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A PLANT-WIDE INDUSTRIAL PROCESS CONTROL PROBLEM

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Abstract—This paper describes a model of an industrial chemical process for the purpose of developing, studying and evaluating process control technology. This process is well suited for a wide variety of studies including both plant-wide control and multivariable control problems. It consists of a reactor/separator/recycle arrangement involving two simultaneous gas–liquid exothermic reactions of the following form:

$$A(g) + C(g) + D(g) \rightarrow G(liq), \quad \text{Product 1,}$$
$$A(g) + C(g) + E(g) \rightarrow H(liq), \quad \text{Product 2.}$$

Two additional byproduct reactions also occur. The process has 12 valves available for manipulation and 41 measurements available for monitoring or control.

The process equipment, operating objectives, process control objectives and process disturbances are described. A set of FORTRAN subroutines which simulate the process are available upon request.

INTRODUCTION

For several years we have heard the chemical engineering process control academic community express interest in having a realistic problem for testing process control technology. We first heard the topic discussed at the second Engineering Foundation Conference on Chemical Process Control meeting in 1981 (Denn, 1982). The topic was also discussed at the first Engineering Foundation Conference on Chemical Process Control meeting in 1976 (Foss and Denn, 1976). Shell presented a test problem at their process control workshop (Prett and Morari, 1986) and Ed Bristol discussed the characteristics of a test problem in a recent paper (Bristol, 1987). Most recently, AIChE initiated a session on the topic of industrial-based test problems in which this problem first appeared (Downs and Vogel, 1990).

As the corporate process control group for Eastman Chemical Company, we see a wide variety of chemical processes. A few years ago we encountered a process which we believe is particularly well suited for use as a test problem. Although we have modified the components, kinetics, process and operating conditions to protect the proprietary nature of the process, this test problem is based on an actual industrial process (not a contrived problem). Bill Luyben of Lehigh University and Charlie Moore of The University of Tennessee looked at this problem and encouraged us to offer it for study. Both Bill and Charlie teach courses and guide research in the process control field.

We believe that this problem is well-suited for studying process control technology and that it is applicable to a wide variety of control issues. The process model has been coded into a set of FORTRAN subroutines which describe the nonlinear relationships in the unit operations and the material and energy balances.

This paper contains a description of the process, the process control objectives, suggestions for potential applications and details for using the model.

PROCESS DESCRIPTION

The process produces two products from four reactants. Also present are an inert and a byproduct making a total of eight components: A, B, C, D, E, F, G, and H. The reactions are:

$$A(g) + C(g) + D(g) \rightarrow G(liq), \quad \text{Product 1,}$$
$$A(g) + C(g) + E(g) \rightarrow H(liq), \quad \text{Product 2,}$$
$$A(g) + E(g) \rightarrow F(liq), \quad \text{Byproduct,}$$
$$3D(g) \rightarrow 2F(liq), \quad \text{Byproduct.}$$

All the reactions are irreversible and exothermic. The reaction rates are a function of temperature through an Arrhenius expression. The reaction to produce G has a higher activation energy resulting in more sensitivity to temperature. Also, the reactions are approximately first-order with respect to the reactant concentrations.

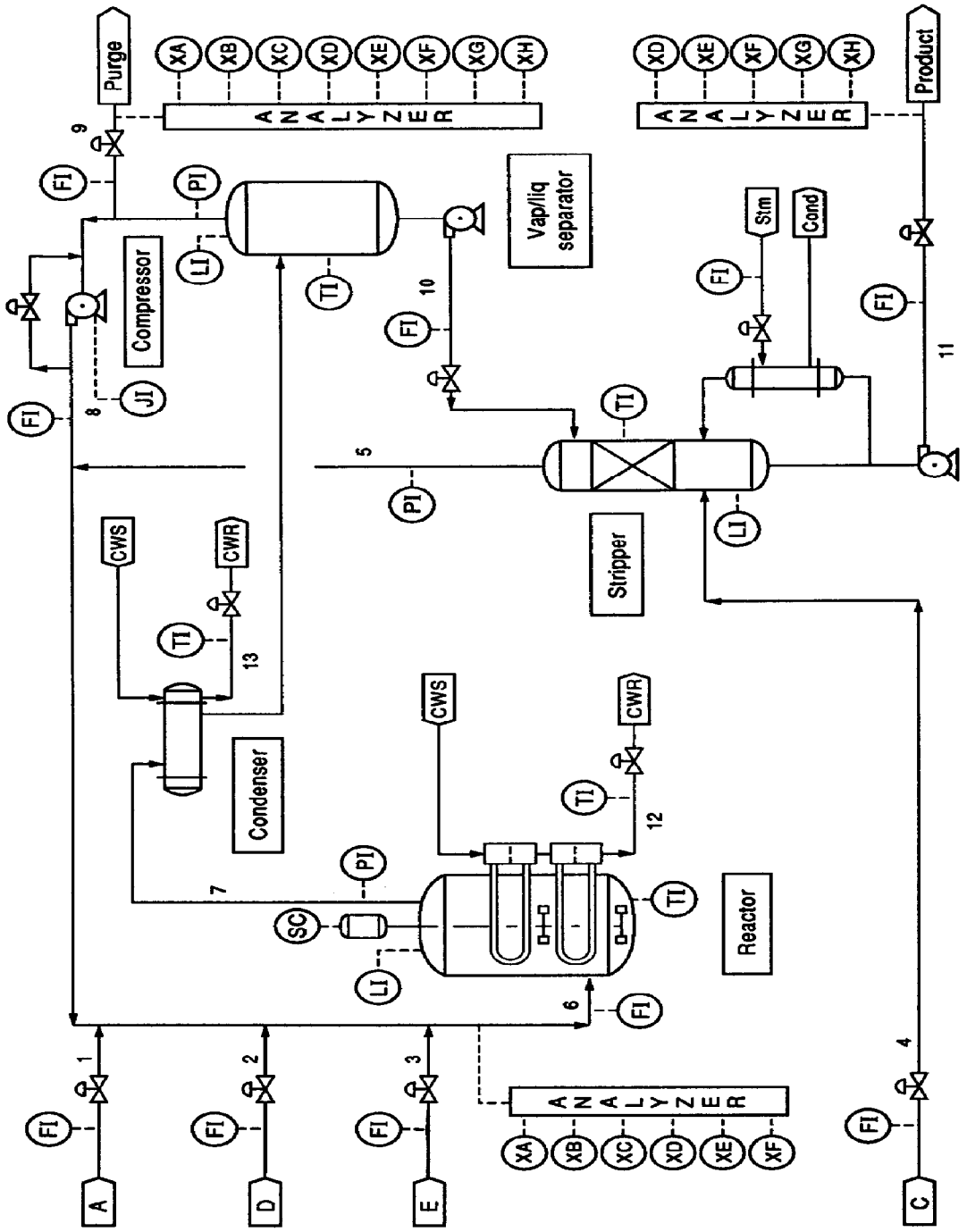

Fig. 1. Tennessee Eastman test problem.

The process has five major unit operations: the reactor, the product condenser, a vapor–liquid separator, a recycle compressor and a product stripper. Figure 1 shows a diagram of the process. Table 1 provides the base case steady-state heat and material balance data for the process and Table 2 lists the component physical properties.

The gaseous reactants are fed to the reactor where they react to form liquid products. The gas phase reactions are catalyzed by a nonvolatile catalyst dissolved in the liquid phase. The reactor has an internal cooling bundle for removing the heat of reaction. The products leave the reactor as vapors along with the unreacted feeds. The catalyst remains in the reactor.

The reactor product stream passes through a cooler for condensing the products and from there to a vapor–liquid separator. Noncondensed components recycle back through a centrifugal compressor to the reactor feed. Condensed components move to a product stripping column to remove remaining reactants by stripping with feed stream number 4. Products G and H exit the stripper base and are separated in a downstream refining section which is not included in this problem. The inert and byproduct are primarily purged from the system as a vapor from the vapor–liquid separator.

There are six modes of process operation at three different G/H mass ratios (stream 11):

Mode	G/H mass ratio	Production rate (stream 11)
1	50/50	7038 kg h^{-1} G and 7038 kg h^{-1} H (base case)
2	10/90	1408 kg h^{-1} G and 12,669 kg h^{-1} H
3	90/10	10,000 kg h^{-1} G and 1111 kg h^{-1} H
4	50/50	maximum production rate
5	10/90	maximum production rate
6	90/10	maximum production rate

Mode 1 is the base case. The product mix is normally dictated by product demands. The plant production rate is set by market demand or capacity limitations.

Table 1. Heat and material balance data (Mode 1, base case)

Process stream data							
Stream name		A feed	D feed	E feed	C feed	Strp Ovhd	Reactor feed
Stream number		1	2	3	4	5	6
Molar flow (kgmol h^{-1})		11.2	114.5	98.0	417.5	465.7	1890.8
Mass flow (kg h^{-1})		22.4	3664.0	4509.3	6419.4	8979.6	48015.4
Temperature (°C)		45.0	45.0	45.0	45.0	65.7	86.1
Mole fractions	A	0.99990	0.00000	0.00000	0.48500	0.43263	0.32188
	B	0.00010	0.00010	0.00000	0.00500	0.00444	0.08893
	C	0.00000	0.00000	0.00000	0.51000	0.45264	0.26383
	D	0.00000	0.99990	0.00000	0.00000	0.00116	0.06882
	E	0.00000	0.00000	0.99990	0.00000	0.07256	0.18776
	F	0.00000	0.00000	0.00010	0.00000	0.00885	0.01657
	G	0.00000	0.00000	0.00000	0.00000	0.01964	0.03561
	H	0.00000	0.00000	0.00000	0.00000	0.00808	0.01659
Stream name		Reactor product	Recycle	Purge	Separation liquid	Product	
Stream number		7	8	9	10	11	
Molar flow (kgmol h^{-1})		1476.0	1201.5	15.1	259.5	211.3	
Mass flow (kg h^{-1})		48,015.4	30,840.0	386.5	16,788.9	14,288.6	
Temperature (°C)		120.4	102.9	80.1	80.1	65.7	
Mole fractions	A	0.27164	0.32958	0.32958	0.00000	0.00479	
	B	0.11393	0.13823	0.13823	0.00000	0.00009	
	C	0.19763	0.23978	0.23978	0.00000	0.01008	
	D	0.01075	0.01257	0.01257	0.00222	0.00018	
	E	0.17722	0.18579	0.18579	0.13704	0.00836	
	F	0.02159	0.02263	0.02263	0.01669	0.00099	
	G	0.12302	0.04844	0.04844	0.47269	0.53724	
	H	0.08423	0.02299	0.02299	0.37136	0.43828	

Unit operation data	Reactor	Separator	Condenser	Stripper
Temperature (°C)	120.4	80.1	—	65.7
Pressure (kPa gauge)	2705.0	2633.7	—	3102.2
Heat duty (kW)	−6468.7	—	−2140.6	1430.0
Liquid volume (m^3)	16.55	4.88	—	4.43

Utilities	
Reactor cooling water flow (m^3 h^{-1})	93.37
Condenser cooling water flow (m^3 h^{-1})	49.37
Stripper stream flow (kg h^{-1})	230.31

Table 2. Component physical properties (at 100°C)

Component	Molecular weight	Liquid density ($kg\ m^{-3}$)	Liquid heat capacity ($kJ\ kg^{-1}\ °C^{-1}$)	Vapor heat capacity ($kJ\ kg^{-1}\ °C^{-1}$)	Heat of vaporization ($kJ\ kg^{-1}$)
A	2.0	—	—	14.6	—
B	25.4	—	—	2.04	—
C	28.0	—	—	1.05	—
D	32.0	299	7.66	1.85	202
E	46.0	365	4.17	1.87	372
F	48.0	328	4.45	2.02	372
G	62.0	612	2.55	0.712	523
H	76.0	617	2.45	0.628	486

Vapor pressure (Antoine equation):
$P = \exp[A + B/(T + C)]$
P = pressure (Pa)
T = temperature (°C)

Component	Constant A	Constant B	Constant C
D	20.81	−1444.0	259
E	21.24	−2114.0	266
F	21.24	−2144.0	266
G	21.32	−2748.0	233
H	22.10	−3318.0	250

Vapor pressure parameters are not listed for components A, B and C because they are effectively noncondensible.

CONTROL OBJECTIVES

The process has 41 measurements and 12 manipulated variables as listed in Tables 3–5. A prerequisite for most studies on this problem is a process control strategy for operating the plant. The control objectives for this process are typical for a chemical process:

1. Maintain process variables at desired values.
2. Keep process operating conditions within equipment constraints.
3. Minimize variability of product rate and product quality during disturbances (stream 11).
4. Minimize movement of valves which affect other processes (in this case the gas feeds as described below).
5. Recover quickly and smoothly from disturbances, production rate changes or product mix changes.

Process constraints

Table 6 lists the specific operational constraints that the control system should respect. These constraints are primarily for equipment protection. The high and low shutdown limits are part of the process interlock strategy and are used to shutdown the process in the event the process conditions get out of hand.

Product variability

The variability of the product stream is important with regard to the downstream distillation system which refines products G and H. Flowrate changes of stream 11 greater than ±5% with significant frequency content in the range 8–16 h^{-1} are particularly harmful. In addition, composition variability greater than ±5 mol% G with significant frequency content in the range 6–10 h^{-1} are equally harmful.

Table 3. Process manipulated variables

Variable name	Variable number	Base case value (%)	Low limit	High limit	Units
D feed flow (stream 2)	XMV (1)	63.053	0	5811	$kg\ h^{-1}$
E feed flow (stream 3)	XMV (2)	53.980	0	8354	$kg\ h^{-1}$
A feed flow (stream 1)	XMV (3)	24.644	0	1.017	kscmh
A and C feed flow (stream 4)	XMV (4)	61.302	0	15.25	kscmh
Compressor recycle valve	XMV (5)	22.210	0	100	%
Purge valve (stream 9)	XMV (6)	40.064	0	100	%
Separator pot liquid flow (stream 10)	XMV (7)	38.100	0	65.71	$m^3\ h^{-1}$
Stripper liquid product flow (stream 11)	XMV (8)	46.534	0	49.10	$m^3\ h^{-1}$
Stripper steam valve	XMV (9)	47.446	0	100	%
Reactor cooling water flow	XMV (10)	41.106	0	227.1	$m^3\ h^{-1}$
Condenser cooling water flow	XMV (11)	18.114	0	272.6	$m^3\ h^{-1}$
Agitator speed	XMV (12)	50.000	150	250	rpm

Each of the manipulated variables is specified by setting the corresponding XMV variable to a value between 0 and 100. The base case values are the initial values of the XMV variables. The ranges of all the XMV variables are 0–100. The low limits shown here are the actual process variable values which correspond to XMV (i) = 0.0. Likewise, the high limits shown here are the actual process variable values which correspond to XMV (i) = 100.0.

The user can manipulate the XMV variables outside the 0–100 limits. However, within the function evaluator (TEFUNC), the XMV vector is copied to another vector which has hard constraints of 0 and 100. Thus, if an XMV variable goes beyond the 0–100 limits, its effect is constrained to 0 or 100, but the XMV variable value is not changed.

Table 4. Continuous process measurements

Variable name	Variable number	Base case value	Units
A feed (stream 1)	XMEAS (1)	0.25052	kscmh
D feed (stream 2)	XMEAS (2)	3664.0	kg h^{-1}
E feed (stream 3)	XMEAS (3)	4509.3	kg h^{-1}
A and C feed (stream 4)	XMEAS (4)	9.3477	kscmh
Recycle flow (stream 8)	XMEAS (5)	26.902	kscmh
Reactor feed rate (stream 6)	XMEAS (6)	42.339	kscmh
Reactor pressure	XMEAS (7)	2705.0	kPa gauge
Reactor level	XMEAS (8)	75.000	%
Reactor temperature	XMEAS (9)	120.40	°C
Purge rate (stream 9)	XMEAS (10)	0.33712	kscmh
Product separator temperature	XMEAS (11)	80.109	°C
Product separator level	XMEAS (12)	50.000	%
Product separator pressure	XMEAS (13)	2633.7	kPa gauge
Product separator underflow (stream 10)	XMEAS (14)	25.160	$m^3 h^{-1}$
Stripper level	XMEAS (15)	50.000	%
Stripper pressure	XMEAS (16)	3102.2	kPa gauge
Stripper underflow (stream 11)	XMEAS (17)	22.949	$m^3 h^{-1}$
Stripper temperature	XMEAS (18)	65.731	°C
Stripper steam flow	XMEAS (19)	230.31	kg h^{-1}
Compressor work	XMEAS (20)	341.43	kW
Reactor cooling water outlet temperature	XMEAS (21)	94.599	°C
Separator cooling water outlet temperature	XMEAS (22)	77.297	°C

Table 5. Sampled process measurements

Reactor feed analysis (stream 6)

Component	Variable number	Base case value	Units	Sampling frequency = 0.1 h Dead time = 0.1 h
A	XMEAS (23)	32.188	mol%	
B	XMEAS (24)	8.8933	mol%	
C	XMEAS (25)	26.383	mol%	
D	XMEAS (26)	6.8820	mol%	
E	XMEAS (27)	18.776	mol%	
F	XMEAS (28)	1.6567	mol%	

Purge gas analysis (stream 9)

Component	Variable number	Base case value	Units	Sampling frequency = 0.1 h Dead time = 0.1 h
A	XMEAS (29)	32.958	mol%	
B	XMEAS (30)	13.823	mol%	
C	XMEAS (31)	23.978	mol%	
D	XMEAS (32)	1.2565	mol%	
E	XMEAS (33)	18.579	mol%	
F	XMEAS (34)	2.2633	mol%	
G	XMEAS (35)	4.8436	mol%	
H	XMEAS (36)	2.2986	mol%	

Product analysis (stream 11)

Component	Variable number	Base case value	Units	Sampling frequency = 0.25 h Dead time = 0.25 h
D	XMEAS (37)	0.01787	mol%	
E	XMEAS (38)	0.83570	mol%	
F	XMEAS (39)	0.09858	mol%	
G	XMEAS (40)	53.724	mol%	
H	XMEAS (41)	43.828	mol%	

The analyzer sampling frequency is how often the analyzer takes a sample of the stream. The dead time is the time between when a sample is taken and when the analysis is complete. For an analyzer with a sampling frequency of 0.1 h and a dead time of 0.1 h, a new measurement is available every 0.1 h and the measurement is 0.1 h old.

Table 6. Process operating constraints

	Normal operating limits		Shut down limits	
Process variable	Low limit	High limit	Low limit	High limit
Reactor pressure	none	2895 kPa	none	3000 kPa
Reactor level	50% (11.8 m^3)	100% (21.3 m^3)	2.0 m^3	24.0 m^3
Reactor temperature	none	150°C	none	175°C
Product separator level	30% (3.3 m^3)	100% (9.0 m^3)	1.0 m^3	12.0 m^3
Stripper base level	30% (3.5 m^3)	100% (6.6 m^3)	1.0 m^3	8.0 m^3

Table 7. Setpoint changes for the base case

Process variable	Type	Magnitude
Production rate change	Step	−15% Make a step change to the variable(s) used to set the process production rate so that the product flow leaving the stripper column base changes from 14,228 to 12,094 kg h^{-1}
Product mix change	Step	50 G/50 H to 40 G/60 H Make a step change to the variable used to ensure correct product composition so that the product production rates of G and H change from 7038 kg h^{-1} G to 5630 kg h^{-1} G and from 7038 kg h^{-1} H to 8446 kg h^{-1} H
Reactor operating pressure change	Step	−60 kPa Make a step change so that the reactor operating pressure changes from 2705 to 2645 kPa
Purge gas composition of component B change	Step	+2% Make a step change so that the composition of component B in the gas purge changes from 13.82 to 15.82%

Similar setpoint changes can also be made with the other operating modes.
To realize the full effect of these setpoint changes, we suggest a simulation time of 24–48 h.

Control strategies should attempt to minimize this type of variability on stream 11.

Feed flow variability

The four feed streams are products of other production facilities within the plant complex. Significant holdup is available for feed stream 3, component E. However, less holdup is available for feed streams 1 and 2, components A and D, and very little holdup is available for feed stream 4, components A and C. For those components which have little holdup, changes in their feed flowrates to this process are product demand changes to the processes producing those components. As a result, flow variability of three of the four feed streams is of concern, particularly for stream 4. It is desired first to minimize flow variability having frequency content in the range 12–80 h^{-1} for stream 4. For feed stream 1 and 2, the A and D feeds, they should be protected from variability having frequency content in the range 8–16 h^{-1}. Finally, variability in the feed rate of E is not of major concern. However, excessive movement or high-frequency ringing or chatter is undesirable for any of the manipulated variables.

Dynamic performance measure

We have provided no mathematical measure for evaluating the "performance" of the many ways to control this process. Although the dynamic performance objectives have been described in the sections above, we felt that the tradeoffs among the possible control strategies and techniques involve much more than a mathematical expression. Issues such as tolerance to measurement failure or drift, understandability by the plant operators, hardware implementation considerations, maintenance, etc. make a mathematical evaluation of control strategies difficult.

Dynamic performance comparisons

The testing and evaluation of various process control technologies can be done with the setpoint changes listed in Table 7 or the load changes listed in Table 8. These setpoint and load disturbances

Table 8. Process disturbances

Variable number	Process variable	Type
IDV (1)	A/C feed ratio, B composition constant (stream 4)	Step
IDV (2)	B composition, A/C ratio constant (stream 4)	Step
IDV (3)	D feed temperature (stream 2)	Step
IDV (4)	Reactor cooling water inlet temperature	Step
IDV (5)	Condenser cooling water inlet temperature	Step
IDV (6)	A feed loss (stream 1)	Step
IDV (7)	C header pressure loss—reduced availability (stream 4)	Step
IDV (8)	A, B, C feed composition (stream 4)	Random variation
IDV (9)	D feed temperature (stream 2)	Random variation
IDV (10)	C feed temperature (stream 4)	Random variation
IDV (11)	Reactor cooling water inlet temperature	Random variation
IDV (12)	Condenser cooling water inlet temperature	Random variation
IDV (13)	Reaction kinetics	Slow drift
IDV (14)	Reactor cooling water valve	Sticking
IDV (15)	Condensor cooling water valve	Sticking
IDV (16)	Unknown	Unknown
IDV (17)	Unknown	Unknown
IDV (18)	Unknown	Unknown
IDV (19)	Unknown	Unknown
IDV (20)	Unknown	Unknown

Disturbances 14–20 should be used in conjunction with another disturbance from this table or a setpoint change.
To realize the full effect of these disturbances, we suggest a simulation time of 24–48 h.

represent a set of tests that can be used to compare and contrast alternative approaches to operating and automatically controlling this process. Each disturbance illustrates a different aspect of operating the process. We encourage users to try all the disturbances and to try them at the different modes of process operation.

To provide the common basis needed for the purpose of publishing and comparing results, we suggest disturbing the process at the base case (Mode 1) with the four setpoint changes listed in Table 7 and the following four load disturbances from Table 8:

IDV(1)	Step change
IDV(4)	Step change
IDV(8)	Random variation
IDV(12), IDV(15)	Simultaneous random variation and sticking valve.

A qualitative comparison of the time responses of at least the following process variables is desired: A feed flowrate (stream 1), D feed flowrate (stream 2), E feed flowrate (stream 3), C feed flowrate (stream 4), product flowrate (stream 11), product compositions (stream 11) and reactor pressure.

PROCESS OPTIMIZATION

The process has more manipulated variables than necessary for controlling inventories and product quality making optimization feasible. An objective function based on operating costs is listed in Table 9. Operating costs for this process are primarily determined by the loss of raw materials. Raw materials are lost in the purge gas, the product stream and by means of the two side reactions. Economic costs for the process are determined by summing the costs of the raw materials and the products leaving in the purge stream, the costs of the raw materials leaving in the product stream, and using an assigned cost to the amount of F formed. Costs of the compressor work and steam to the stripping column are also included. Component values and a sample costs calculation for the base case are listed in Table 9.

POTENTIAL APPLICATIONS

This problem can be used for studying a wide variety of topics:

1. **Plant-wide control strategy design**—There are many control strategies that can be used to control this plant. Steady-state analysis tools such as RGA can be used to screen possible

Table 9. Process operating costs

Component	Cost ($ kgmol^{-1})
A	2.206
C	6.177
D	22.06
E	14.56
F	17.89
G	30.44
H	22.94

Compressor costs: \$0.0536 (kW-h)$^{-1}$

Stripper steam costs: \$0.0318 kg^{-1}

Operating costs at the base case:

Purge losses:	Component	Mole fraction	Molar costs	
	A	0.32958	2.206	0.7271
	C	0.23978	6.177	1.4811
	D	0.01257	22.06	0.2773
	E	0.18579	14.56	2.7051
	F	0.02263	17.89	0.4049
	D	0.04844	30.44	1.4745
	H	0.02299	22.94	0.5274
			Costs per kgmol of purge	7.5973

Losses in the product:	Component	Mole fraction	Molar costs	
	D	0.00018	22.06	0.0040
	E	0.00836	14.56	0.1217
	F	0.00099	17.89	0.0177
			Costs per kgmol of product	0.1434

Total operating costs at base case:

(purge costs)(purge rate) + (product stream costs)(product rate)
+ (compressor costs)(compressor work) + (steam costs)(steam rate) = total costs

$$7.5973\frac{\$}{\text{kgmol}}\left(44.79\frac{\text{kgmol h}^{-1}}{\text{kscmh}}0.3371\ \text{kscmh}\right)+0.1434\frac{\$}{\text{kgmol}}\left(9.21\frac{\text{kgmol}}{\text{m}^3}\frac{\text{h}^{-1}}{\text{h}^{-1}}22.95\ \text{m}^3\text{h}^{-1}\right)$$
$$+0.0536\frac{\$}{\text{kWh}}(341.4\ \text{kW})+0.0318\frac{\$}{\text{kg}}(230.3\ \text{kg h}^{-1})=170.6\ \$\,\text{h}^{-1}$$

schemes. Dynamic simulation can then be used to test the performance of the schemes with the disturbances listed in Tables 7 and 8. Control strategies can be designed to reject disturbances for all six modes of operation given in the section titled "Process Description".

2. **Multivariable control**—Many of the process measurements respond to many of the manipulated variables. Consequently, multivariable control may be beneficial for reducing interaction.
3. **Optimization**—Both steady-state and dynamic optimization problems may be studied. Determine the optimum operating conditions for the six modes of operation. Table 9 provides an objective function.
4. **Predictive control**—The application of predictive control techniques containing identification, constraint handling and optimization can be evaluated.
5. **Estimation/adaptive control**—Variation in production rate and product mix may cause the process dynamics to change sufficiently to merit on-line controller adaptation.
6. **Nonlinear control**—The reaction and vapor–liquid equilibrium equations are quite nonlinear and control may benefit from a nonlinear approach to the problem.
7. **Process diagnostics**—Expert systems and fault diagnostics can be tested to evaluate their performance and reaction to new or unknown conditions.
8. **Education**—This problem could be used as a study in process control courses to illustrate the concepts of control strategy design, controller tuning, control loop troubleshooting and applications of advanaced control.

This list is intended to generate ideas for some of the possible applications of this test problem. No doubt there are other possible topics for study as well.

MODEL DESCRIPTION

We chose to present the test problem in the form of FORTRAN subroutines, hoping that this form would be the easiest to use for the most people and promote widespread use.

Below is a list of points that may be useful in using the model:

- The vapors all behave as ideal gases.
- The vapor–liquid equilibrium follows Raoult's Law with the vapor pressure calculated using the Antoine equation.
- All the vessels are well mixed and contain no distributed parameters.
- The list of manipulated variables, Table 3, includes some variables listed as thousand standard cubic meters per hour (kscmh), kilograms per hour ($kg\,h^{-1}$), or as cubic meters per hour ($m^3\,h^{-1}$), and some variables listed as valve position (%). For those manipulated variables listed as kscmh, $kg\,h^{-1}$, or $m^3\,h^{-1}$, the flowrate is not a function of upstream or downstream pressure. For those manipulated variables listed as valve position (%), the flowrate is a function of pressure. If a constant flowrate in the presence of pressure changes is desired, a flow controller should be included. The text at the bottom of Table 3 discusses how constraints on the manipulated variables are handled.
- The reactor is agitated. Agitation speed only affects the heat transfer coefficient.
- The recycle gas compressor is a centrifugal type and has internal surge protection by means of a mechanical bypass arrangement. The relation between flow through the compressor and inlet–outlet pressure difference follows a typical centrifugal compressor curve.
- All process measurements include Gaussian noise with standard deviation typical of the measurement type.
- Table 6 lists the process constraints, both normal operating limits and process shutdown limits. The process should be operated within the normal operating limits. If the process exceeds the shutdown limits, it will automatically be shut down as described in the section below.
- The model is not intended for simulating process start-up and shutdown procedures.
- Modeling the process presented a tradeoff between rigor and model stiffness due to the gas phase dynamics during pressure change. In developing the process model, a compromise was made to ensure realistic behavior for the dynamics of primary interest while not having the system become too stiff. The model is sufficiently rigorous to capture the important process dynamics. We did not include fast dynamics such as transmitter lags. A linear eigenvalue analysis at the base case was used to find the fastest mode of the system. The largest negative eigenvalue is $1968\,h^{-1}$ for a time constant of about 1.8 s. The step size used in the sample program (TEMAIN, discussed below) is 1 s and was sufficient for integration stability.

USE OF THE MODEL SUBROUTINES

The model consists of 10 FORTRAN subroutines: TEFUNC, TEINIT and TESUB1, . . . , TESUB8.

To run the model, the user must provide a main program, an integration algorithm, control algorithms and output routines. A simple example main program, TEMAIN, is included with the subroutines and illustrates their use as well as all of the elements needed to run the model. TEMAIN linked with the 10 subroutines forms a sample executable program.

TEFUNC

TEFUNC is the function evaluator to be called from an integration subroutine. It calculates current process variable measurements and derivatives from the current states provided from the integrator. The user must provide the integration algorithm.

TEFUNC is called as follows:

CALL TEFUNC(NN, TIME, YY, YP).

TEFUNC's inputs are:

NN = Number of variables (states) to integrate. There are 50 states for simulating the process.
(Subroutine argument list.)

TIME = Current time in hours. Updated by the integrator.
(Subroutine argument list.)

YY = Vector containing the current values of the states. Calculated by the integrator.
(Subroutine argument list.)

XMV = Vector of manipulated variables.
(Common block: PV.)

IDV = Vector of disturbance flags.
(Common block: DVEC.)

TEFUNC's outputs are:

YP = Vector containing the current derivatives of the states.
(Subroutine argument list.)

XMEAS = Vector of process variable measurements.
(Common block: PV.)

TEINIT

TEINIT is the initialization subroutine. It specifies the initial values of the states (the variables that are integrated) and the initial values of the manipulated variables. It also specifies the values of variables that are constant, such as physical properties. The values of the states and manipulated variables as specified by TEINIT correspond to the base-case, steady-state operating condition (as shown in Tables 1, 3, 4 and 5). TEINIT calls TEFUNC to calculate the initial process measurement values. After calling TEINIT, the values of the derivatives will all be close to zero. TEINIT should be called when first starting the simulation program and anytime the user wishes to return the simulation to the base-case, initial condition.

TEINIT is called as follows:

CALL TEINIT(NN, YY, YP).

TEINIT's inputs are

NN = No. of variables (states) to integrate.
(Subroutine argument list.)

TEINIT's outputs are

YY = Vector containing the initial values of the states.
(Subroutine argument list.)

YP = Vector containing the initial derivatives of the states.
(Subroutine argument list.)

Utility subroutines

There are 8 utility subroutines, TESUB1, . . . , TESUB8. They are all called by TEFUNC, and the user need not call any of them.

Constraints

TEFUNC tests the process variables which have shutdown constraints as listed in Table 6. If any variable violates a shutdown constraint, the process will automatically be shut down. More specifically, TEFUNC sets all the derivatives to zero, because it is invalid to operate the process outside these limits. Restarting the process requires calling TEINIT which resets the process to the base case condition and enables TEFUNC to again calculate derivatives.

User's interface

The user's "interface" to the model is through two common blocks as explained below.

COMMON/PV/XMEAS(41), XMV(12): XMEAS is the vector of process measurements which are calculated in TEFUNC from the current states. The measurements contained in this vector are listed in Tables 4 and 5. Elements of XMEAS are REAL*8 variables.

XMV is the vector of manipulated variables which the user specifies either as constant values or as outputs of control algorithms. The variables contained in this vector are documented in Table 3. When specifying values for the manipulated variables through XMV, the range for *all* of the manipulated variables is 0–100. The manipulated variables are then scaled by TEFUNC according to the ranges listed on Table 3. Table 3 also discusses how constraints on the XMVs are handled. Elements of XMV are REAL*8 variables.

COMMON/DVEC/IDV(20): IDV is a vector of disturbance flags which the user sets as either on (1) or off (0). The disturbances corresponding to the elements of IDV are listed in Table 8. Setting an element to 1 turns on the disturbance. Setting an element to 0 turns off the disturbance. The user may turn any of the disturbances on or off at any time separately or simultaneously and they are applicable to all six modes of process operation. The variables changed for the disturbance return to their base case values upon setting the disturbance flag back to 0. Elements of IDV are INTEGER*4 variables.

TEMAIN

Figure 2 shows a flowchart for TEMAIN. The process is initialized with a call to TEINIT. Disturbance flags, manipulated variables to be held constant (different from their initial values), and setpoints are specified. The remainder of TEMAIN is the simulation loop. The loop begins by executing the discrete control algorithms which update their manipulated variables. Next, desired measurements and manipulated variables for the current time step are saved for later printing or plotting. Last, the integrator is called to integrate the process ahead to the next time step. TEMAIN uses a simple Euler integrator for example.

Saving process operating conditions

The operating conditions may be saved for purpose of restoring the simulation to a condition other than the base case by writing the state vector (YY) and the manipulated variable vector (XMV) to a file. After reading the YY and XMV variables, the user must set the variable TIME to zero and then call TEFUNC to update all the other measurements. Setting TIME to zero, causes the sampled process measurements to be re-initialized correctly.

Controllers

The user may implement controllers as either discrete or continuous algorithms. The simulation loop in TEMAIN illustrates the implementation of discrete controllers. Comment statements in TEINIT and TEFUNC show where additional states needed for continuous controllers may be appended to the process model and included in the integration.

Steady-state convergence

In addition to integrating TEFUNC to perform dynamic simulation, TEFUNC may also be used to converge the test problem to new steady-states. A convergence algorithm such as Newton or Broyden can be used to drive the values of the derivatives returned from TEFUNC to zero. The user will need to append any controllers or design specifications to the states and derivatives of TEFUNC. When converging to steady-state, call TEFUNC with TIME = 0. Only when TIME = 0 is there no noise on the measurements.

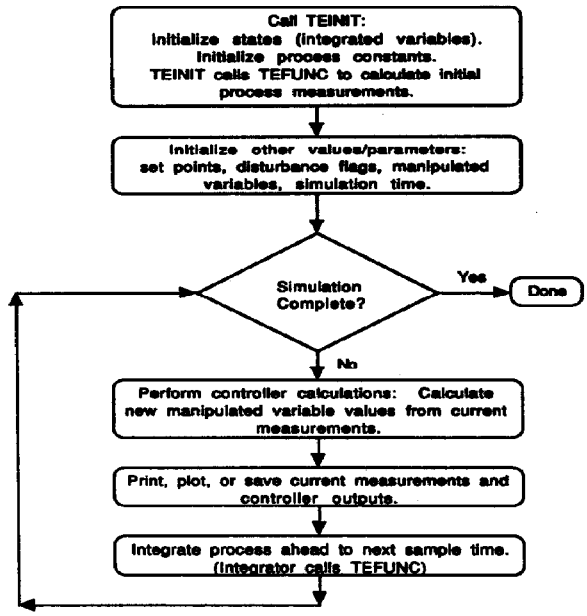

Fig. 2. Flowchart of TEMAIN.

Program code

The subroutines were developed on a DEC VAX system, however standard FORTRAN was used so that the routines can be compiled on any machine. All the subroutines use REAL*8 variables (double precision arithmetic). The source code includes documentation regarding its application. However, by intention, the calculations are not documented and the variable names are somewhat cryptic. We prefer that the study issues focus on process control, as opposed to modeling topics. Further, for the sake of meaningful comparisons, we do not want to encourage modification of the model.

Example simulation

Figure 3 shows the open-loop dynamic responses for eight process measurements to a step change in the reactor cooling water flow rate. XMV(10) = 41.106 $m^3 h^{-1}$ was changed to XMV(10) = 38.00 $m^3 h^{-1}$ and held constant throughout the simulation. All other manipulated variables were constant at their base case values (no controllers in automatic). No other disturbances were present (all IDVs = 0), other than the normal measurement noise. This simulation was performed with an Euler integrator

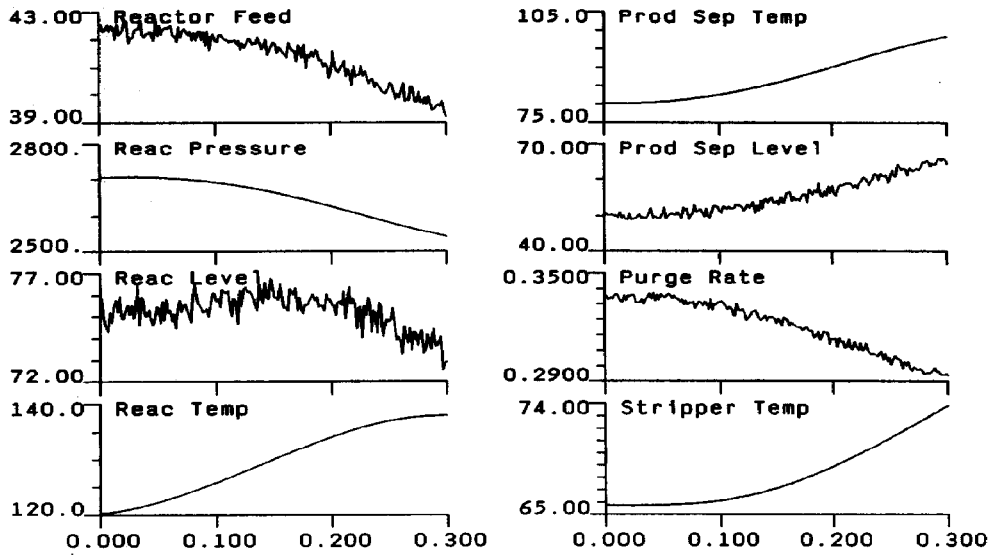

Fig. 3. Open-loop responses for step change in reactor cooling water flow.

(constant step size of 1 s) and the response data was plotted every sixth step.

OBTAINING THE SOURCE CODE

The FORTRAN source code is available by request from either author. We can send it by electronic mail (Internet or BITNET) or on $3\frac{1}{2}$" floppy (IBM PC or Macintosh format). We recommend that you obtain a copy directly from us. By requesting the program from us, we will know who has a copy and we can notify users of any future modifications.

SUMMARY

The chemical process model presented here is a challenging problem for a wide variety of process control technology studies. Even though this process has only a few unit operations, it is much more complex than it appears on first examination. We hope that this problem will be useful in the development of the process control field. We are also interested in hearing about applications of the problem.

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