/10)
1	D Feed, %	63.053	62.935	12.637	89.130	*100.00*	13.098	*100.000*
2	E Feed, %	53.980	53.147	96.216	8.381	86.715	*100.000*	9.438
3	A Feed, %	24.644	26.248	30.412	19.114	49.477	32.009	21.543
4	A+C Feed, %	61.302	60.566	56.092	51.368	96.595	58.155	57.640
5	Recycle valve, %	22.210	*1.000*	*1.000*	77.621	*1.000*	*1.000*	71.166
6	Purge valve, %	40.064	25.770	44.347	9.501	48.742	47.095	10.654
7	Separator valve, %	38.100	37.266	35.799	29.146	60.960	37.422	32.685
8	Stripper valve, %	46.534	46.444	42.865	39.425	74.522	44.491	44.251
9	Steam valve, %	47.446	*1.000*	*1.000*	*1.0000*	*1.000*	*1.000*	*1.000*
10	Reactor coolant, %	41.106	35.992	25.257	35.550	60.794	26.070	40.538
11	Condenser coolant, %	18.113	12.431	12.907	99.000	35.534	14.115	99.000
12	Agitator speed, %	50.000	*100.000*	*100.000*	*100.000*	*100.000*	*100.000*	*100.000*

3.1. *Effect of reactor pressure*

The optimal reactor pressure y_7 is always at an upper bound. To obtain the results given in Tables 2–4, the maximum pressure was set at 2800 kPa—judged to be safely below the high-alarm limit of 2895 kPa. For control-system design, one would like to know the potential benefits of operating closer to the high-alarm. Therefore, the sensitivity of operating cost to reactor pressure was determined by calculation of the minimum cost for three specified reactor pressures. For each pressure, the product composition and rate, and the reactor liquid level were held at the base-case values given by Downs and Vogel. Table 5 summarizes the results.

An increase in the pressure has two important beneficial effects:

1. The partial pressure of the inerts can increase without depressing the reactant partial pressures (which would tend to decrease the production rate). The increase in inerts concentration reduces the purge rate. As shown in Table 5, the concentration of B in the purge is at least a factor of 1.45 higher under optimal operation, and for the three optimal solutions, the purge rate decreases steadily with increasing pressure. This has a large impact on cost.
2. One can also decrease the reactor temperature, which improves the selectivity for G and H. Table 5 shows that the production of F decreases with decreasing temperature. In fact, the base case, which has the minimum reactor temperature in Table 5, makes about half as much as F as the maximum temperature. The optimal strategies operate at higher temperatures in order to cut the purge rate, even though selectivity suffers.

Increasing reactor pressure increases compression costs, all other things being equal, but this is a small effect. Overall, Table 5 shows that if the variables are otherwise optimal, increasing the pressure by 100 kPa (at constant liquid level) reduces costs by about 10%—a significant saving.

3.2. *Effect of reactor liquid level*

The optimal reactor liquid level is also at its lower bound. The gas residence time is inversely proportional to the liquid level, so a decrease in reactor level is similar to an increase in pressure, i.e. it allows one to achieve the same production at a higher inerts concentration (lower purge rate) and/or a lower reactor temperature (better selectivity). The results in Tables 2–4 are for a *specified* minimum reactor level of 65%—judged to be safely above the lower alarm at 50%.

Table 5 shows the effect of variations in level (with pressure held constant at 2800 kPa, and production of G and H as in the base case). For example, at a constant pressure of 2800 kPa, a reduction in level from 75 to 65% allows one to operate at a lower reactor temperature *and* a slightly higher concentration of B in the purge, and the operating cost decreases by about 8%.

Table 4. Operating costs for the base case (from Downs and Vogel, 1993) and for optimal operation in the six modes listed in Table 1

Cost items	Base case	Mode 1 (50/50)	Mode 2 (10/90)	Mode 3 (90/10)	Mode 4 (50/50)	Mode 5 (10/90)	Mode 6 (90/10)
Purge losses, \$/h	114.71	73.75	130.03	138.49	142.29	138.49	23.91
Product losses, \$/h	30.28	25.46	36.18	41.38	87.29	41.38	9.43
Compressor, \$/h	18.30	14.95	14.72	14.61	14.11	14.56	15.72
Steam, \$h	7.32	0.15	0.16	0.17	0.22	0.16	0.18
Total cost, \$/h	170.61	114.31	181.09	43.93	243.92	194.59	49.23
Per unit product, ¢/kg	1.21	0.81	1.29	0.40	1.09	1.33	0.39

Table 5. Effect of reactor pressure and liquid level on key process variables. Production rates of G and H are as for the base case. Steam costs are negligible for optimal operation (steam valve is closed). The steam cost for the base case is $7.32/h

	Base case	Optimal operation Constant reactor level			Optimal operation Constant reactor pressure		
Reactor pressure, kPa	2705	*2750*	*2800*	*2895*	*2800*	*2800*	*2800*
Reactor level, %	75	*75*	*75*	*75*	*60*	*65*	*70*
Reactor temperature, °C	120.4	126.0	125.7	125.2	122.8	123.1	123.3
Separator pressure, kPa	2634	2704	2752	2843	2706	2706	2706
Separator temperature, °C	80.1	76.7	77.3	78.3	91.7	92.1	92.4
Stripper pressure, kPa	3102	3004	3066	3184	3326	3326	3326
Stripper temperature, °C	65.7	54.8	55.4	56.4	66.7	66.9	67.1
Recycle valve, %	22.21	59.28	56.17	50.38	*1.0*	*1.0*	*1.0*
Purge rate, kscmh	0.337	0.234	0.224	0.207	0.206	0.212	0.219
Purge %B, mol%	13.82	19.96	20.86	22.49	22.37	21.72	21.04
Product %E, mol%	0.84	0.86	0.82	0.75	0.55	0.56	0.57
F production, kmol/h	0.6	1.3	1.2	1.1	0.9	0.9	1.0
Purge losses, $/h	114.71	69.61	65.63	59.27	71.30	74.34	77.74
Product losses, $/h	30.28	40.11	38.33	35.37	24.51	24.93	25.36
Compression, $/h	18.30	17.77	18.09	18.67	15.02	14.96	14.91
Total cost, $/h	170.61	127.69	122.25	113.51	110.98	114.37	118.15

As for the pressure, the appropriate safety margin for the reactor level depends on the ability of the control system to reject disturbances. The reactor must normally operate above the lower alarm limit of 50%. The main danger is loss of heat-transfer surface for cooling, which becomes increasingly serious as the level drops below 50%. Once the level goes below 10%, the cooling rate goes to zero, which normally leads to a process shutdown.

3.3. *Discontinuity in operating strategy*

There is an interesting change in operating strategy as one goes from 75 to 70% at 2800 kPa. As shown in Table 5, the compressor recycle valve jumps from 56 to 1% (the specified lower limit). There is a corresponding *increase* of nearly 300 kPa in the stripper pressure, and a 50 kPa *decrease* in the product separator pressure. Simultaneously, the separator temperature increases by 15 °C (the condenser coolant valve goes from 48% open to 12%—not shown). The concentration of E in the product decreases from 0.82 to 0.57% (because less is condensed in the product separator). This, combined with improved selectivity (because of a lower reactor temperature) cuts product losses by $13/h. Compression costs also drop by $3/h. On the other side of the ledger, the purge losses increase by $12/h (even though the purge rate is lower) because the new separator conditions increase the mole fractions of valuable G and H in the purge. The net effect of these competing factors is a savings of $4/h.

These two very different operating strategies have essentially equal costs between 70 and 75% (at 2800 kPa). For example, at 70%, we can operate in a manner similar to the 75% strategy in Table 5, and the cost is $118.49 (compared to $118.15 for optimal operation). The insensitivity of the objective function to large changes in the states may be a cause of convergence problems. It was observed, for example that MINOS could converge to the wrong solution (depending on the starting point).

3.4. *Effect of production composition*

For the six standard operating modes, the stoichiometry of the two main reactions dictates the optimal reactant feed rates. Regardless of product composition, the combined feed must be about 50% A + C and 50% D + E on a molar basis (actually $49.5 \pm 0.2\%$ D + E for the six modes in Tables 2–4). Similarly, of the total A + C fed, about half must be A ($50.0 \pm 0.3\%$). Figure 2 shows that the optimal feed rates of D and E correlate very well with the desired product compositions. This is also reflected in the composition of the reactor feed and purge streams (Table 2). Note, however, that certain disturbances can change the picture. An important one is the loss of the A feed (see Section 3.8).

Production of G is relatively inexpensive. D reacts rapidly, and is always dilute in the purge gas, even when the product is 90% G. One can exploit this by increasing the inerts partial pressure. For the optimal 90/10 cases, there is more than 45 mol% B in the purge, so the purge rate is only 1/3 that of the base case (Table 2). Also, the relatively low concentration of E in the system reduces product losses.

3.5. *Effect of compressor recycle valve*

Another distinction of modes 3 and 6 is that the compressor recycle valve is about 70% open (it is closed for the other modes—see Table 3). This increases the pressure in the separator, as explained in the previous section. Also, the condenser coolant valve is wide open. Both actions promote condensation to reduce the losses of D and G to the purge.

It is possible to operate with the compressor recycle valve closed, as in the other modes, but

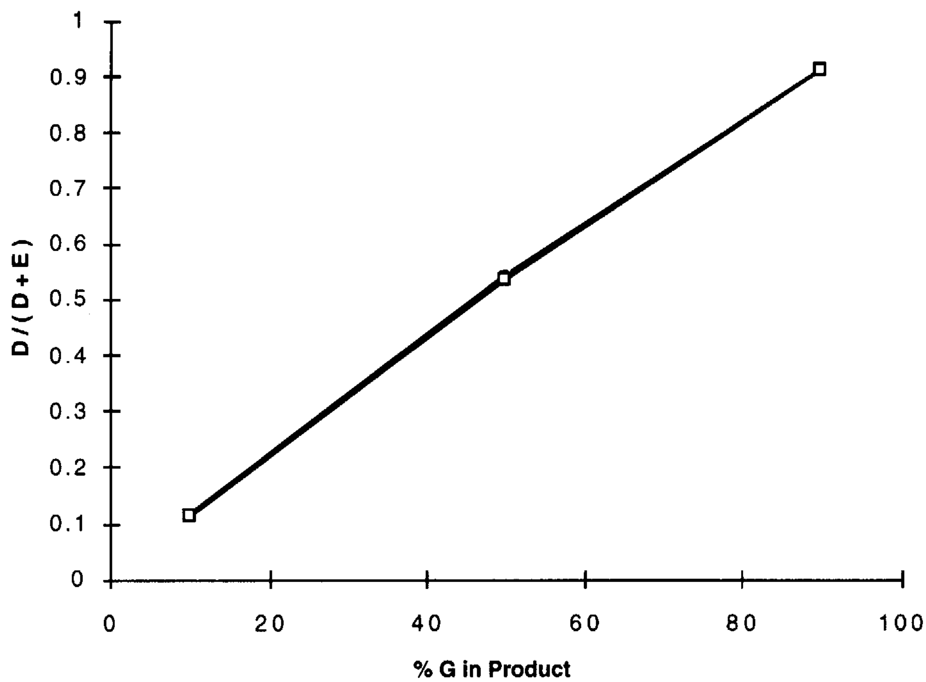

Fig. 2. Correlation of product composition with relative molar amounts of D and E fed. There are actually 2 lines in this figure, one for normal production and one for maximum production. They overlap almost perfectly.

there is a cost penalty of more than 10%. Table 6 shows how the key variables from Tables 2–4 would change if the valve were closed for modes 3 and 6. The recycle flow increases by about 50%. Consequently, the condenser must operate at a higher temperature (97.1 °C, an increase of about 16 °C)†. The high separator temperature increases the loss of G to the purge significantly, and is the main reason for the \$8.2/h increase in purge costs. On the positive side, the reactor temperature is slightly lower, improving selectivity. Also, product losses and compression costs decrease by about \$1/h each.

3.6. *Effect of production rate*

The constraints on flows of reactants D and E determine the maximum production rate for all cases considered here. Table 3 shows that when the desired product ratio is G:H = 1:9, E is limiting. Otherwise, D is limiting. Other manipulated variables may also be at their bounds (e.g. the compressor recycle valve in modes 4 and 5), but these do not limit production.

For the 50:50 product composition, one can react all the available D and about 87% of the E. Since the base case uses only about 63 and 53% respectively, there is considerable flexibility in the production rate. The maximum (mode 4) is about 59% above the base (mode 1). On the other hand, when the desired product is 1:9 (G:H), we can only increase production by about 4% (relative to mode 2), and when it is 9:1, we are limited to a 12% increase (relative to mode 3).

The sustained disturbances described by Downs and Vogel (1993) should have little impact on the maximum production rates, except for mode 4. In that case, about 97% of the available A + C is being used. Thus, a decrease in the percentage of C in stream 4 could cause C to become the limiting reactant. Similarly, either a loss of the auxiliary A feed (stream 1), or a large decrease in the percentage of A in stream 4 could cause A to be limiting.

3.7. *Agitation speed and steam consumption*

Downs and Vogel (1993) note that the agitation rate (u_{12}) affects the heat transfer coefficient for reactor cooling only. From the steady-state point of view, the choice of the agitation rate is arbitrary as long as the coolant flow (u_{10}) is unconstrained. Thus, a value of $u_{12} = 100\%$ was used for all cases presented here. This provides the maximum operating range.

Table 3 shows that optimal steady-state operation uses *no* steam in the stripper, relying instead on stream 4 to recover reactants D and E from the

† The increase in temperature brings the rate of condensation in the partial condenser back into balance with the rate of liquid production in the reactor.

Table 6. Comparison of two strategies for production of 90% G, 10% H (by mass). Italicized variables are either specified, or at an upper or lower bound

	Minimum cost	Sub optimal
Manipulated variables		
D Feed, %	*100.000*	*100.000*
E Feed, %	9.438	9.445
A Feed, %	21.543	20.800
A+C feed, %	57.640	57.611
Recycle valve, %	71.166	*1.000*
Purge valve, %	10.654	12.623
Separator valve, %	32.685	33.480
Stripper valve, %	44.251	44.171
Steam valve, %	*1.000*	*1.000*
Reactor coolant, %	40.538	41.340
Condenser coolant, %	*99.000*	9.516
Agitator speed, %	*100.000*	*100.000*
Measured variables		
Reactor pressure, kPa	*2800*	*2800*
Reactor level, %	*65.0*	*65.0*
Reactor temperature, °C	123.0	121.9
Recycle flow, kscmh	20.08	32.11
Reactor feed, kscmh	34.02	46.17
Purge, rate, kscmh	0.099	0.098
Separator temperature, °C	80.9	97.1
Separator pressure, kPa	2761	2707
Separator underflow, m^3/h	19.60	20.87
Stripper pressure, kPa	3015	3316
Stripper underflow, m^3/h	20.20	20.45
Stripper temperature, °C	60.5	71.3
Purge %A, mol%	28.61	20.50
%B, mol%	44.41	44.83
%C, mol%	9.76	8.72
%D, mol%	2.09	3.13
%E, mol%	4.00	5.95
%F, mol%	1.91	2.46
%G, mol%	8.76	13.66
%H, mol%	0.46	0.74
Product %E, mol%	0.18	0.16
%F, mol%	0.08	0.06
Costs		
Purge losses, $/h	23.91	32.13
Product losses, $/h	9.43	8.00
Compression, $/h	15.72	14.82
Total, $/h	49.23	55.07
Per unit production ¢/kg	0.39	0.44

Table 7. Comparison of two strategies for production of 50% G, 50% H (by mass) when the auxiliary A feed (stream 1) is lost. Italicized variables are either specified, or at an upper or lower bound

	P = 2815	P = 2895
Manipulated variables		
D Feed, %	63.489	63.383
E Feed, %	56.142	55.444
A Feed, %	*0.000*	*0.000*
A+C Feed, %	65.510	65.398
Recycle valve, %	41.050	44.398
Purge valve, %	*100.000*	91.902
Separator valve, %	37.421	36.943
Stripper valve, %	46.675	46.628
Steam valve, %	*1.000*	*1.000*
Reactor coolant, %	34.398	34.073
Condenser coolant, %	*99.000*	*99.000*
Agitator speed, %	*1000.000*	*100.000*
Measured variables		
Reactor pressure, kPa	*2815*	*2895*
Reactor level, %	*60.0*	*60.0*
Reactor temperature, °C	126.8	127.4
Recycle flow, kscmh	19.88	19.96
Reactor feed, kscmh	35.70	35.66
Purge rate, kscmh	0.762	0.725
Separator temperature, °C	77.1	76.0
Separator pressure, kPa	2761	2707
Separator underflow, m^3/h	2757	2839
Stripper pressure, kPa	24.53	24.11
Stripper underflow m^3/h	22.93	22.89
Stripper temperature, °C	54.5	54.2
Purge %A, mol%	17.86	18.14
%B, mol%	6.53	6.85
%C, mol%	50.04	52.01
%D, mol%	0.77	0.64
%E, mol%	16.31	14.03
%F, mol%	2.20	2.34
%G, mol%	4.26	4.06
%H, mol%	2.03	1.92
Product %E, mol%	1.01	0.90
%F, mol%	0.13	0.14
Costs		
Purge losses, $/h	279.23	256.29
Product losses, $/h	36.69	33.72
Compression, $/h	15.69	15.65
Total, $/h	331.82	305.86
Per unit production, ¢/kg	2.36	2.17

product. Experience with the dynamic simulation suggests that the concentration of D and E in the product is never large enough to have a significant impact on product purity (Downs and Vogel stipulate a tolerance of ±5 mol% G). Use of steam may be justified during transients to minimize product losses, however.

3.8. *Sustained loss of auxiliary A feed*

Of the 20 disturbances listed by Downs and Vogel (1993), 6 is the most difficult to handle. The auxiliary A feed (stream 1) goes to zero. This throws the A and C reactants out of balance. To maintain the desired production rate, the rate of stream 4 must increase (to provide the required A) and the purge rate must increase (to get rid of the excess C introduced with stream 4).

Table 7 compares two modes of optimal operation under these conditions. The first column corresponds to $P_{max} = 2815$ kPa, and the second to $P_{max} =$ 2895 (the shutdown limit). In both cases, the minimum liquid level in the reactor was set at 60%. The optimal condenser coolant setting was at its upper bound.

The specified production rate is infeasible at reac tor pressures below 2815 kPa (given all the other constraints on the process). The limiting factor is the mol fraction of C in the purge. The lower the C concentration, the higher the required purge rate. The purge valve must be wide open at a reactor pressure of 2815 kPa (Table 7), where the C concentration in the purge is 50.04 mol%. A further increase in the C concentration is prevented by the need to maintain production. The main reactions are relatively sensitive to the partial pressures of A, D and E. At 2815 kPa, a further increase in C would force a decrease in the production rate. Increasing the pressure to 2895 kPa (the high alarm limit) allows a higher C mole fraction, and the constraint on the purge is no longer limiting.

In both cases, the cost is roughly three times that of the optimal base case (mode 1). The main reason is the huge increase in the purge losses.

4. CONCLUSIONS—IMPLICATIONS FOR CONTROL SYSTEM DESIGN

The optimal steady-state conditions for the Tennessee Eastman Challenge Process provide important insights related to control-system design.† These are summarized as follows:

1. Reactor pressure and liquid level are critical operating variables. Optimal operation calls for the *maximum* feasible reactor pressure and the *minimum* feasible liquid level. The control strategy should be flexible enough to maintain these values, regardless of the constraints. One possibility is to adjust reactor temperature to control pressure, and adjust either recycle rate or condenser cooling rate to control level. This avoids the use of reactant flows, which are often constrained.
2. Most of the process variables are strong functions of the desired product rate and composition. For example, the optimal concentration of E in the reactor feed (and the purge) changes by a factor of 7 (Table 2). An attempt to hold this variable at an arbitrary, constant setpoint will limit productivity and/or increase costs. The same can be said of most other temperatures, pressures, and compositions in the process. Thus, the variables to be controlled must be carefully chosen; arbitrary use of feedback control loops should be avoided.
3. Purge losses dominate the operating costs. There is a large economic incentive to maximize the percentage of inerts in the purge, thereby reducing the losses of the other chemicals.
4. Per unit of production, operating costs triple as the production of H varies from 10% to 90% by mass (Table 4).
5. Optimal steady-state sets the steam flow in the stripper to zero for all cases studied. There may be transients that require steam to minimize losses of D and E to the product, but that has yet to be demonstrated.
6. The agitator speed and reactor coolant rate are interdependent. One can set the agitator speed at its upper bound, which maximizes the range of cooling duties the process can handle.
7. The maximum production rate is limited by a reactant flowrate in all cases. For the 10/90 product composition, the limiting reactant is E. Otherwise it is D. For the 50/50 product composition, production can be increased by a factor of 1.59. The 10/90 and 90/10 cases are more restrictive (factors of 1.04 and 1.12, respectively). A general-purpose control strategy must be able to regulate product composition when either D or E is at its upper bound.

† McAvoy and Ye (1994) have recently published a control strategy consisting of conventional feedback loops and overrides. Ricker and Lee (1995) review other work on control system design, and demonstrate the use of nonlinear model predictive control.

It is emphasized that these results were obtained using information that would not be available in an industrial setting—the full state vector of the plant, and noise-free measurements. Thus, the results should be regarded as a *benchmark* for more realistic studies of on-line optimization. Moreover, direct use of the numerical results (e.g. as setpoints) in a "solution" of the challenge problem might be criticized, since such information would not be available in practice. On the other hand, many of the more qualitative conclusions, such as points 1, 2, 3 and 6 above, could have been reached through a careful analysis of the process, i.e. without doing a numerical optimization, and are therefore "fair game" for exploitation.

Despite the ideal conditions exploited here and the availability of a well-developed optimization method (MINOS), the problem was difficult to solve in some cases. A more robust approach would be needed for on-line use, and is the subject of current research.

Those wishing to use the steady-state conditions of Tables 2–4 as the starting point for simulations may obtain the state vectors and manipulated variables for each mode. This information is available in electronic form as an ASCII tab-delimited text file. Send requests by e-mail to RICKER@CHEME.WASHINGTON.EDU.

Acknowledgement—I am grateful to J. Downs and E. Vogel of the Tennessee Eastman Company for taking the trouble to develop this challenge problem. They have provided an important service to the control research community.

REFERENCES

Bailey J. K., A. N. Hrymak, S. S. Treiber and R. B. Hawkins, Nonlinear optimization of a hydrocracker fractionation plant, *Computers chem. Engng* **17**, 123–138 (1993).

Downs J. J. and E. F. Vogel, A plant-wide industrial process control problem. *Computers chem. Engng* **17**, 245–255 (1993).

Edgar T. E. and D. M. Himmelblau, *Optimization of Chemical Processes*, Chap. 8. McGraw-Hill, New York (1988).

McAvoy T. J. and N. Ye, Base control for the Tennessee Eastman problem. *Computers chem. Engng* **18**, 383–413 (1994).

Murtagh B. A. and M. Saunders, *MINOS 5.1 User's Guide*. Technical Report SOL 83-20R, Stanford University (1987).

Ricker N. L. and J. H. Lee, Nonlinear model predictive control of the Tennessee Eastman challenge process. *Computers chem. Engng* **19**, 961–981 (1995).