

Design and Control Degrees of Freedom

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One of the central problems in developing a steady-state process flowsheet is finding the number of variables that must be specified to completely define the process. This number is called the *design degrees of freedom*. Once this number has been found, the number of design optimization variables can be calculated by subtracting all variables that are set by specifications on production rate, product qualities, safety constraints, and environmental limitations. In principle, the design degrees of freedom are easily calculated by simply subtracting the number of equations from the number of variables. However, for typically complex industrial processes, there are many hundreds of variables and equations, and it is not a trivial job to make sure that the correct variables and equations have been defined. In addition, this conventional variables-minus-equations approach requires that a detailed model of the process be available. Once the plant has been specified, the design of a control structure requires that the *control degrees of freedom* be known. This is the number of variables that *can* be controlled. It is very easy to calculate this number, even for quite complex processes, because it is equal to the number of manipulated variables (the number of control valves in the process). These variables are different than the design optimization variables. This paper illustrates that the number of *design* degrees of freedom is equal to the number of *control* degrees of freedom for an important class of processes. For a much broader class of processes a slight modification of this equality must be used. Several progressively more complex recycle process case studies are used to demonstrate these results. The practical significance of this approach is that we do not need a model and we can avoid the tedious and error-prone procedure of accounting for all variables and equations.

Introduction

A. Design Degrees of Freedom: Competitive pressures have resulted in chemical process flowsheets that are increasingly complex and multivariable. It is often difficult to determine the design degrees of freedom of the process, i.e., the number of parameters or variables that must be specified to completely define the system (to yield a square set of equations). This number is important because subtracting one for production rate and subtracting the number of product-quality, safety, and environmental constraints from the degrees of freedom gives the number of design optimization variables available to the designer for maximizing some appropriate measure of profitability. Typical design optimization variables are reactor sizes, number of reactors, number of column trays, recycle flow rates, and recycle purities.

Conceptually, the determination of the design degrees of freedom is a simple job of subtracting the number of chemical and physical equations describing the system from the total number of variables. In very simple systems, this is easy. However, typical industrial chemical processes have many hundreds of variables and many hundreds of equations. It is quite easy to *not* do the accounting precisely and to calculate an incorrect number. Equations can be written that are not independent. Variables can be forgotten. Since we are taking the difference between two very large numbers, any small error in either the number of variables or the number of equations can produce a large error in the degrees of freedom.

Of course this variables-minus-equations approach also requires that a detailed steady-state model of the entire process be available. Deriving such models for a complex, multiunit plant can be quite difficult.

Modern steady-state flowsheeting and optimization software packages provide some assistance in finding the degrees of freedom, but they do not eliminate all of the problems in determining how many design optimization parameters are available and what variables are appropriate.

B. Control Degrees of Freedom: The discussion above applies to the steady-state design of a process. The concept of steady-state *design degrees of freedom* is different than the concept of dynamic *control degrees of freedom*. The control degrees of freedom are the number of variables that *can* be controlled in the process, and it is important to know this number when developing a control system for the process. Some of the variables that can be chosen to satisfy the control degrees of freedom are different than those chosen to satisfy the design degrees of freedom. At the design stage, we can set equipment sizes (number of trays in each column section and reactor size) in addition to setting stream flow rates, compositions, temperatures, and/or pressures. At the control stage (operating an existing plant), we can only set stream flow rates (change control valve openings).

In satisfying the control degrees of freedom we use one to set production rate. All liquid levels (except in recycle systems) and all gas pressures must be controlled, so these controlled variables consume an equivalent number of degrees of freedom. Additional degrees of freedom are used to control product qualities and to satisfy safety, environmental, and regulatory constraints. Any remaining degrees of freedom can be used to achieve optimum operation (e.g., minimize energy consumption, maximize yield, etc.) or to improve dynamic performance (e.g., maintain purities in recycle streams, hold pressures or temperatures at intermediate locations in the flowsheet, etc.).

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Unlike the design degrees of freedom, which are difficult to calculate, the control degrees of freedom are easily determined. Since all variables are stream flow rates, we simply count up the number of control valves in the plantwide process. Of course it is vital that good engineering practices are followed in installing all control valves. For example, there should never be two control valves in series in a liquid-filled line.

C. Design and Control Experience: During a number of plantwide studies dealing with a large variety of processes over the last decade, an interesting observation has been made: the number of *design* degrees of freedom seemed to be equal to the number of *control* degrees of freedom in many of these processes. Since the latter is so easy to calculate compared to the former, it would be very useful to know for what class of processes this relationship is true and how can it be modified to handle a more general class of chemical processes.

The purpose of this paper is to demonstrate that this equivalence of design and control degrees of freedom does hold in many processes and that it can be extended to a broader class of process. Many different cases have been studied, but only 11 cases are reported here. They span the range from simple ideal systems with two components, one reactor, and one column up to systems with seven chemical components, nonideal vapor–liquid equilibrium, nonequimolar overflow, three columns, and three reactors.

Previous Work

One would think that the literature on the subject of design degrees of freedom would be extensive. However, there have been relatively few discussions of these concepts. If we look at the standard undergraduate textbooks for process design, we find that Peters and Timmerhaus (1991) devote one page to it, while Douglas (1988) and Ulrich (1984) do not even mention it. The books by Rudd and Watson (1968) and Westerberg et al. (1979) discuss the conventional variables-minus-equations approach. The book on material and energy balance by Reklaitis and Schneider (1983) use degrees of freedom extensively. A very general mathematical approach is given by Georgiou and Floudas (1989).

The book by Henley and Seader (1981) discusses degrees of freedom for individual units of increasing complexity, starting from simple mixers and building up through individual trays to complete distillation columns, absorbers, liquid–liquid extraction columns, etc. The basic approach is the conventional variables-minus-equations technique.

The conventional approach has two problems. First, it is complex and prone to errors. Second, it requires that a model of the process be explicitly known. For a complex multiunit plantwide design, the modeling can be quite difficult, as we will demonstrate in some of the cases considered in this paper.

The pioneering work by Hanson et al. (1962) is in spirit similar to the approach used in this paper. They proposed the use of *The Description Rule*, which attempts to avoid the complexities of developing a model and counting variables and equations. The Description Rule states that, for any multistage contacting unit, the number of independent variables is equal to the number of variables that can be set by *construction* or *controlled by external means*. The construction variables are items like the number of trays in a section of the column. The variables that can be externally controlled are streams

like the feed rate, the heat input to the reboiler, the pressure in system, etc. This paper can be considered an extension of this approach. We desire a quick way to calculate degrees of freedom that avoids all the complexities of the rigorous conventional approach.

Most process control textbooks discuss control degrees of freedom (Seborg et al. (1983), Marlin (1995)) but most use the variables-minus-equations approach. Stephanopoulos (1984) uses the concept of *dynamic* degrees of freedom to account for nonzero derivatives during transients. This is different than the *control* degrees of freedom used in this paper.

Scope of This Paper

The case-study approach is used to illustrate the calculation of the design degrees of freedom and the control degrees of freedom for a number of increasingly complex processes. We begin with the simple reactor/stripper binary process with the $A \rightarrow B$ reaction, making all the usual simplifying assumptions: constant relative volatility, equimolar overflow, etc. Next we remove these assumptions one by one to see the effect of each on the degrees of freedom. Then we explore more complex flowsheets: multiple columns, multiple recycles, etc. Three quite complex processes conclude the study:

1. Luyben Challenge Process (Luyben and Luyben, 1995) involving three reactors, three columns, two recycles, three fresh feed streams, and six components.
2. Eastman Plantwide Problem (Downs and Vogel, 1993) involving a two-phase reactor, a condenser/separator, a stripper, a gas recycle stream, four fresh feeds, and seven components.
3. Vinyl Acetate Process involving a vaporizer, a gas-phase reactor, a condenser/separator, an absorber, an inert-removal unit, a gas recycle, two liquid recycles, and a heterogeneous azeotropic distillation column with a decanter.

The first part of the paper presents a restricted but important class of process in which design and control degrees of freedom are shown to be equal. The second part of the paper extends the approach to a broad spectrum of chemical processes.

Processes with Simple Columns and Liquid-Phase Reactors

Case 1: Figure 1 shows the process flow sheet. The chemistry consists of the reaction $A \rightarrow B$ taking place in a continuous liquid-phase stirred-tank reactor. The fresh feed stream is fed into the reactor along with a recycle stream from the top of a stripping column. Reactant A is not completely converted in one pass through the reactor, so the reactor effluent, which is binary mixture of A and B , is fed into a stripping column. The volatility of A is higher than that of B , so product B is removed from the bottom and reactant A is taken out the top for recycle back to the reactor.

We make as many simplifying assumptions as possible so as to strip away all but the essential parameters. We assume equimolar overflow in the stripper, which means that neither energy balances nor total balances are needed in the stripper (steady-state liquid and vapor rates are the same on all trays). Other assumptions are constant relative volatility (so there is only one vapor–liquid equilibrium equation per stage in this binary system and pressure and tray temperatures do not have to be explicitly listed as variables), isothermal

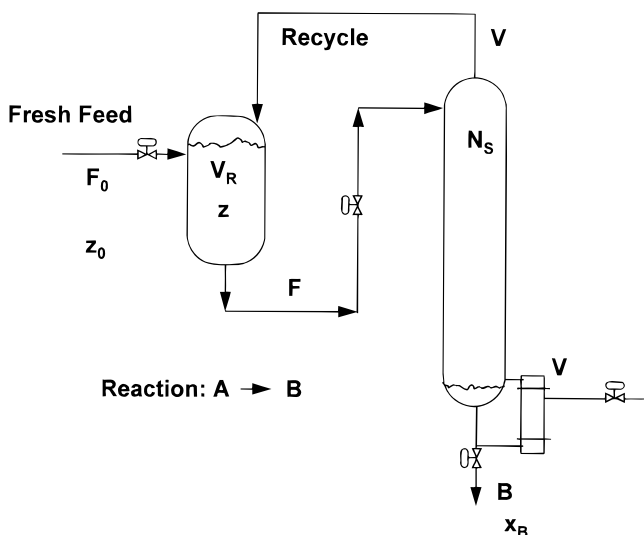


Figure 1. Reactor/stripper binary process.

operation of the reactor (specific reaction rate k is constant), theoretical trays, saturated liquid feed to the stripper, and partial reboiler. We will relax most of these in later cases.

There are many alternative ways of counting variables and equations. For example, if there are N_C chemical components in the process, we could consider that there are $N_C - 1$ component composition variables for each stream in the system, implicitly using the relationship that the sum of mole fractions must be unity. Alternatively we could use N_C component composition variables for each stream, but then we would add to our list of equations the relationship that the sum of mole fractions must be unity. Since the number of variables and the number of equations are both reduced by using the implicit sum-of-mole-fraction relationships for both vapor and liquid phases, we adopt this accounting system. In all our cases we try to use as few equations as possible so that we do not lose engineering insight about the problem variables and equations.

For similar reasons, in most of the cases studied we assume constant temperatures in all reactors and constant pressures in all columns. These temperatures and pressures and the corresponding heat transfer rates could be added to the list of variables, but then additional energy balance equations could also be added. The degrees of freedom would increase by one for each temperature and each pressure. Reactor temperatures and column pressures are important design optimization variables, but we do not include them in our accounting system in most of the cases.

We also do not include chemical reaction rates explicitly in the list of variables. They could be included, but then additional kinetic equations could be added, showing the dependence of reaction rates on compositions, temperature, and pressure. The degrees of freedom would remain the same.

A. Design Degrees of Freedom: Let the number of trays in the stripper be N_S . Assuming the fresh feed composition z_0 is given, we can list the variables and equations shown in Table 1.

The design degrees of freedom for this process are 4. Typically one of these is set by production rate (e.g., setting fresh feed flow rate F_0). A second would be consumed by specifying product purity (x_B , the mole fraction of component A in the stripper bottoms). This leaves two remaining variables for design optimization.

Table 1. Case 1: Binary Reactor/Stripper

		Variables	
compositions	reactor	z	1
	tray liquid	x_n	N_S
	tray vapor	y_n	N_S
	base liquid	x_B	1
	base vapor	y_B	1
flows	fresh feed	F_0	1
	reactor effluent	F	1
	vapor boilup	V	1
	bottoms	B	1
holdup	reactor	V_R	1
number of trays		N_S	1
total number variables = $2N_S + 9$			
component balances	Equations		
	reactor		1
	trays		N_S
total balances	base		1
	reactor		1
	base		1
VLE	trays		N_S
	base		1
total number equations = $2N_S + 5$			

Common choices are reactor holdup V_R and number of trays in the stripper N_S .

B. Control Degrees of Freedom: Now if we look again at Figure 1 and count the number of control valves, we find that the control degrees of freedom are also 4. So for this simple process, the design and control degrees of freedom are equal.

A typical control structure for this process would use F_0 to set production rate, V to hold product quality (x_B), F to hold reactor level, and B to hold base level. This consumes all of the control degrees of freedom.

C. The Effect of Surge Tanks: Note that the vapor from the stripper shown in Figure 1 is sent directly into the reactor. The reactor temperature is assumed constant, so the energy balance in the reactor would have to account for the vapor recycle stream. Suppose we make an equipment modification to the process, adding a condenser and a liquid surge drum at the top of the stripper and returning liquid to the reactor instead of vapor. We have added more variables (condensate composition and flow rate), but we have added exactly the same number of equations. Since the condenser is a total condenser, the compositions and flow rates of the vapor stream and the liquid stream are exactly the same under steady-state conditions. So the degrees of freedom remain the same.

However, we have added a control valve in the liquid line to the reactor. This valve would typically be used to control drum level. It appears that this now gives us a process in which the control degrees of freedom (5 from the five control valves) differ from the design degrees of freedom (4). Exactly the same dilemma would occur if we placed a surge tank between the reactor and the stripper.

Therefore, whenever we encounter a tank that serves only as surge with no flow splitting of its exiting stream, we do not count the control valve on this stream in our calculation of the *net* control degrees of freedom. The design degrees of freedom are equal to the net control degrees of freedom (with surge-drum valves not counted). We discuss the effects of liquid level control for more complex plants later in this paper.

Case 2: In the next series of case studies we want to see the effects of relaxing some of the simplifying assumptions. In Case 2 we remove the constant relative volatility assumption and use the appropriate bubble-

Table 2. Case 2: Nonconstant Relative Volatility

		Variables	
compositions	reactor	z	1
	tray liquid	x_n	N_S
	tray vapor	y_n	N_S
	base liquid	x_B	1
	base vapor	y_B	1
flows	F_0, F, V, B		4
temperatures	trays	T_n	N_S
	base	T_B	1
holdup	reactor	V_R	1
number of trays		N_S	1
total number variables = $3N_S + 10$			
		Equations	
component balances	reactor		1
	trays		N_S
	base		1
total balances	reactor		1
	base		1
VLE	trays		$2N_S$
	base		2
total number equations = $3N_S + 6$			

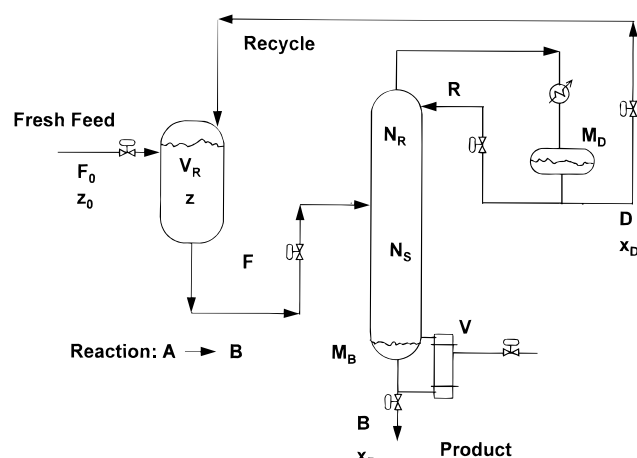
Table 3. Case 3: Nonequimolal Overflow and Nonconstant Relative Volatility

		Variables	
compositions	reactor	z	1
	tray liquid	x_n	N_S
	tray vapor	y_n	N_S
	base liquid	x_B	1
	base vapor	y_B	1
flows	F_0, F, B		3
	tray liquid	L_n	N_S
	tray vapor	V_n	N_S
	reboiler vapor	V_B	1
	reboiler	Q_R	1
heat transfer rate	trays	T_n	N_S
	base	T_B	1
	reactor	V_R	1
number of trays		N_S	1
total number variables = $5N_S + 11$			
		Equations	
component balances	reactor		1
	trays		N_S
	base		1
total balances	reactor		1
	trays		N_S
	base		1
VLE	trays		$2N_S$
	base		2
energy balances	trays		N_S
	reboiler		1
total number equations = $5N_S + 7$			

point calculations (whatever their degree of complexity) to relate vapor and liquid compositions. The only restriction we place on the VLE is that there is only one liquid phase. The model that we are using assumes only one liquid phase in equilibrium with a vapor phase. If the system is highly nonideal and multiple liquid phases are present, we need a different model.

Now we have more variables (tray temperatures and base temperature), but there are also more equations. There are two VLE equations per tray instead of only one in this binary system (one equation for each component that equates chemical potentials in the two phases). As mentioned earlier, we assume a constant and known pressure throughout the column. This would usually be held by condenser cooling. We continue to assume equimolal overflow.

As shown in Table 2, the design degrees of freedom are still 4 even though we have increased the number of variables and the number of equations. Thus we have

**Figure 2.** Reactor/column binary process.

illustrated that the complexity of the vapor–liquid equilibrium does not affect the degrees of freedom (provided no new phases are produced). Since the number of control valves remains unchanged, the control degrees of freedom are also still 4.

Case 3: Now we drop the equimolal overflow assumption.

A. Design Degrees of Freedom: Nonequimolal overflow means that each tray has its own liquid and vapor flow rates and energy balances must be used. We choose to not add vapor and liquid enthalpies to the list of variables because there are physical property equations relating temperatures and compositions to enthalpies. Accounting implicitly for these variables and equations reduces the numbers. Table 3 lists variables and equations. Once again the degrees of freedom remain at 4. Even though we now have many more equations and variables, the difference between the two remains the same.

B. Control Degrees of Freedom: Once again, the number of control valves remains unchanged, so the control degrees of freedom are still 4. We see clearly from this example that the use of the control degrees of freedom is much easier than the use of the design degrees of freedom, particularly as we make our models more and more complex and rigorous.

Case 4: Now we illustrate the effect of increasing the complexity of the flowsheet. Instead of using a stripper, we use a full distillation column with both stripping and rectifying sections and with reflux.

A. Design Degrees of Freedom: Figure 2 gives a sketch of the process. We have added a rectifying section, overhead condenser, and reflux drum. Reflux is pumped back to the top of the column, and distillate is recycled back to the reactor. We assume saturated liquid reflux and feed to the column. We assume a total condenser, so we need no VLE relationship in the reflux drum. For simplicity, we go back to the very simple model of equimolal overflow and constant relative volatility. The cases considered above illustrate that these simplifying assumptions do not change the degrees of freedom.

Table 4 lists variables and equations. The number of trays in the stripping section is N_S , and the number in the rectifying section is N_R . The more complex flowsheet gives us 6 degree of freedom. After specifying production rate (F_0) and product quality (x_B), we have four design optimization variables. These typically would be the number of stripping trays, the number of rectifying trays, the recycle flow rate (D), and the reactor

Table 4. Case 4: Full Distillation Column

compositions	Variables		
	reactor	z	1
	tray liquid	x_n	$N_S + N_R$
	tray vapor	y_n	$N_S + N_R$
	reflux drum	x_D	1
flows	base liquid	x_B	1
	base vapor	y_B	1
	fresh feed	F_0	1
	reactor effluent	F	1
	vapor boilup	V	1
holdup	distillate	D	1
	bottoms	B	1
	reflux	R	1
	reactor	V_R	1
	no. of stripping trays	N_S	1
	no. of rectifying trays	N_R	1

total number variables = $2N_S + 2N_R + 13$

component balances	Equations	
	reactor	1
	trays	$N_S + N_R$
	base	1
	reflux drum	1
total balances	reactor	1
	base	1
	reflux drum	1
VLE	trays	$N_S + N_R$
	base	1

total number equations = $2N_S + 2N_R + 7$

holdup (V_R). A four-dimensional search is required to optimize the steady-state design.

Since trays are integer variables, the rigorous solution of this type of problem uses mixed-integer nonlinear programming. It is often possible to greatly simplify the optimization problem by using heuristics for the design of the column. Two degrees of freedom can be removed by assuming that the optimum column design uses some multiple of the minimum number of trays (typically twice) and uses the optimum feed tray (the feed tray location that minimizes energy consumption). Then we are left with just a two-dimensional optimization problem with continuous variables (reactor holdup and recycle flow rate).

B. Control Degrees of Freedom: As Figure 2 shows, the new flowsheet has 6 control valves. This is exactly the number we found from our rigorous accounting of variables and equations. Thus, the control degrees of freedom give the increase in the number of degrees of freedom as the flowsheet becomes more complex.

These 6 control degrees of freedom would typically be used in a control structure in the following way.

1. One degree of freedom would set production rate by flow controlling F_0 .
2. One would hold product quality (x_B controlled by V).
3. There are three liquid levels, so three manipulated variables must be used (V_R controlled by F , M_D controlled by D , and M_B controlled by B).
4. The one remaining degree of freedom could be used to control recycle composition (x_D controlled by reflux flow rate R).

Case 5: All the preceding cases considered only a binary system with components A and B . Now let us look at a process in which we have three components. An isothermal reaction $A + B \rightarrow C$ occurs in a reactor. There are two fresh feed makeup streams that contain mostly reactants A (F_{0A}) and B (F_{0B}). We assume the compositions of the fresh feed streams ($z_{0A,j}$ and $z_{0B,j}$) are known.

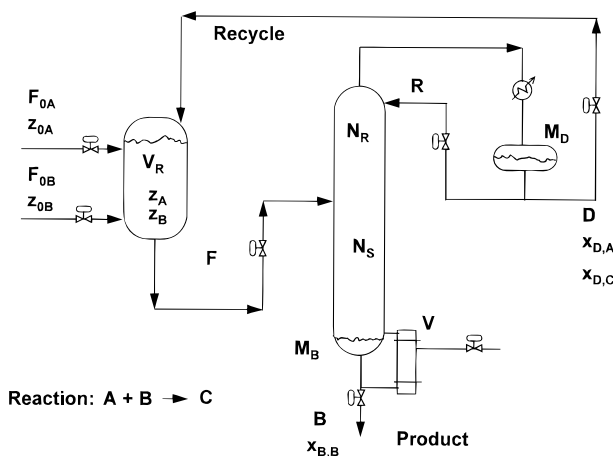


Figure 3. Reactor/column ternary process with one recycle.

Table 5. Case 5: Ternary Reactor/Column with One Recycle

compositions	Variables		
	reactor	z_j	2
	tray liquid	x_{nj}	$2(N_S + N_R)$
	tray vapor	y_{nj}	$2(N_S + N_R)$
	reflux drum	x_{Dj}	2
flows	base liquid	x_{Bj}	2
	base vapor	y_{Bj}	2
	fresh feeds	F_{0A}, F_{0B}	2
	reactor effluent	F	1
	vapor boilup	V	1
holdup	distillate	D	1
	bottoms	B	1
	reflux	R	1
	reactor	V_R	1
	no. stripping trays	N_S	1
	no. rectifying trays	N_R	1

total number variables = $4N_S + 4N_R + 18$

component balances	Equations	
	reactor	2
	trays	$2(N_S + N_R)$
	base	2
	reflux drum	2
total balances	reactor	1
	base	1
	reflux drum	1
VLE	trays	$2(N_S + N_R)$
	base	2

total number equations = $4N_S + 4N_R + 11$

The reactor effluent is fed into a distillation column to separate product C from unreacted reactants A and B (see Figure 3). We assume the relative volatilities are in the following order: $\alpha_A > \alpha_B > \alpha_C$. This means that components A and B both go overhead together in the column, and the single recycle stream D contains essentially all the A in the reactor effluent stream F and most of the B . Some small amount of B goes out in the bottom product stream B as an impurity ($x_{B,B}$). The concentrations in the reactor are z_A , z_B , and z_C .

Since there are three components, the implicit accounting system has two compositions for each stream in the process. For simplicity, we assume constant relative volatilities and equimolar overflow; but as we demonstrated above, these assumptions do not affect the degrees of freedom.

A. Design Degrees of Freedom: Table 5 lists variables and equations. There are 7 degrees of freedom. Comparing these results with case 4 we see that increasing the number of components by one has increased the degrees of freedom by one. The process equipment looks essentially the same: one reactor and

one column. Does this imply that if we added a fourth component, the degrees of freedom would increase to 8? The answer is no. Suppose one of the fresh feed streams contained a fourth component D that had a volatility less than C . What would happen to this component? It would run through the reactor and drop out the bottom of the column in the bottoms product as an additional impurity. There is no way to regulate the amount of D anywhere in the process. Thus the degrees of freedom are unchanged. The presence of D would increase temperatures in the stripping section and base of the column, and it would affect concentrations in the reactor. Of course if D were a very light component, it could not get out of the system, so this flowsheet is an unworkable one in this situation. We will demonstrate this effect in case 9 considered later in this paper.

What has led to the increase in the degrees of freedom? Note that Figure 3 shows there are two fresh feed streams. This is what gives the additional degree of freedom.

One of the design degrees of freedom would be used to specify the purity of the product stream B . If A is much more volatile than B , this impurity specification is $x_{B,B}$. If the volatilities of A and B are close, the impurity specification could be on the sum of $x_{B,A}$ and $x_{B,B}$. Note that we cannot use 2 degrees of freedom by specifying both $x_{B,A}$ and $x_{B,B}$ because the column is separating between B and C . There is no way the separation between A and B can be independently changed if only one simple column is used in the flowsheet.

One of the degrees of freedom can be used to set production rate. One of the fresh feeds, either F_{0A} or F_{0B} , can be used, but not *both*. The other fresh feed must be used to satisfy the reaction stoichiometry and component losses in product streams.

This leaves 5 degrees of freedom, so there are five design optimization variables. These might be reactor holdup V_R , recycle flow rate D , recycle purity $x_{D,C}$, number of stripping section trays N_S , and number of rectifying section trays N_R .

B. Control Degrees of Freedom: Counting control valves in Figure 3 gives 7 degrees of freedom. One is used to set production rate (for example, flow controlling reactor effluent F). One is used to control product purity (the amount of B in the bottoms product, $x_{B,B}$). There are three liquid levels, so 3 degrees of freedom are needed: hold V_R with F_{0B} , hold M_B with B , and hold M_D with D .

There are 2 degrees of freedom left. One must be used to satisfy the chemical stoichiometry; for example, F_{0A} can be manipulated to control the concentration of A in the reactor z_A . The final degree of freedom can be used to control recycle purity $x_{D,C}$ by manipulating R .

Case 6: If the volatilities of the components are changed such that $\alpha_A > \alpha_C > \alpha_B$, we get a more complex flowsheet. Two columns are needed to separate the two reactants from the intermediate-boiling product. Figure 4 shows one possible flowsheet using the indirect separation sequence ("heavy-out-first"). The heaviest component B is recycled from the bottom of the first column in stream B_1 . The lightest component A is recycled from the top of the second column in D_2 . The design and control of this process has been studied in several papers: Tyreus and Luyben (1993); Luyben et al. (1996).

The alternative separation sequence (the direct or "light-out-first") recycles A from the top of the first

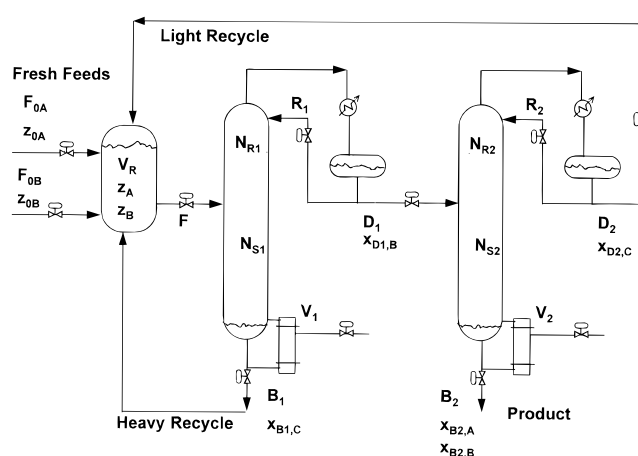


Figure 4. Reactor/two-column ternary process with two recycles.

Table 6. Case 6: Two Distillation Columns, Two Recycles

		Variables	
compositions	reactor	z_j	2
	tray liquid	x_{nj}	$2\sum N_T$
	tray vapor	y_{nj}	$2\sum N_T$
	reflux drums	x_{Dj}	4
	base liquid	x_{Bj}	4
	base vapor	y_{Bj}	4
	fresh feeds	F_{0A}, F_{0B}	2
	reactor effluent	F	1
	vapor boilups	V_n	2
	distillates	D_n	2
flows	bottoms	B_n	2
	refluxes	R_n	2
	reactor	V_R	1
	no. stripping trays	N_{S1}, N_{S2}	2
	no. rectifying trays	N_{R1}, N_{R2}	2
total number variables = $4\sum N_T + 30$			
component balances	Equations		
	reactor		2
	trays		$2\sum N_T$
	bases		4
	reflux drums		4
total balances	reactor		1
	bases		2
	reflux drums		2
VLE	trays		$2\sum N_T$
	bases		4
total number equations = $4\sum N_T + 19$			

column and B from the bottom of the second column. The degrees of freedom of these two processes are the same, so we only consider the first.

A. Design Degrees of Freedom: Table 6 lists variables and equations. The total number of stripping and rectifying trays in both columns is defined as $\sum N_T$. Since there are two columns, there are many more variables, but there are also many more equations. The degrees of freedom have increased from 7 in case 5 with one column to 11 in this case, which has two columns. The degrees of freedom increase by 2 for every column section and reflux drum or column base added. This is exactly what we found in the binary system when we changed from a stripper (case 1) to a full column (case 4).

There are many alternatives for choosing these 11 design degrees of freedom. Those used by Tyreus and Luyben (1993) were as follows:

1. Production rate (1 degree of freedom): F_{0A} .
2. Product quality (2 degrees of freedom): $x_{B2,B}$ and $x_{B2,A}$.

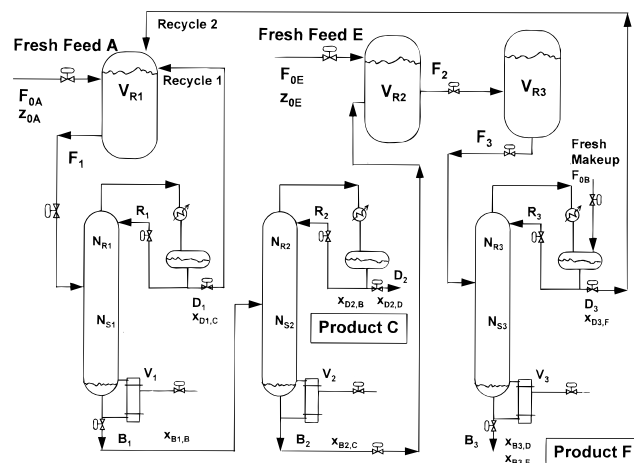


Figure 5. Luyben challenge process.

3. Light recycle flow rate and purity (2 degrees of freedom): D_2 and $x_{D2,C}$.

4. Heavy recycle flow rate and purity (2 degrees of freedom): B_1 and $x_{B1,C}$.

5. Total trays in each column set equal to twice the minimum (2 degrees of freedom).

6. Optimum feed tray locations in both columns (2 degrees of freedom).

B. Control Degrees of Freedom: Figure 4 shows there are 11 control valves in this two-column process, which again matches the more difficultly calculated design degrees of freedom.

As Tyreus and Luyben (1993) demonstrated, there are a large number of control structures for this process, many of which do *not* work. One of the control structures they found to work (CS1) had the 11 control loops listed below. The first two fix the production rate. The next five control liquid inventories. The next two control product quality. The final two improve dynamic performance by ratioing reflux flow rates to column feed flow rates. Note that both fresh feeds are brought in on level control with this control structure.

1. Total B recycle flow controlled ($B_1 + F_{0B}$).
2. Total A recycle flow controlled ($D_2 + F_{0A}$).
3. V_R controlled F .
4. M_{D1} controlled by D_1 .
5. M_{D2} controlled by F_{0A} .
6. M_{B1} controlled by F_{0B} .
7. M_{B2} controlled by B_2 .
8. Impurity of B in product ($x_{B2,B}$) controlled by V_1 , using a cascade $x_{D1,B}$ to V_1 secondary loop.
9. Impurity of A in product ($x_{B2,A}$) controlled by V_2 .
10. Reflux flow rate R_1 ratioed to F .
11. Reflux flow rate R_2 ratioed to D_1 .

Case 7: A recent paper (Luyben and Luyben, 1995) discusses a chemical process containing two reaction steps, three distillation columns, two recycle streams, and six chemical components. Figure 5 shows the flowsheet. The overall effect of the process is to feed A and E and make products C and F . This is accomplished in two reaction steps with intermediate components B and D circulating around inside the process. Component relative volatilities are $\alpha_A > \alpha_B > \alpha_C > \alpha_D > \alpha_E > \alpha_F$.

In the first reaction step, the reaction $A + B \rightarrow C + D$ takes place. Fresh feed of A and two recycle streams are fed into this first reactor. The reactor effluent is separated in a distillation column that produces a mixture of A and B overhead and recycles this stream back to the reactor. The bottoms stream from this

Table 7. Case 7: Luyben Challenge Process

		Variables	
compositions	reactors	$z_{n,j}$	15
	tray liquid	$x_{n,j}$	$5\sum N_T$
	tray vapor	$y_{n,j}$	$5\sum N_T$
	reflux drums	x_{Dj}	15
	base liquid	x_{Bj}	15
	base vapor	y_{Bj}	15
	fresh feeds	F_{0A}, F_{0B}, F_{0E}	3
	reactor effluents	F_n	3
	vapor boilups	V_n	3
	distillates	D_n	3
flows	bottoms	B_n	3
	refluxes	R_n	3
	reactors	$V_{R,n}$	3
	no. stripping trays		3
	no. rectifying trays		3
total number variables = $10\sum N_T + 67$			
		Equations	
component balances	reactors		15
	trays		$5\sum N_T$
	bases		15
	reflux drums		15
total balances	reactors		3
	bases		3
	reflux drums		3
	trays		$5\sum N_T$
VLE	bases		15
total number equations = $10\sum N_T + 69$			

column, containing mostly C and D , is fed to another column that takes a product stream of mostly C overhead.

The bottoms stream from this second column is fed into a second reaction section (two reactors in series) in which the reaction $D + E \rightarrow F + B$ occurs. A fresh feed stream of component E is also fed into this reaction step. Reactor effluent is separated in a third column into a bottoms product of mostly F and a distillate stream that is recycled back to the first reaction section. There is a small makeup stream (F_{0B}) of component B that is added in the reflux drum of the third column. In theory, B and D just recycle around inside the process. However, there are small losses of these components, so there must be some makeup of at least one of these components to satisfy the overall component material balances.

A. Design Degrees of Freedom: Table 7 lists variables and equations. With six components and three columns there are large numbers of equations and variables. We define $\sum N_T$ as the total number of stripping and rectifying trays in all three columns.

The degrees of freedom are 18. In moving from case 6 (which has 11 degrees of freedom) to this case, we have added two columns (4 degrees of freedom) and two reactors (2 degrees of freedom). These account for 6 of the 7 additional degrees of freedom. We have also added another makeup fresh feed stream, which gives us the final degree of freedom.

The design degrees of freedom used by Luyben and Luyben (1995) in their heuristic design were one for production rate (F_{0A}), four for product purities ($x_{D2,B}$, $x_{D2,D}$, $x_{B3,D}$, $x_{B3,E}$), three for recycle purities ($x_{D1,C}$, $x_{B2,C}$, $x_{D3,F}$), six for the number of trays (twice minimum) and feed trays locations (optimum) in the three columns, and one from the assumption of equal volumes in the second and third reactors. The remaining three degrees of freedom were used as design optimization parameters: first reactor holdup V_{R1} , recycle flow rate from the first column D_1 , and recycle flow rate from the third column D_2 .

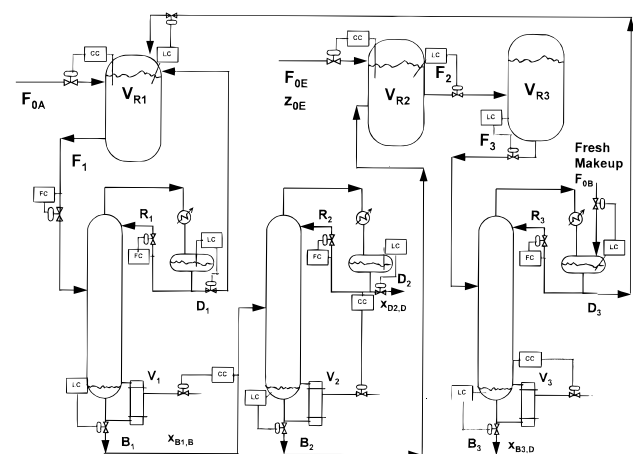


Figure 6. Control structure.

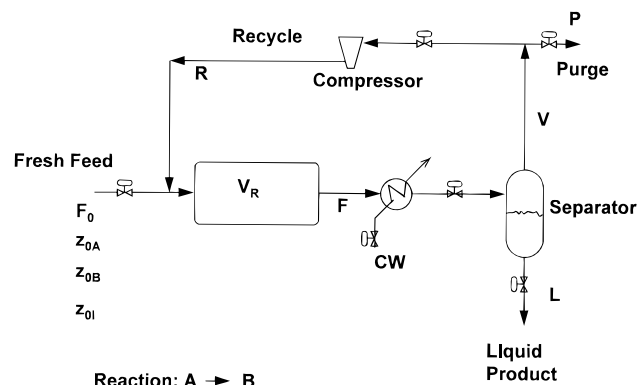


Figure 7. Westerberg process.

B. Control Degrees of Freedom: Counting control valves in Figure 5 quickly gives us the 18 degrees of freedom. Luyben and Luyben (1995) demonstrated that there are many control structures that do *not* work in this complex process, and they presented two that do work. Figure 6 shows one of these control schemes.

Extended Class of Processes

In the seven cases considered above, the design degrees of freedom are equal to the control degree of freedom. All of these processes had liquid-phase reactors and simple distillation columns (single-feed, two-products). In the sequence of cases given below we consider processes with other unit operations: gas-phase reactors, condenser/separators, sidestream columns, etc. We show that a modified, but still very simple procedure, is needed to calculate design degrees of freedom.

Case 8: A somewhat different ternary system discussed by Westerberg et al. (1979) is shown in Figure 7. The fresh feed stream F_0 contains a reactive component A and some inert component I , which is not involved in the reaction $A \rightarrow B$. Fresh gaseous feed and a gas recycle stream R are fed into a gas-phase reactor, and reactor effluent F is cooled in a condenser and flashed into the separator. Liquid product L leaves from the bottom of the drum and the vapor stream from the drum is split into a purge stream P , which is necessary in order to prevent the buildup of the inert component, and the recycle stream R , which is compressed and returned to the reactor inlet.

The reactor is adiabatic and reactor temperature T_R is a variable in this example. The pressures in the reactor (P_R) and in the separator (P_S) are also variables.

Table 8. Case 8: Westerberg Process with Inert Component

Component	Variables		
compositions	reactor	z_j	2
	separator liquid	x_j	2
	separator vapor	y_j	2
flows	fresh feed	F_0	1
	reactor effluent	F	1
	separator liquid	L	1
	separator vapor	V	1
	purge	P	1
	recycle	R	1
	Fresh Makeup	F_{0B}	1
holdup	reactor	V_R	1
	reactor	T_R	1
	separator	T_S	1
heat transfer rate	condenser	$Q_{condenser}$	1
pressures	reactor	P_R	1
	separator	P_S	1
total number variables = 18			
component balances	Equations		
	reactor		2
total balances	separator		2
	reactor		1
VLE	separator		1
	purge splitter		1
energy balances	separator		3
	reactor		1
	condenser		1
total number equations = 12			

Energy balances for the reactor and around the cooler/separator are included.

Note that this process is similar to case 1. The reaction is the same, and the flowsheet looks somewhat similar, but now there is an inert component, and we have two streams exiting the process. Table 8 lists variables and equations. The design degrees of freedom are 6. The number of control valves is also 6. So it appears that this type of process can be analyzed in the same way. However, as we will show in later cases, we need to modify our method.

A. Reactor Effects: A liquid-phase reactor has 3 degrees of freedom: throughput, holdup, and temperature. Pressure is usually not a factor. A liquid-phase reactor also has three control valves: inlet, exit, and coolant. A gas-phase reactor has the additional degree of freedom of pressure, but it has the same number of valves. Therefore, we can take the number of valves and add one to get degrees of freedom for a gas-phase reactor.

B. Liquid Surge Effects: The liquid level in a liquid-phase reactor is a degree of freedom because holdup in reactive systems affects the steady-state conditions in the process. The liquid holdups in all nonreactive vessel have no effect on the steady state, and therefore they should not be included in the design degrees of freedom. Surge tanks were mentioned earlier in the paper, but reflux drums, column bases, separators, decanters, and vaporizers are in the same category: their sizes do not affect the steady state. Yet we need control valves to hold these liquid levels. Therefore, we should take the total number of control valves and subtract the number of nonreactive liquid holdups. If we did this in the first seven cases, we would not get the correct design degrees of freedom, so we must correct our number by considering the number of column sections.

C. Column Section Effects: For a single-feed, two-product column there are two sections: rectifying and stripping. The number of trays in each section is a design degree of freedom. There are also two nonreac-

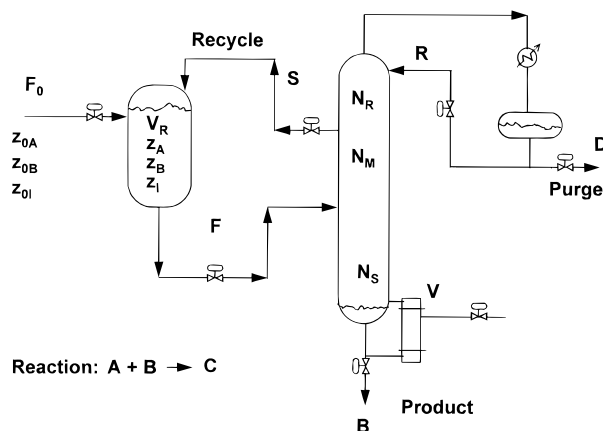


Figure 8. Reactor/sidestream column process.

tive liquid inventories in this plain-vanilla column: reflux drum and column base. These two numbers fortuitously compensate for each other in our degrees of freedom count. In a more general case the simple relationship does not hold.

Let us return to Case 8 and use the new accounting system. There are six valves in the process. There is one gas-phase reactor, which increases the count by one, and one nonreactive liquid holdup, which decreases the count by one. The following equation predicts the degrees of freedom (DOF) for a broad class of chemical processes, as the remaining cases demonstrate.

$$N_{\text{valves}} + N_{\text{sections}} + N_{\text{gas reactors}} - N_{\text{nonreactive levels}} = \text{DOF}$$

Case 9: Figure 8 shows a flowsheet in which a sidestream column is used for separation. The chemistry is the same as in case 8: two reactive components *A* and *B* and one inert *I*. The column has three sections with N_S stripping trays, N_R rectifying trays, and N_M trays between the feed tray and the sidestream drawoff tray. The column separates the reactor effluent into a bottoms product stream *B* (most component *B*), a sidestream recycle stream *S* (mostly component *A*), and a purge stream *D* (mostly component *I*). Table 9 lists variable and equations, giving 8 degrees of freedom. There are seven control valves, three column sections, and two nonreactive liquid holdups. The equation above gives

$$\text{DOF} = 7 + 3 - 2 = 8$$

Case 10: The Eastman Plantwide Control process presented by Downs and Vogel (1993) contains seven components, a liquid-phase reactor (with only a vapor stream leaving the reactor), a stripper, and a gas recycle stream. Figure 9 gives a sketch of the process. There are four reactions occurring: $A + C + D \rightarrow G$, $A + C + E \rightarrow H$, $A + E \rightarrow F$, $3D \rightarrow 2F$. Four gas fresh feed streams enter the process. One of these is fed into the bottom of the stripper. The vapor stream leaving the reactor is cooled before entering a separator. Liquid from the separator is fed into a stripper, which produces a bottoms product stream. Vapor from the separator is split between a gas purge and a recycle stream back to the reactor. The vapor from the stripper is also fed into the reactor. The reactor is cooled by manipulating cooling water flow rate to cooling coils.

In our analysis we use nonideal VLE and do not assume equimolal overflow. Reactor temperature and

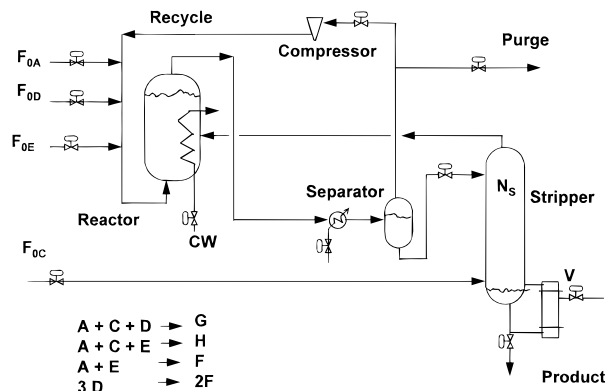


Figure 9. Eastman process.

Table 9. Case 9: Sidestream Column

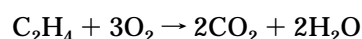
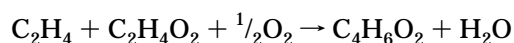
Variables			
compositions	reactor	z_j	2
	tray liquids	$x_{n,j}$	$2N_T$
	tray vapors	$y_{n,j}$	$2N_T$
	reflux drum	$x_{D,j}$	2
	base liquid	$x_{B,j}$	2
flows	base vapor	$y_{B,j}$	2
	fresh feed	F_0	1
	reactor effluent	F	1
	bottoms	B	1
	purge	P	1
	reflux	R	1
	vapor boilup	V	1
	sidestream	S	1
holdup	reactor	V_R	1
number of trays	three section	N_S, N_M, N_R	3
total number variables = $4N_T + 19$			
Equations			
component balances	reactor		2
	trays		$2N_T$
	reflux		2
	base		2
total balances	reactor		1
	base		1
	reflux drum		1
VLE	trays		$2N_T$
	base		2
total number equations = $4N_T + 11$			

pressure are not assumed constant. Pressure drops around the gas loop are neglected, so there is only one pressure in the system. Since there are seven chemical components, there are six composition variables for each stream. The compositions of the separator vapor and purge and recycle streams are the same.

Table 10 lists variables and equations for this process. The design degrees of freedom are 10. The number of control valves in the process is 11. The number of separators and column bases is two. The number of column sections is one. Applying the DOF equation gives 10 degrees of freedom.

$$\text{DOF} = 11 + 1 - 2 = 10$$

Case 11: As our final case we consider the vinyl acetate process sketched in Figure 10. This process contains seven components. The chemistry consists of two reactions, which produce vinyl acetate ($C_4H_6O_2$) from ethylene, oxygen, and acetic acid ($C_2H_4O_2$) and form byproducts of water and carbon dioxide.



Fresh acetic acid and a liquid acetic acid recycle

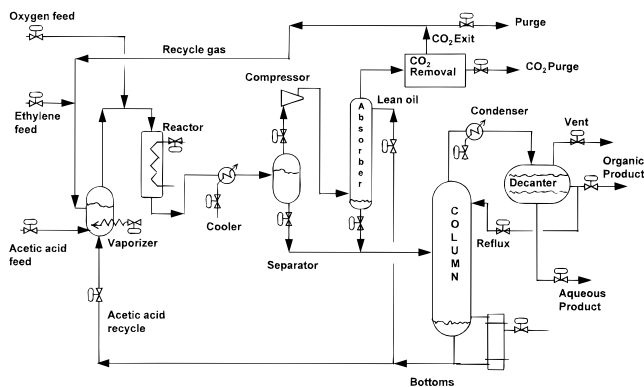


Figure 10. Vinyl acetate process.

Table 10. Case 10: Eastman Process

	Variables		
compositions	reactor liquid	$x_{R,j}$	6
	reactor vapor	$y_{R,j}$	6
	stripper liquids	$x_{n,j}$	$6N_S$
	stripper vapors	$y_{n,j}$	$6N_S$
	base liquid	$x_{B,j}$	6
	base vapor	$y_{B,j}$	6
flows	separator liquid	$x_{S,j}$	6
	separator vapor	$y_{S,j}$	6
	fresh feeds	$F_{0,n}$	4
	reactor vapor	$V_{reactor}$	1
	tray vapors	V_n	N_S
	tray liquids	L_n	N_S
	reboiler vapor	V_B	1
	bottoms	B	1
	separator vapor	V_S	1
	separator liquid	L_S	1
	purge	P	1
	recycle	R	1
	reactor	$Q_{reactor}$	1
	condenser/sep.	Q_{cond}	1
	reboiler	$Q_{reboiler}$	1
holdup	reactor	V_R	1
number of trays		N_S	1
temperatures	trays		N_S
	base		1
	reactor		1
	separator		1
pressure		P	1
total number variables = $15N_S + 56$			
component balances	Equations		
	reactor		6
	separator		6
	stripper trays		$6N_S$
	stripper base		6
	reactor		1
total balances	separator		1
	purge splitter		1
	stripper trays		N_S
	stripper base		1
	reactor		7
	separator		7
VLE	stripper trays		$7N_S$
	stripper base		7
	reactor		1
	condenser/separator		1
energy balances	stripper trays		N_S
	stripper base		1
	reactor		1
	condenser/separator		1
total number equations = $15N_S + 46$			

stream are fed into a vaporizer along with a gas recycle stream and fresh ethylene feed. Oxygen is added after the vaporizer, and reactions occur in a gas-phase reactor. Reactor effluent is cooled and fed into a separator. Vapor from the separator is compressed and fed into an absorber to recover vinyl acetate. Recycled acetic acid is used as lean oil in the absorber. Exit gas from the absorber is sent to a CO₂-removal unit, which

Table 11. Case 11: Vinyl Acetate Process

	Variables	
compositions	vaporizer x and y	12
	reactor	6
	separator x and y	12
	absorber x and y	$12N_A$
	CO ₂ unit streams	12
	column trays x and y	$12N_T$
	base x and y	12
	decanter x's and y	18
	fresh feeds	3
	recycle gas	1
	recycle acetic acid	1
	vaporizer exit	1
flows	reactor exit	1
	separator liquid and vapor	2
	absorber liquids and vapors	$2N_A$
	absorber lean oil and bottoms	2
	CO ₂ purge and exit	2
	purge	1
	column reflux and bottoms	2
	column liquids and vapors	$2N_T$
	column reboiler vapor	1
	decanter vent	1
	decanter liquids	2
	decanter vapors	2
temperatures	vaporizer and reactor	2
	separator and decanter	2
	absorber trays	N_A
	column trays	N_T
pressures	column base	1
	separator, absorber, column	3
heat transfer rates	vaporizer, reactor, cooler	3
	reboiler, condenser	2
number of trays	absorber, stripping, rectifying	3
	reactor	1
total number variables = $15(N_A + N_T) + 109$		
component balances	Equations	
	vaporizer	6
	reactor	6
	separator	6
	absorber	$6N_A$
	CO ₂ unit streams	6
	column trays	$6N_T$
	base	6
	decanter	6
	vaporizer	1
	reactor	1
	separator	1
total balances	absorber trays	N_A
	CO ₂ unit	1
	column trays	N_T
	column base	1
	decanter	1
	purge split	1
	acetic acid split	1
	vaporizer	7
	separator	7
	absorber trays	$7N_A$
	column trays	$7N_T$
	column base	7
phase equilibrium	decanter	14
	CO ₂ unit	7
	pressure drop	1
	energy balances	1
component splits	vaporizer	1
	reactor	1
	cooler/separator	1
	absorber trays	N_A
	column trays	N_T
	column base	1
	condenser/decanter	1
	total number equations = $15(N_A + N_T) + 92$	

produces a CO₂ purge stream and gas recycle. Another purge stream is used to remove the small amount of ethane that is in the fresh ethylene makeup feed.

The liquid streams from the separator and the bottom of the absorber are combined and fed into a distillation

column. The bottoms from the column are split into two streams: absorber lean oil and recycled acetic acid. The overhead vapor condenses into two liquid phases because of the nonideality of the phase equilibrium. The aqueous phase from the decanter (mostly water) is removed as product and sent to further processing, which we do not consider here. Some of the organic phase (mostly vinyl acetate) is refluxed back to the column, and some is removed for further processing.

The CO₂-removal unit is modeled as a simple component splitter with the recoveries of all seven components specified. The pressures in the vaporizer and reactor are assumed to be the same as the pressure in the separator. The pressure in the absorber is calculated from the pressure drop through the CO₂-removal unit.

Table 11 gives the very long list of variables and equations. The degrees of freedom of this complex process are 17. There are 19 control valves, one gas-phase reactor, six nonreactive levels (vaporizer, separator, absorber base, column base, aqueous phase in the decanter, and organic phase in the decanter), and three column sections (one in the absorber and two in the column). The DOF equation gives

$$\text{DOF} = 19 + 3 + 1 - 6 = 17$$

Conclusions

This paper has demonstrated that there is an easy way to determine the design degrees of freedom. For a certain class of processes, we just count the number of control valves in the process. The design and the control degrees of freedom are same in number, but different parameters are used to satisfy them. For a broader class of processes, we must modify the procedure to account for nonreactive liquid levels, column sections, and gas-phase reactors.

Several case studies of increasing complexity have been presented to show the effects of various types of flowsheets and physical properties. The complexity of the phase equilibrium and the physical properties does not affect the degrees of freedom. The structure of the flowsheet is what determines the design degrees of freedom.

As a qualitative explanation of why there is an equivalence between design and control degrees of freedom, consider the following simple processes.

(1) Distillation: Separation in a distillation column is affected by both reflux ratio and number of trays. In design we fix the reflux ratio (at 1.1 times the minimum) and calculate the number of trays. In control, since the

number of trays is fixed, we use reflux ratio to affect separation (a control valve on the reflux, distillate, or steam line).

(2) Reactor: Reaction rates in a reactor are affected by holdup, concentrations, and temperature. In design, we fix temperature and concentrations and calculate the required reactor size. In control, with reactor size fixed, we use temperature and/or concentrations to affect reaction rates (a control valve on reactor cooling water or a reactant recycle stream).

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