Design and Control of the Ethyl Benzene Process

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The ethyl benzene (EB) process involves the reaction of benzene with ethylene to form the desired EB product. However, ethylene can also react with EB to form an undesired product of di-ethyl benzene (DEB) if reactor temperatures or ethylene concentrations are high. An unusual feature of the EB process is the ability to recycle "to extinction" all the DEB formed in the reactor (no net DEB product produced), since DEB reacts with benzene to form EB. Since DEB is the highest-boiling component in the system, it comes out the bottom of the two distillation columns, so there is little energy penalty in having a large DEB recycle. Recycling benzene is more expensive because it goes overhead in the first distillation column. The economic optimum steady-state design is developed that minimizes total annual cost (capital and energy). An effective plantwide control structure is also developed. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 655–670, 2011

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Introduction

Ethyl benzene (EB) is an important commodity chemical. Much of its production is used to make styrene. The process considered in this article has two reactors in series, two distillation columns and two liquid recycle streams. Thus it provides a nice example of a multiunit complex process that is typical of many chemical plants found in industry.

An interesting and unusual feature of the EB process is the recycle to extinction of the DEB by-product. A significant amount of DEB circulates around through the system, and the per-pass EB selectivity is quite low. But the overall selectivity is essentially 100% since all of the fresh reactant feeds (ethylene and benzene) end up leaving in the single product stream as EB.

The purpose of this article is to present the details of the process, discuss the important economic trade-offs in its steady-state design, and demonstrate the effectiveness of a plantwide control structure. It is hoped that other workers will find the EB process useful in their research for testing other design and control methodologies.

The EB process provides a good example of the application of several fundamental principles of design. We can look at the chemistry and immediately know that there will be a trade-off between reactor size and selectivity because the activation energy of the undesirable reaction is larger than that of the desirable reaction. So low reactor temperatures will be favored, but this requires larger reactors for a given conversion. The chemistry also tells right up front that there will be a trade-off between recycle costs and selectivity because the concentrations of the components that react in the undesirable reaction must be kept small. These design trade-offs are discussed in detail in this article.

Process Studied

Figure 1 shows the flowsheet studied in this article. The process is a modified version of the process explored earlier[1] when it was used to illustrate dynamic plantwide simulation methods. The economics of the design were not considered in this previous work. Kinetic parameters have been adjusted

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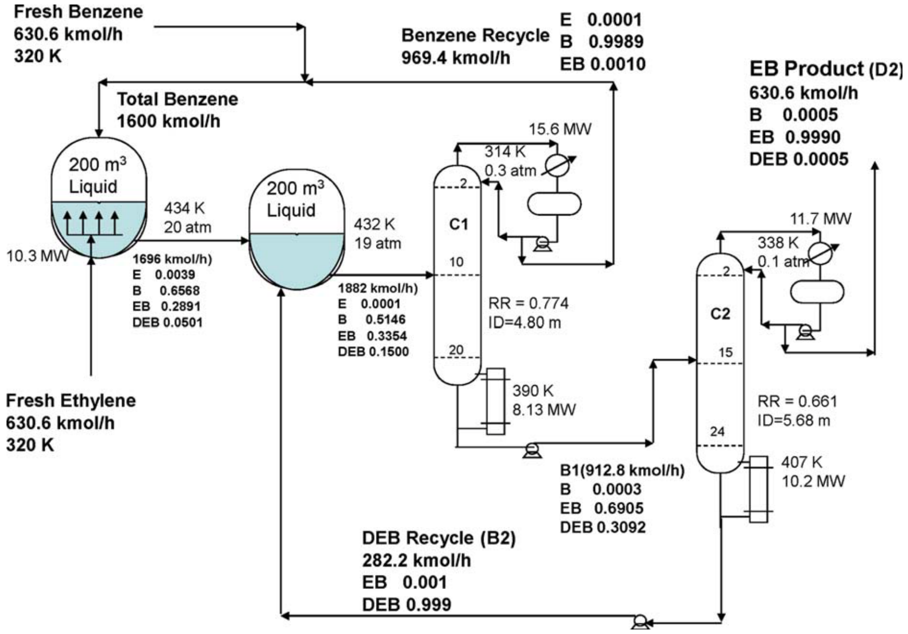

Figure 1. Ethyl benzene flowsheet.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

to give reasonable rates of generation of the two components of interest (EB and DEB) in the reactors.

The EB process involves sparging gaseous ethylene into the liquid phase of the first of two CSTR reactors in series. Both reactors operate at high pressure (20 atm) to maintain liquid in the reactor at the high temperatures required for reasonable reaction rates (433 K). A large liquid benzene stream is also fed to the first reactor. The heat of the exothermic reaction is removed by generating 2.5 atm steam in this reactor.

The effluent from the first reactor is fed into the second reactor along with a recycle stream of DEB. This reactor is adiabatic. The effluent from the second reactor is fed to a distillation column that produces a distillate that is mostly benzene, which is recycled to the first reactor along with the fresh feed of make-up benzene. The bottoms stream is a mixture of EB and DEB. It is fed to a second distillation column that produces an EB distillate and a DEB bottoms, which is recycled back to the second reactor.

Note that a two-reactor flowsheet is used so that high conversion of the ethylene can be achieved in the first reactor and conditions are favorable in the second reactor for the reaction of DEB back to EB (higher concentration of DEB).

Reaction kinetics

The production EB involves the liquid-phase reaction of ethylene with benzene

$$C_2H_4 + C_6H_6 \rightarrow C_8H_{10} \tag{1}$$

There are other undesirable reactions that we assume can be represented by the formation of di-ethyl benzene (DEB) from the reaction of EB with ethylene.

$$C_8H_{10} + C_2H_4 \rightarrow C_{10}H_{14} \tag{2}$$

A third reaction also occurs in which DEB reacts with benzene to form EB.

$$C_{10}H_{14} + C_6H_6 \rightarrow 2C_8H_{10} \tag{3}$$

This reaction makes it possible to recycle the DEB back to the second reactor where an excess of benzene exists and drives the reaction to the right to produce EB. Thus there is essentially no DEB leaving the system despite the fact that a large amount is produced in the first reactor and passes through the two distillation columns.

Table 1 gives the reaction kinetics assumed in this article. All reaction rates have units of kmol/(s m^3) (consistent with Aspen simulation requirements). Concentration units are molarity (kmol/m^3).

Notice that the activation energy of the undesirable reaction (Reaction 2) is larger than that of the desirable reaction. Therefore low reactor temperatures improve selectivity. In addition, selectivity is improved by keeping low concentrations of ethylene and EB in the reactor. This can be achieved by using a large excess of benzene, but the excess must be recovered and recycled.

A high conversion of ethylene in the first reactor is desired so that the ethylene concentration is low. This

Table 1. Ethyl Benzene Reaction Kinetics

	$\mathfrak{R}1$	$\mathfrak{R}2$	$\mathfrak{R}3$
k	1.528×10^6	2.778×10^7	1000
E (cal/mol)	17,000	20,000	15,000
Concentration terms (kmol/m^3)	$C_E C_B$	$C_E C_{EB}$	$C_B C_{DEB}$

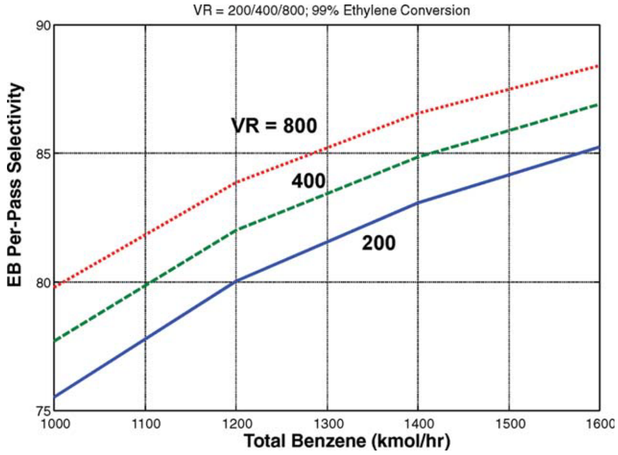

Figure 2. Per-pass selectivity.

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reduces the production of DEB and results in only a small amount of ethylene that is recycled in the benzene recycle stream. Ethylene conversion is set at 99% for all the cases considered by adjusting the temperature of the first reactor.

Figure 2 illustrates how the important design optimization variables affect EB selectivity, which is defined as the molar flowrate of EB leaving the reactor divided by the sum of the molar flowrates of EB and DEB. This is *per-pass* selectivity, not the overall selectivity of the entire process. Selectivity is increased by increasing the recycle flowrate of benzene or by increasing reactor size. The larger the reactor, the lower the temperature required for the fixed ethylene conversion of 99%. The 200 m^3 reactor requires temperatures around 430 K. The 400 m^3 reactor requires temperatures around 416 K. The 800 m^3 reactor requires temperatures around 403 K. Lower temperature favors EB production because of the higher activation energy of the DEB reaction.

Phase equilibrium

The two separations required are the removal of benzene from EB and the removal of EB from DEB. The Choa-Seader physical property package is used in the Aspen simulations. The normal boiling points of these components are 353 K for benzene, 409 K for EB, and 457 K for DEB. The significant differences mean that the two distillation columns have a fairly small number of trays and required a low reflux ratio. In a later section of this article, the optimum designs of these two columns are developed based on minimizing total annual cost (capital and energy). The design optimization variables are pressure, number of trays, and feed locations.

Notice that the normal boiling points are considerably higher than the temperatures that can be achieved in a water-cooled condenser (314 K). This means that the columns could be operated under vacuum conditions if this is economically attractive. This question is quantitatively addressed in a later section.

Flowsheet

Figure 1 shows the flowsheet of the EB process with the equipment sizes and conditions that are the economic optimum, as discussed in the next section. Reactors of equal size are assumed. The economic optimum combination of reactor size and benzene recycle flowrate is reactors containing 200 m^3 of liquid (half full) and a total benzene stream of 1600 kmol/h. The total benzene stream is the distillate from the first column (969.4 kmol/h) and the fresh benzene feed.

The two fresh feeds (ethylene and benzene) are each 630.6 kmol/h, as is the production rate of EB because only a negligible amount of DEB leaves the system. Essentially all of the ethylene and benzene reactant leave as EB product in the distillate D2 from the second column.

The first reactor operates at 434 K and 20 atm. It is cooled by generating steam. About 80.5 kmol/h of DEB is generated in the first reactor along with 464.4 kmol/h of EB, leaving 6.3 kmol/h of unreacted ethylene. So the per-pass EB selectivity is only 85% in the first reactor.

$$\text{EB Selectivity} = \frac{464.4}{464.4 + 80.5} = 0.852$$

The first reactor is cooled by generating steam in internal cooling coils. The temperature of the saturated steam is 414 K with a reactor temperature of 434 K. In the Aspen Dynamics simulation, the heat removal option is *constant medium temperature*. A heat transfer coefficient of 203 cal/(s m^2 K) is assumed, which requires 602 m^2 of heat-transfer area to remove the 2.46 $\times$ 10^6 cal/s of heat. Jacket heat-transfer area in the reactor (diameter = 7.53 m and length = 6.34 m) is only 151 m^2, so internal coils are required.

The effluent from the first reactor is fed into the second reactor in which essentially all the DEB generated in the first reactor is converted to EB by reaction with benzene. The recycled DEB from the bottom of the second column is also fed into the second reactor at a molar flowrate of 282.2 kmol/h. The DEB leaving in the effluent of the second reactor is this same 282.2 kmol/h. So the second reactor is able to convert essentially all the DEB formed in the first reactor back to EB. Thus the DEB is recycled to extinction.

The effluent from the second reactor is at high pressure and high temperature. It is fed into the first distillation column C1. The high feed temperature results in the vapor load in the rectifying section being higher than that in the stripping section. Notice that the condenser heat duty (15.6 MW) is much higher than the reboiler duty (8.13 MW) because of the high temperature of the feed stream. The first column has 21 stages and a reflux ratio of 0.774. It operates under moderate vacuum at 0.3 atm, which gives a reflux-drum temperature of 314 K and permits the use of cooling water in the condenser. The base temperature is 390 K, which permits the use of low-pressure steam (433 K, 4 atm) in the reboiler. The distillate is mostly benzene, which is mixed with the fresh benzene makeup feed and recycled to the first reactor. Figure 3 gives temperature and composition profiles in Column C1.

The second column C2 has 25 stages and a reflux ratio of 0.661. It operates under low vacuum at 0.1 atm, which gives a reflux-drum temperature of 338 K and permits the use of cooling water in the condenser. The base temperature is 407 K, which permits the use of low-pressure steam in the reboiler. The distillate is high-purity EB (99.9 mol%). The bottoms B2 is recycled to the second reactor. Figure 4 gives temperature and composition profiles in Column C2.

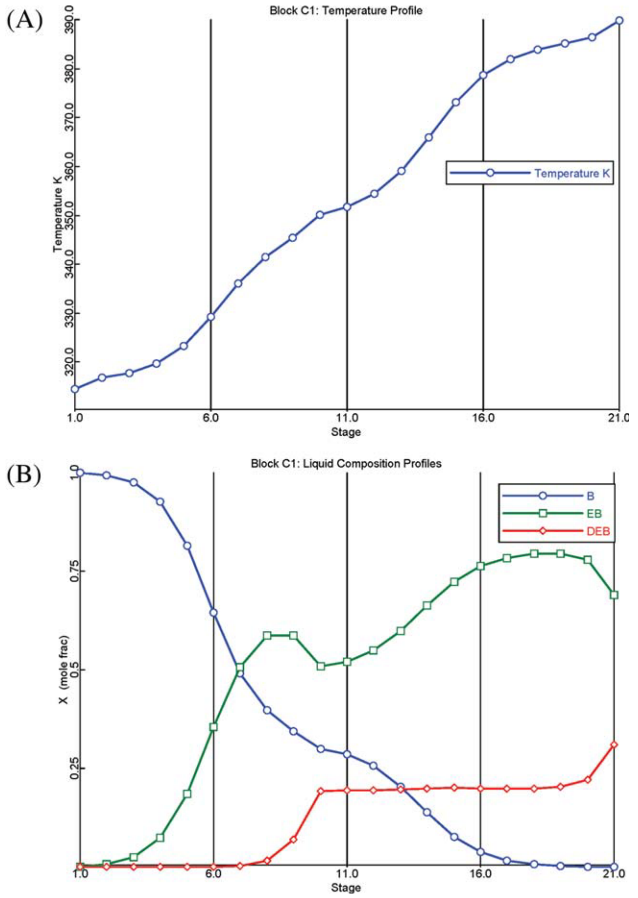

Figure 3. A: C1 temperature profile. B: C1 composition profiles.

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Design of Distillation Columns

A common procedure for optimizing the design of a distillation column is to determine the values of the design optimization variables that minimize total annual cost (see Table 2). The parameters that must be given are the feed conditions and the desired product specifications. The design optimization variables include pressure, total number of trays, and feed tray location.

An iterative sequential optimization procedure was used to optimize the entire process. First, preliminary estimates of reactor conditions were used to determine distillation column feed compositions and flowrates. The columns were then optimized for these values. Next, the overall process was optimized in terms of reactor size and recycle flowrates using the preliminary column designs. Once new column feed conditions were determined, the columns were reoptimized and the procedure repeated until design optimization variables stopped changing.

In many systems, decreasing pressure increases relative volatilities, which decreases energy requirements. This can reduce steam consumption and capital investment in column shell and in heat exchanger area (condenser and reboiler). Since the components to be separated in this system have fairly high normal boiling points, pressure can be reduced to vacuum conditions.

Lower pressure also gives a lower base temperature, which means a lower-temperature, less-expensive energy source can be used in the reboiler or the area of the reboiler can be smaller. However, lower column pressure gives a lower condenser temperature, which increases the required area in the condenser. All of these interacting effects must be quantitatively evaluated.

Column pressure selection

A number of cases are run with different operating pressures to assess the economic impact of pressure. The sizing relationships and cost estimations for the equipment are based on information from Douglas[2] and Turton et al.[3] and are summarized in Table 2. Note that the cost of steam at different pressures is given.

The feed flowrates and compositions used in the cases are those found in the final optimum design. The number of

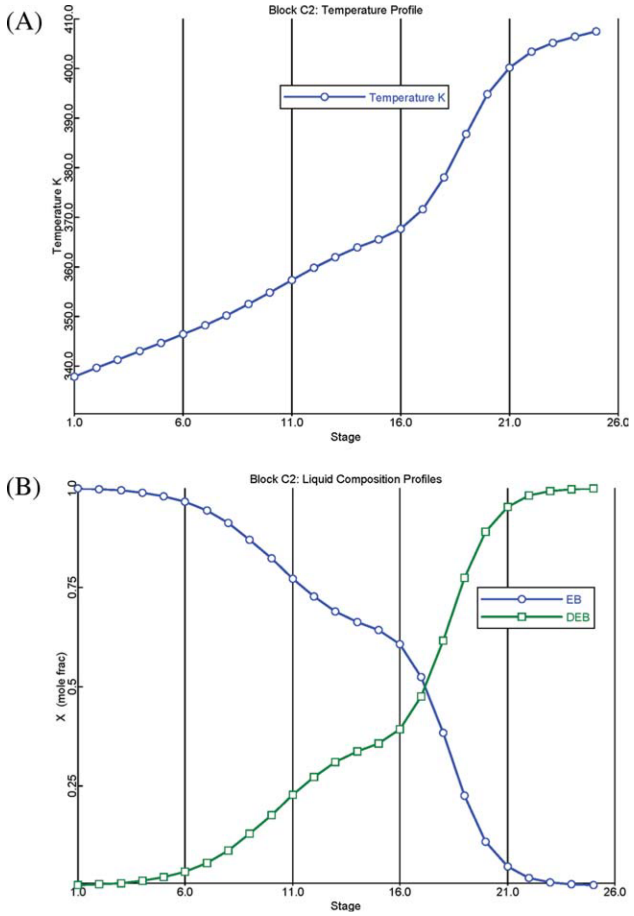

Figure 4. A: C2 temperature profile. B: C2 composition profiles.

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Table 2. Basis of Economics and Equipment Sizing

- Column diameter: Aspen Tray Sizing using double-pass trays
- Column length: NT trays with 2 ft spacing plus 20% extra length
- Column vessel (diameter and length in meters)
- Capital cost = 17,640 $(D)^{1.066}$ $(L)^{0.802}$
- Condensers (area in m^2)
  - Heat-transfer coefficient = 0.852 kW/K m^2
  - Differential temperature = Reflux drum temperature − 310 K
  - Capital cost = 7296 $(\text{area})^{0.65}$
- Reboilers (area in m^2):
  - Heat-transfer coefficient = 0.568 kW/K m^2
  - Differential temperature = Steam temperature – Base temperature
  - Capital cost = 7296 $(\text{area})^{0.65}$
- Reactor (diameter and length in meters)
  - Half full of liquid
  - Aspect ratio = 1
  - Capital cost = 17,640 $(D)^{1.066}$ $(L)^{0.802}$
- Energy cost
  - LP steam (433 K) = $7.78 per GJ
  - MP steam (457 K) = $8.22 per GJ
  - HP steam (537 K) = $9.83 per GJ
  - Value of steam generated in reactor;
    - LP steam (410 K) = $6.00 per GJ
- $\text{TAC} = \frac{\text{Capital Cost}}{\text{Payback Period}} + \text{Energy Cost}$
- Payback period = 3 years

trays and the feed tray locations are also those found in the final optimum design (see Figure 1). The determination of the optimum number of trays is discussed in the next section.

The specifications for the design of Column C1 are 0.1 mol % EB in the distillate and a ratio of benzene to EB in the bottoms of 0.0005. This latter specification is needed to make sure the purity of the final EB product leaving the second column can be achieved. Distillate flowrate and reflux ratio are varied to achieve these specification for each case. The specifications for the design of column C2 are 0.1 mol % EB in the bottoms and 0.05 mol % DEB in the distillate.

Table 3 gives detailed results for both columns over a range of pressures. Note that the pressure of the steam used in the reboiler changes from case to case. In both columns energy costs decrease as pressure is decreased because reboiler heat inputs decrease. In addition, lower-pressure, less-expensive steam can be used as base temperatures (TB) decrease. As shown in Figure 5, Column C1 diameters increase monotonically as pressure decreases. However, in Column C2 there is an initial decrease in diameter before it begins to increase as pressure is reduced. This is due to the interaction between vapor flowrates (which decrease as pressure decreases) and vapor velocities (which increase as vapor density decreases). Notice the rapid increase in the required condenser area as pressures are reduced because of the smaller temperature difference between cooling water (310 K) and the reflux-drum temperature. Pressures lower than 0.3 atm cannot be used in Column C1 and still use cooling water as the heat-removal medium.

It is assumed that the minimum practical pressure is 0.1 atm (76 mm Hg) in the condenser. Therefore, the pressure selected for Column C2 is 0.1 atm and for Column C1 is 0.3 atm.

Only steady-state issues have been considered in this analysis. However, running distillation column under vacuum can significantly impact dynamic control strategies. In a vacuum column, the pressure changes from tray to tray are a significant portion of the total pressure. Tray pressure drop changes with vapor rates, so pressures on the column trays can vary, which affects tray temperatures. Therefore it is sometimes necessary to use direct composition control instead of temperature control. A practical alternative in some systems is to use "pressure-compensated" temperature

Table 3. Column Pressure Selection

C1 21/11	Pressure (atm)	0.1	0.3	0.4	0.5	0.7	1.0
	TD (K)	289	316	324	331	341	353
	TR(K)	373	392	398	405	415	426
	Steam	LP	LP	LP	LP	MP	HP
	ID (m)	6.5	4.80	4.44	4.17	3,85	3.62
	QR (10^6 cal/s)	1.57	1.91	2.11	2.17	2.40	2.69
	QC (10^6 cal/s)	3.89	3.72	3.69	3.66	3.63	3.63
	AR (m^2)	–	343	443	570	420	638
	AC (m^2)	–	3040	1292	854	574	414
	Capital (10^6 $)	–	2.44	1.86	1.76	1.44	1.36
	Energy (10^6 $/year)	–	1.97	2.17	2.23	2.60	2.92
	TAC (10^6 $/year)	–	2.77	2.788	2.80	3.08	3.37
C2 22/13	Pressure (atm)	0.1	0.3	0.5	0.7	1.0	
	TD (K)	338	369	386	397	411	
	TR (K)	405	426	440	451	464	
	Steam	MP	MP	MP	MP	HP	
	ID (m)	5.78	4.44	4.17	4.17	4.20	
	QR (10^6 cal/s)	2.30	2.74	3.05	3.31	3.65	
	QC (10^6 cal/s)	2.90	2.95	3.04	3.13	3.27	
	AR (m^2)	325	648	258	328	426	
	AC (m^2)	508	245	196	176	159	
	Capital (10^6 $)	1.72	1.49	1.20	1.22	1.27	
	Energy (10^6 $/year)	2.49	2.97	3.96	4.29	4.73	
	TAC (10^6 $/year)	3.07	3.46	4.35	4.70	5.16	

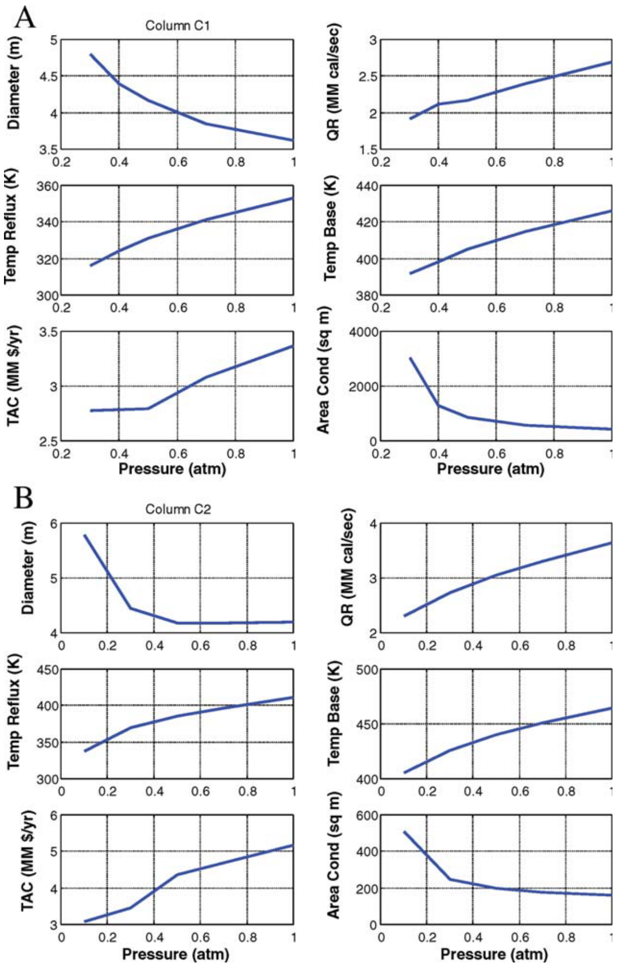

Figure 5. A: Effect of pressure in C1. B: Effect of pressure in C2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

control. Control of these vacuum columns is discussed later in this article.

Number of column trays

Having established the operating pressures in the columns, we must find the economic optimum number of trays. Using more trays reduces reboiler heat input, which reduces column diameter and heat exchanger area (reboiler and condenser). But using more trays increases the height of the column, which increases capital cost.

Table 4 gives results for both columns over a range of tray numbers. The pressure in C1 is 0.3 atm. The pressure in C2 is 0.1 atm. The feed tray location is optimized for each case by minimizing reboiler heat input. Increasing the number of trays reduces energy cost and the capital cost of the heat exchangers. However, the capital cost of the vessel shell increases as more trays are used.

Total annual cost is minimized by using a 21-stage C1 column and a 25-stage C2 column.

Economic Optimization of Entire Process

The design optimization variables in the EB process are reactor size and benzene recycle flowrate. Ethylene conversion in the first reactor is fixed at 99%. Increasing reactor size means lower reactor temperatures, better EB selectivity, and lower DEB recycle flowrates. The result is higher reactor capital cost but lower separation costs. Increasing benzene recycle also gives better EB selectivity and lower DEB recycle, but separation costs increase because recycling benzene is more expensive than recycling DEB since benzene must be vaporized and taken overhead in the first distillation column. The DEB recycle, on the other hand, comes out the bottom of both distillation columns and does not have to be vaporized.

Figure 6 shows the economic impact of these two variables. The minimum TAC is achieved using 200 m^3 reactors and a total benzene flowrate of 1600 kmol/h. Figure 7 shows the effect of the two design optimization variables on the recycle flowrate of DEB from the bottom of Column C2. Bigger reactors and higher benzene recycle flowrates produce less DEB in the reactor and result in smaller DEB recycle. Table 5 provides more detailed information about the alternative designs.

Plantwide Control

The flowsheet shown in Figure 1 does not include all the pumps and control valves needed in the process. The first step in studying dynamics using a pressure-driven dynamic simulation is to add these items and to determine the volumes of all vessels. The reactor sizes and column diameters are known, but the liquid surge capacities of the column reflux drums and column bases must be specified. These are all sized to provide 5 min of holdup when at 50% level. The steady-state conditions found in the dynamic simulation using Aspen Dynamics have only minor differences from

Table 4. Column Tray Number Optimization

	C1 (0.3 atm)			C2 (0.1 atm)		
NT	16	21	26	22	25	32
NF	8	10	13	13	15	18
ID (m)	5.14	4.81	4.77	5.82	5.78	5.64
QR (10^6 cal/s)	2.26	1.96	1.95	2.55	2.46	2.44
QC (10^6 cal/s)	4.07	3.73	3.68	2.93	2.83	2.77
Shell (10^6 \$)	0.653	0.776	0.929	0.992	1.10	1.33
Heat exchangers (10^6 \$)	1.78	1.67	1.66	0.756	0.739	0.732
Total capital (10^6 \$)	2.43	2.45	2.58	1.75	1.84	2.06
Energy (10^6 \$/year)	2.32	2.01	2.00	2.77	2.67	2.65
TAC (10^6 \$/year)	3.131	2.828	2.864	3.348	3.282	3.333

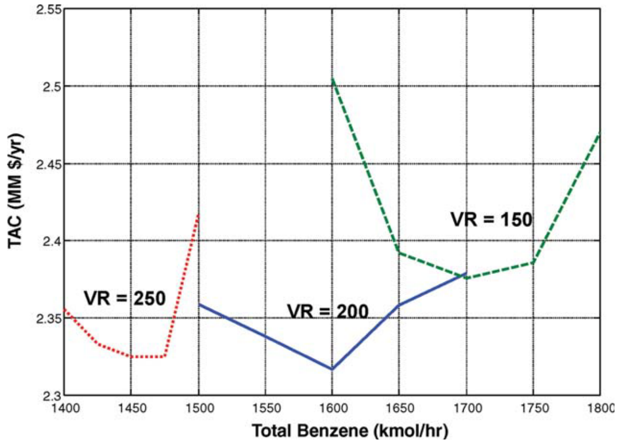

Figure 6. Effect of benzene recycle and reactor size on TAC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

those found in the steady-state simulation using Aspen Plus. The most significant difference is the DEB recycle B2, which is 282.2 kmol/h in Aspen Plus and 251.2 kmol/h in Aspen Dynamics.

Figure 8 shows the plantwide control structure developed. Conventional PI controllers are used in all loops. The recycles and the EB product are streams from the two distillation columns, so we first discuss the control schemes used for these units.

Distillation column control structure

Most industrial distillation columns use inferential temperature control instead of the ideal direct composition control because of practical issues in dealing with on-line analyzers of reliability, expense, and high maintenance. In many columns a single temperature controller is used to maintain a temperature on an appropriate tray by manipulating reboiler heat input. Several methods for selecting the best tray have been proposed, but the most simple is to use the location where the temperature profile is steep. Then a reflux-to-feed ratio or a reflux ratio structure is selected based on which can better handle feed composition disturbances. This approach is employed for the two columns in this study.

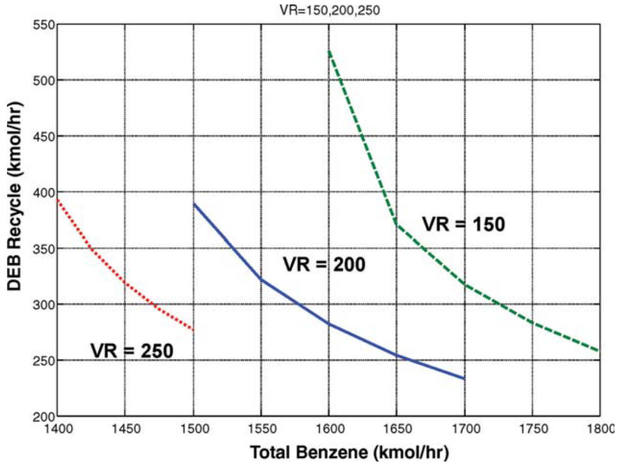

Figure 7. Effect of benzene recycle and reactor size on DEB recycle.

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Table 5. Effects of Reactor Size and Recycle

VR = 150 (m^3)			
Total benzene (kmol/h)	1600	1700	1800
DEB recycle (kmol/h)	525.9	317.3	258.0
TR1 (K)	440	442	442
ID1 (m)	4.99	5.03	5.15
QR1 (10^6 cal/s)	2.09	2.01	2.07
QC1 (10^6 cal/s)	4.02	4.09	4.29
ID2 (m)	6.10	5.74	5.64
QR2 (10^6 cal/s)	2.83	2.49	2.40
QC2 (10^6 cal/s)	3.21	2.86	2.77
Total energy cost (10^6 $/year)	0.941	o.846	0.867
Total capital (10^6 $)	4.69	4.59	4.88
Total annual cost (10^6 $/year)	2.505	2.376	2.470
VR = 200 (m^3)			
Total benzene (kmol/h)	1500	1600	1700
DEB recycle (kmol/h)	389.6	282.2	233.3
TR1 (K)	433	434	434
ID1 (m)	4.70	4.80	4.93
QR1 (10^6 cal/s)	1.92	1.94	2.02
QC1 (10^6 cal/s)	3.58	3.74	3.94
ID2 (m)	5.86	5.68	5.61
QR2 (10^6 cal/s)	2.60	2.44	2.37
QC2 (10^6 cal/s)	2.97	2.80	2.73
Total energy cost (10^6 $/year)	0.761	0.725	0.778
Total capital (10^6 $)	4.79	4.77	4.80
Total annual cost (10^6 $/year)	2.359	2.317	2.379
VR = 250 (m^3)			
Total benzene (kmol/h)	1400	1450	1500
DEB recycle (kmol/h)	393.1	319.0	276.9
TR1 (K)	427	427	428
ID1 (m)	4.50	4.54	4.60
QR1 (10^6 cal/s)	1.85	1.84	1.87
QC1 (10^6 cal/s)	3.28	3.34	3.43
ID2 (m)	5.87	5.74	5.67
QR2 (10^6 cal/s)	2.61	2.50	2.43
QC2 (10^6 cal/s)	2.98	2.86	2.79
Total energy cost (10^6 $/year)	0.696	0.673	0.766
Total capital (10^6 $)	4.98	4.96	4.96
Total annual cost (10^6 $/year)	2.356	2.325	2.418

Figure 3A gives the temperature profile in Column C1. The primary control objective in this column is to keep the benzene from dropping out the bottoms, so temperature in the lower part of the column should be used. The location where temperatures are changing rapidly from tray to tray is around Stage 14, so the temperature on this stage is controlled by reboiler heat input. Figure 4A gives the temperature profile in Column C2. The location where temperatures are changing rapidly from tray to tray is around Stage 20, so the temperature on this stage is controlled by reboiler heat input.

Now we must decide whether to use a reflux-to-feed ratio (R/F) structure or a reflux ratio structure (RR). From a steady-state perspective, either scheme can handle feed flowrate disturbances since all flowrates just ratio up or down with feed flowrate (if changes in pressure and tray efficiencies are neglected). However, their performances with feed composition changes are quite different.

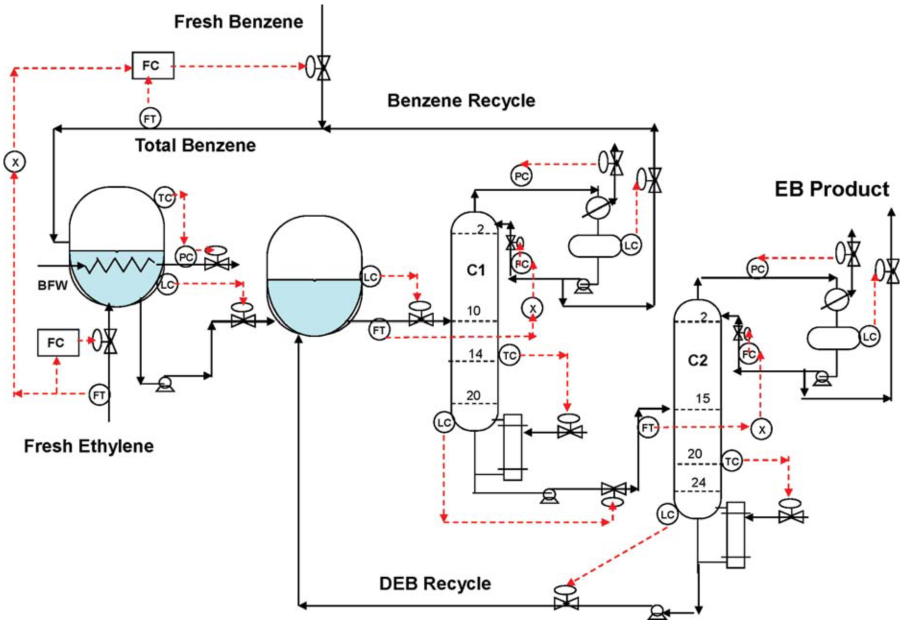

Figure 8. Ethyl benzene plantwide control structure.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

To see which is better, feed compositions are changed around their design conditions in a steady-state simulation in which the two product streams are held at their specified values. In Aspen Plus, this is achieved by using the *Design Spec/Vary* feature. Table 6 gives the required changes in R/F and RR as feed compositions are changed in terms of the light and heavy key components in the two columns. In Column C1, the key components are benzene and EB. In Column 2, the key components are EB and DEB.

The results given in Table 6 indicate that R/F structures are better than RR structures in both columns. They are more effective in Column C2 than in Column C1 since the RR changes are only 3% in the former but 15% in the latter. The performances of the R/F structures are evaluated in the next section.

Plantwide control structure

The various loops shown in Figure 8 are listed below with their controlled and manipulated variables.

(1) Fresh ethylene feed is flow controlled

(2) The total benzene (distillate from Column C1 plus fresh benzene) is flow controlled by manipulating the fresh benzene feed. The setpoint of the flow controller comes from a multiplier. The input signal to the multiplier is the fresh ethylene flowrate. The constant in the multiplier is the desired total benzene-to-ethylene ratio.

(3) The liquid levels in each reactor are controlled by manipulating the liquid streams leaving the reactor.

(4) The temperature in the first reactor TR1 is controlled by changing the setpoint of a steam pressure controller. Not shown in Figure 8 are the details of adding boiler feed water to maintain a liquid level in the steam drum and coils in the reactor.

(5) The pressures in both columns are controlled by condenser heat removal.

(6) Base levels in both columns are controlled by manipulating bottoms flowrates.

(7) Reflux drum levels in both columns are controlled by manipulating flowrates of the distillate stream. Reflux ratios are small in both columns, so using distillate instead of reflux is an acceptable choice.[4]

(8) The temperature on Stage 14 in Column C1 is controlled by manipulating reboiler heat input.

(9) The temperature on Stage 20 in Column C2 is controlled by manipulating reboiler heat input.

Controller tuning

Deadtimes of 1 min are inserted in column temperature loops. A deadtime of 3 min is used in the reactor temperature loop because of the dynamics of the steam coils and steam drum with the steam pressure controller. The very convenient relay-feedback feature in Aspen Dynamics is used to find ultimate gains and periods. The Tyreus-Luyben tuning rules are used. Table 7 gives controller tuning parameters.

Table 6. Effect of Column Feed Compositions

		Base		Percentage Change Over Range
C1				
z1(B)	0.4601	0.5102	0.5601	
z1(EB)	0.3825	0.3325	0.2825	
R/F	0.4332	0.4018	0.3725	15%
RR	0.9407	0.7870	0.6644	35%
C2				
z2(EB)	0.6283	0.6783	0.7283	
z2(DEB)	0.3714	0.3214	0.2714	
R/F	0.4655	0.4582	0.4530	3%
RR	0.6753	0.6216	0.7406	18%

Table 7. Controller Parameters

	Reactor TCR 1	C1 Stage 14 TC1	C2 Stage 20 TC2	VPC FCB2
SP	433.7 K	365.8 K	394.5 K	251.2 kmol/h
Transmitter range	400–500 K	300–400 K	350–450 K	0–500 kmol/h
OP	414.9 K	1.99×10^6 cal/s	2.42×10^6 cal/s	2.537
OP range	350–450 K	$0 - 6.6 \times 10^6$ cal/s	$0–6.6 \times 10^6$ cal/s	0–5
Deadtime	3 min	1 min	1 min	0
K_C	1.5	0.54	1.5	0.6
τ_I (min)	26	13	9.2	9999

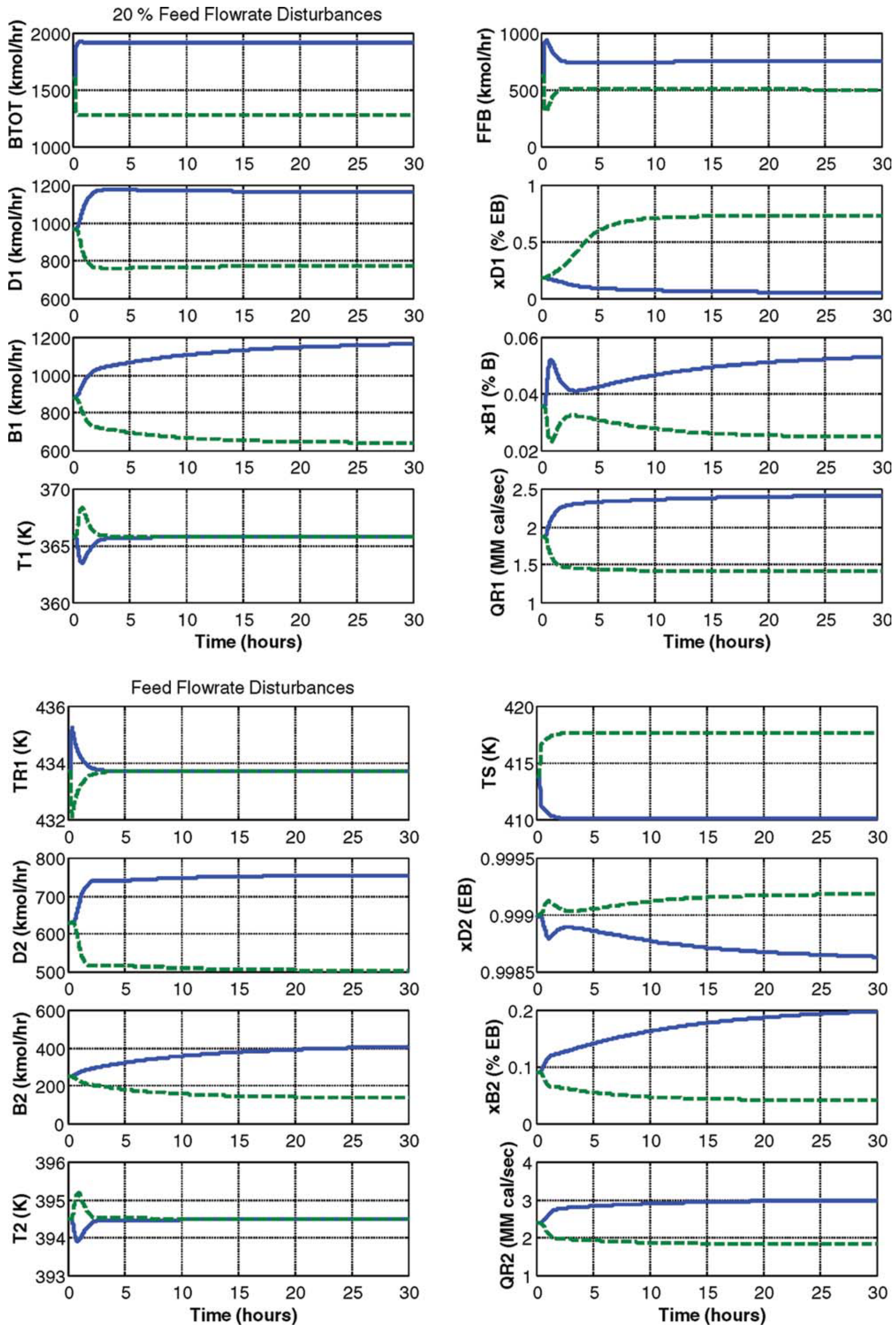

Figure 9. Ethylene feed flowrate disturbances.

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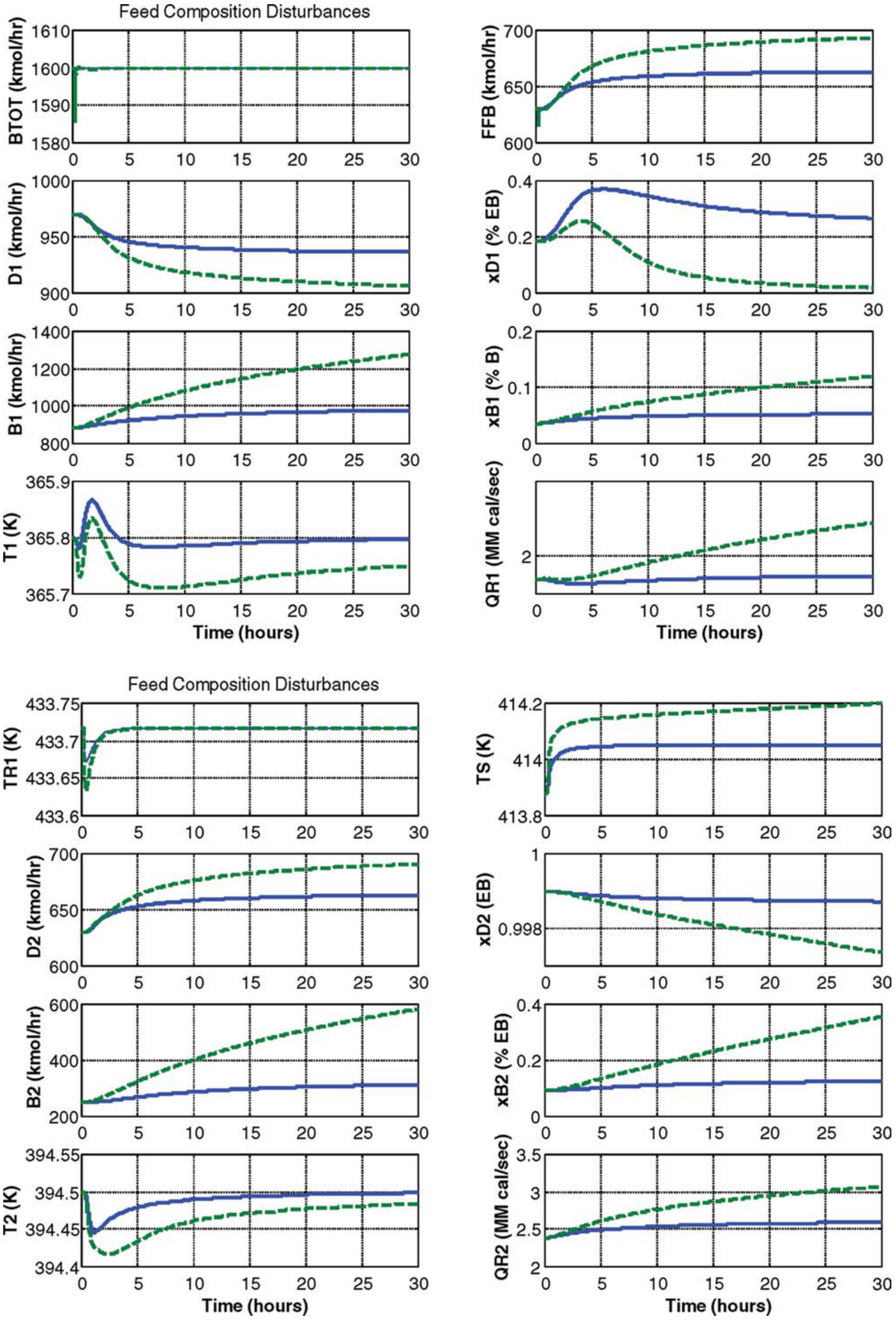

Figure 10. Feed composition disturbances.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Reactor level controllers are proportional with $K_c = 5$. Column base and reflux-drum level loops are proportional with $K_c = 2$.

Dynamic performance

Figure 9 shows the responses of the entire process for 20% disturbances in the setpoint of the ethylene feed flow controller. The solid lines are for a 20% increase. The dashed lines are for a 20% decrease. An increase in fresh ethyl feed produces increases in benzene fresh feed (FFB) and the EB product (D2), while flowrates increase throughout the plant. The purity of the EB product XD2(EB) is maintained quite close to its specified value of 99.9 mol % for these large disturbances.

Notice the large change in the DEB recycle flow (B2) from the second column. It increases from 251 up to 415 kmol/h, a

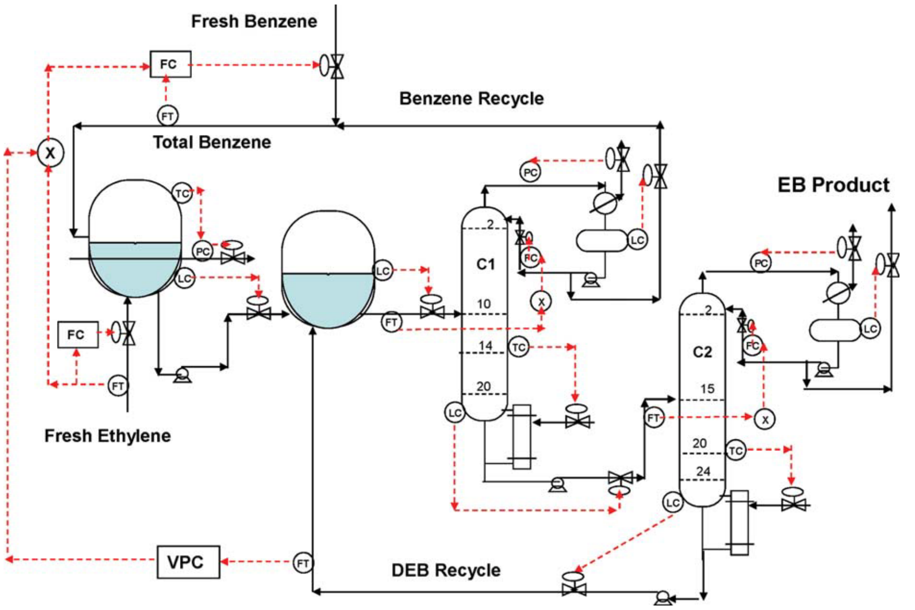

Figure 11. Modified plantwide control structure using VPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

65% increase for the 20% increase in ethylene fresh feed. This is a classical example of the "snowball effect" (a small change in throughput results in a large change in recycle flowrate). We return to this issue in the next section.

Figure 10 shows responses for two different feed composition disturbances. The solid lines are when the fresh benzene composition is changed from pure benzene to 95 mol % benzene and 5 mol % EB. For this disturbance, since the ethylene fresh feed is constant, the fresh feed of benzene must be increased to provide the benzene reactant required by the reaction stoichiometry. The same amount of EB is produced in the reactors, but there is some EB in the benzene fresh feed. So the distillate D2 from the second column increases. There is a fairly small change in the DEB recycle (B2), increasing from 251 to 319 kmol/h.

The other more significant disturbance shown as dashed lines in Figure 10 is when the fresh benzene composition is changed from pure benzene to 95 mol % benzene and 5 mol % DEB. We are putting more DEB into the system that must be converted into EB in the second reactor since DEB is recycled to extinction. There is a very large increase in B2 that climbs from 251 to almost 600 kmol/h after 30 h. The purity of the EB product in D1 drops well below its specification because there is more benzene dropping out the bottom of the first column [see xB1(B)]. In addition, the temperature controllers in both columns are unable to maintain their setpoint because of the gradual ramp disturbances that this column sees. Reboiler heat inputs are increasing, but temperatures hang below their setpoints.

The control structure shown in Figure 8 cannot handle this severe and difficult disturbance. Are there better control structures?

Modified control structure

The control structure shown in Figure 8 handles most disturbances fairly well but results in large changes in the DEB recycle flowrate. The disturbance in which DEB impurity is added into the fresh benzene feed cannot be handled because of extremely large changes in DEB recycle needed to recycle to extinction this component.

Several modified control structures were tested to overcome these problems. The generation of DEB depends on both reactor temperature and DEB concentrations in the reactors. As reactor volumes are fixed by the steady-state design, reactor temperature cannot be reduced without adversely affecting ethylene conversion. However, DEB concentrations can be affected by changing benzene recycle. Figure 7 illustrates the strong dependence of DEB recycle flowrate on total benzene flowrate. This suggests that using benzene recycle to lessen the impact of large DEB recycle flowrates may be possible.

In the original control structure, the total benzene flowrate is ratioed to the fresh ethylene flowrate using a fixed ratio. Therefore total benzene recycle is only changed if there is a change in the ethylene fresh feed flowrate. A modified control structure was developed that adjusts this ratio on the basis of changes in the DEB recycle flowrate (B2). This structure is a type of "valve position controller" (VPC). The B2 flowrate signal is the process variable signal to a proportional-only controller whose setpoint signal is the steady-state value of the B2 flowrate (251.2 kmol/h). The controller output signal of this controller is the BTOT/FFE ratio (2.537 at design conditions) and is fed into the multiplier. The other input to the multiplier is the flowrate of the ethylene fresh feed.

A proportional-only VPC controller is used because we do not want to maintain a constant B2 flowrate. We merely want to change benzene recycle somewhat to reduce the magnitude of the changes in DEB recycle. Several values of controller gain were evaluated using gains from 0.1 to 1. A controller gain of $K_c = 0.6$ was found to give good dynamic responses with very little oscillation (see Table 7).

Figure 11 shows the modified control structure with the VPC controller adjusting the BTOT/FFE ratio. All other

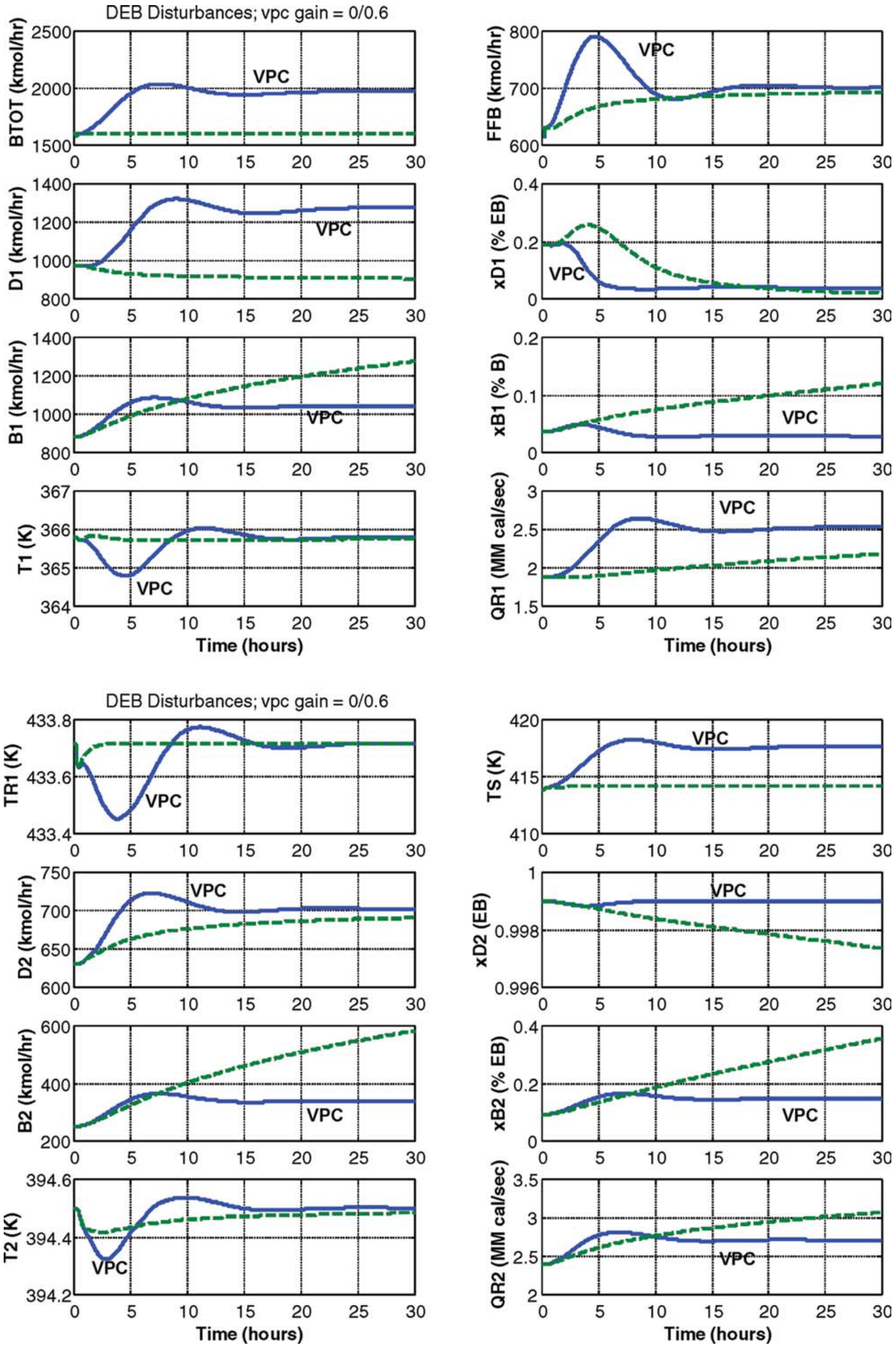

Figure 12. DEB feed composition disturbance with and without VPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

loops are unchanged. No retuning of temperature loops is required.

Figure 12 compares the responses of the system using the original structure (dashed lines) and the VPC structure (solid lines). The disturbance is the severe addition of DEB impurity into the fresh benzene feed. The original structure cannot handle this disturbance. The VPC structure handles it very well. Instead of a large buildup of DEB recycle, there is only a modest increase (from 251 to 337 kmol/h) because the benzene recycle has been increased from 1600 to 1978 kmol/h instead of remaining constant at 1600 kmol/h in the original control structure. EB product purity (xD2) is held very close

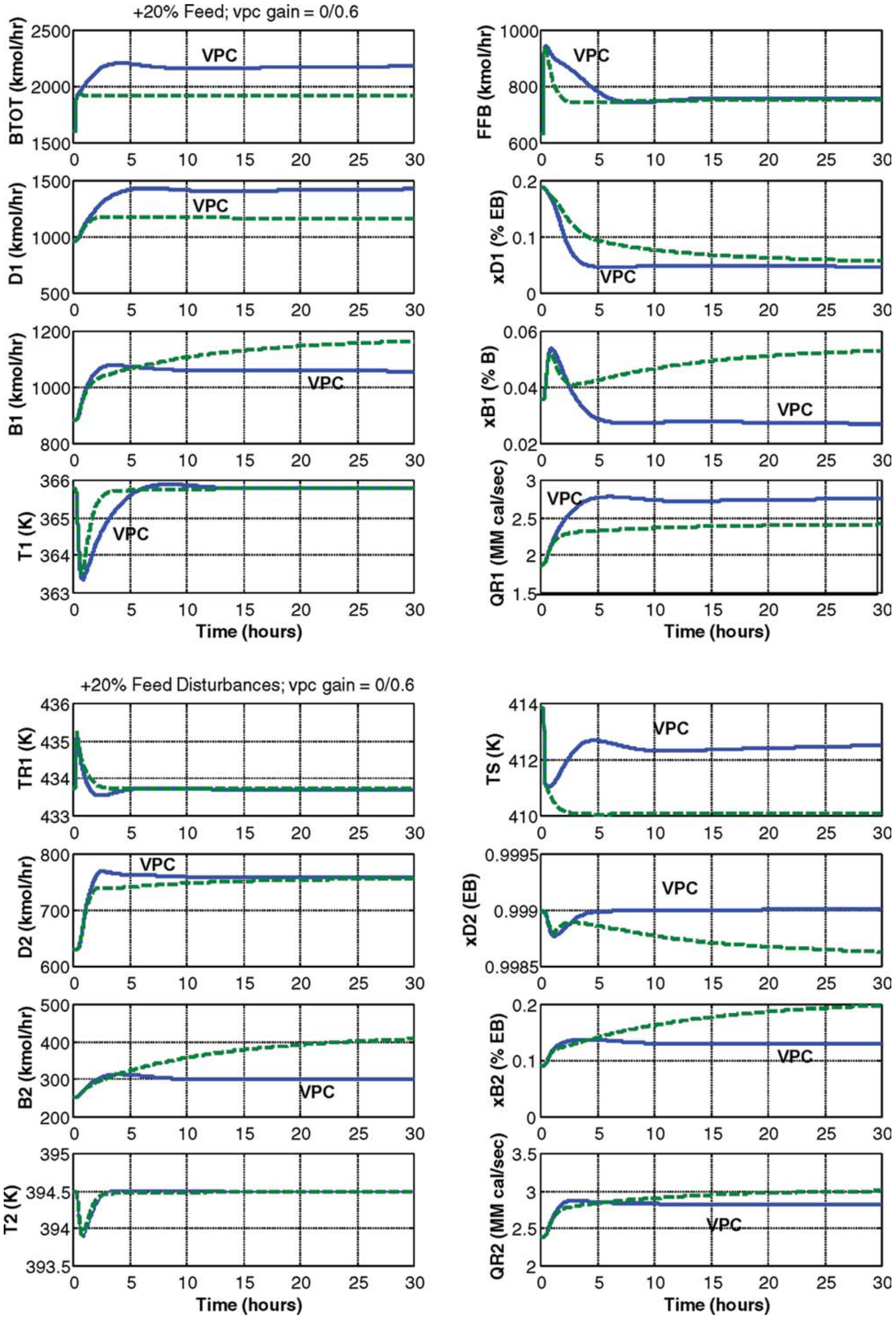

Figure 13. The +20% ethylene feed flowrate disturbance with and without VPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

to its specification. The composition of benzene in the bottoms of C1 is kept small with the VPC control structure instead of increasing significantly as it did in the original structure. The EB impurity in the recycled DEB stream is also kept small in the VPC control structure instead of increasing significantly as it did in the original structure.

The effect of the control structure change on reactor temperature control is interesting. As benzene recycle is increased in the VPC control structure and this stream is colder than the temperature of the first reactor, less heat has to be removed. The result is an increased in the required steam temperature TS.

Figures 13 to 15 give direct comparisons of the responses of the original control structure and the VPC control structure for the same feed flowrate and feed composition disturbances. The VPC control structure provides

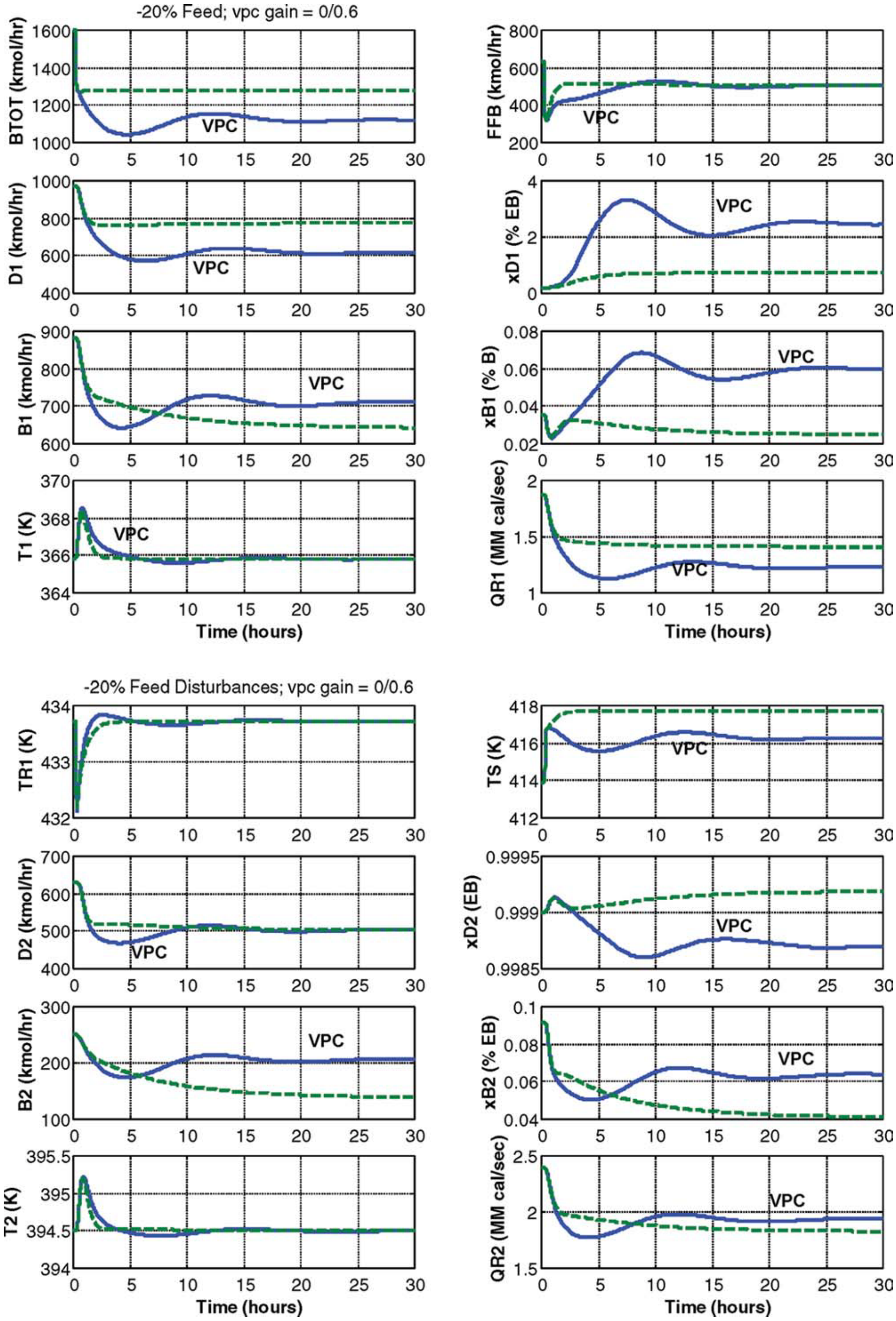

Figure 14. The −20% ethylene feed flowrate disturbance with and without VPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

improved dynamic control in terms of tighter product quality control and smaller changes in the DEB recycle flowrate.

These results demonstrate that the proposed plantwide control structure provides effective dynamic control of the EB process in the face of quite large disturbances.

Conclusion

The design and control of an interesting multiunit process has been explored. The two-reactor, two-column, two-recycle process presents challenging problems. The EB process displays several unusual features. The most unusual is the recycling to extinction of an undesirable byproduct DEB.

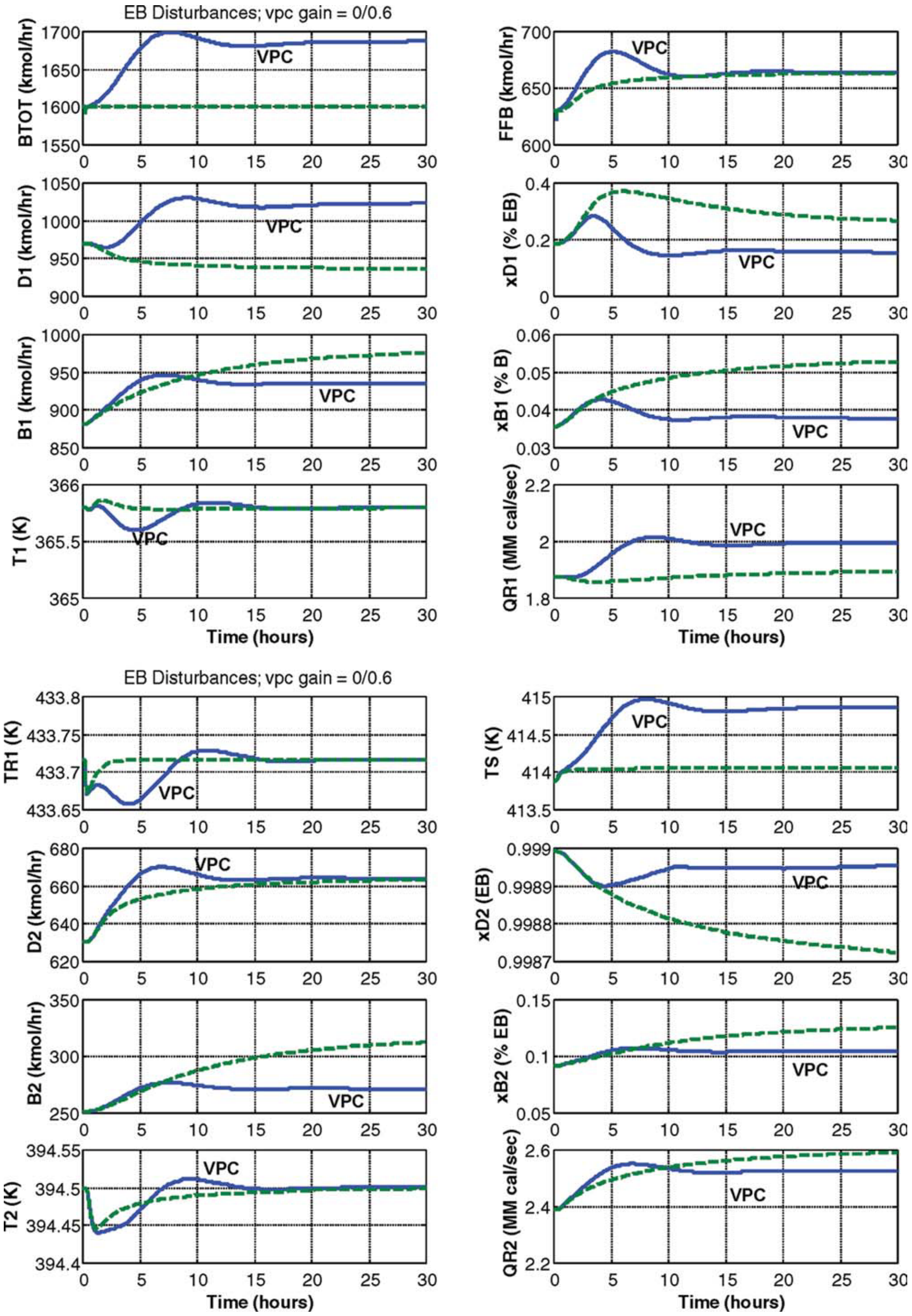

Figure 15. EB feed composition disturbance with and without VPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Significant design trade-offs between reactor size and recycle flowrates exist that require detailed economic analysis to find the optimum design that balances the competing effects of the design optimization variables.

Effective dynamic control of the multiunit process is achieved by the use of conventional controllers but configured in an unusual control structure. The straight-forward structure that simply ratios the total benzene recycle to the ethylene feed stream leads to very large changes in the recycle of the DEB and fails for some disturbances. A modified valve position control structure solves these problems by changing the benzene-to-ethylene ratio in response to changes in the DEB recycle flowrate. Very large disturbances can be effectively handled with the EB purity being maintained very close to its specification.

The Aspen Plus and Aspen Dynamics files for the EB process are available from the author upon request.

Notation

AC = condenser area (m^2)
AR = reboiler area (m^2)
D = distillate flowrate (kmol/h)
F = feed flowrate (kmol/h)
ID = column diameter
HP = high-pressure steam
K_C = controller gain (dimensionless)
LP = low-pressure steam
MP = medium-pressure steam
NF = feed stage
NT = total number of stages
OP = controller output signal
QC = condenser duty (MW)
QR = reboiler duty (MW)
R = reflux flowrate (kmol/h)
RR = reflux ratio (R/D)
SP = setpoint signal
TAC = total annual cost (10^6 \$/year)
TB = base temperature (K)
TD = reflux-drum temperature (K)
TR = reactor temperature (K)
VPC = valve-position controller
VR = reactor size (m^3)
zn(j) = column n feed composition (mole fraction j)
τ_I = controller integral time (min)

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