USE OF DYNAMIC SIMULATION TO CONVERGE COMPLEX PROCESS FLOWSHEETS

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Commercial process simulators are widely used for designing new processes and for analysis of existing processes. Most senior design courses contain a significant component of computer simulation of process flowsheets using these tools. The most widely used commercial process simulation software is that developed by Aspen Technology—AspenPlus for steady-state simulation and AspenDynamics for dynamic simulation—and these tools are used in the examples in this paper. The standard Aspen notation is used. For example, distillation column stages are counted from the top of the column: the condenser is Stage 1 and the reboiler is the last stage.

The simulators contain models of most common unit operations, which can be connected into a process flowsheet. If the units operate in series, with upstream units feeding downstream units, the simulation is usually reasonably straightforward. If the flowsheet contains recycle streams, however, the simultaneous solution of the typically very large number of simultaneous nonlinear algebraic equations that make up the steady-state model can be quite challenging. There is no guarantee that any algorithm will find a solution. In addition, there are sometimes multiple solutions in these nonlinear systems. The convergence of these recycle loops (or "tear" streams) is a major challenge in steady-state process simulation.

Energy integration can also produce complications because of "energy recycle" between different units. These difficulties can sometimes be avoided by using the plant utility system to break the energy linkage.

Commercial steady-state simulators contain a variety of algorithms. For example, the user of AspenPlus can try such methods as Wegstein, Broyden, and Newton. Convergence tolerances and the maximum number of iterations can also be adjusted.

The experience of many users, particularly students, has been that the convergence of recycle loops is the most diffi-cult part of steady-state simulation. The normal procedure is to assume some conditions of a recycle stream (flow, temperature, pressure, and composition) and work down through the flowsheet until the calculated values of the recycle stream are available. If the assumed and calculated values are not sufficiently close, new guesses must somehow be made. The process is repeated until convergence between the assumed and calculated values has been attained. Often, however, convergence does not occur.

One would think that this convergence should be fairly easily achieved if the user has adjusted the design and operating parameters so the assumed and calculated conditions of the recycle stream are fairly close, but this all too frequently does not occur. For example, in one of the cases discussed later, an assumed recycle stream had a composition 98 mol% methanol and 2 mol% water, while the calculated stream is only slightly different (0.4 mol% dimethyl ether; 97.2 mol% methanol; 2.4 mol% water). The assumed flowrate is 72 kmol/hr, while the calculated flowrate is 72.9 kmol/hr. The temperature and pressures are identical. After connecting the recycle stream and defining it as a "tear" stream in the "Convergence" section of the "Data Browser" in AspenPlus, the recycle loop does not converge when using any of the algorithms.

This paper illustrates that recycle loops can be easily converged if the steady-state AspenPlus simulation (with the re-

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cycle loops not connected) is "exported" into the dynamic simulator AspenDynamics and the recycle connections are made on the dynamic model. The steps in going from a steady-state simulation to a dynamic simulation are discussed in the next section.

It should be noted that the issue of requiring good initial guesses of plant conditions in order to converge is not a problem since all the units have been converged individually in AspenPlus before going into dynamics. The "guessed" and the "calculated" values of the tear streams have also been adjusted to be fairly close to each other.

TRANSITION FROM STEADY STATE TO DYNAMIC SIMULATION

There are several items that must be taken care of to convert a steady-state simulation into a dynamic simulation: all equipment must be sized and a control structure must be developed. Luyben[1] presents many details of these necessary steps, which are summarized below. Not all of the units that are available in steady-state AspenPlus are supported in AspenDynamics, so this limitation must be kept in mind. For example, neither the "separator" (a fictitious component splitter) nor a liquid-liquid extractor is supported in the current version (Version 11.1) of AspenDynamics.

When the steady-state simulation in AspenPlus is exported into AspenDynamics, a "pressure-driven" dynamic simulation should be used. This requires that all the "plumbing" must be specified in the flowsheet. Pumps and compressors must be inserted where needed to provide the required pressure drop for material flow. Control valves must be installed where needed, and their pressure drops selected.

This is one of the more important educational aspects of the procedure since most students have a poor grasp of plumbing. Common errors include inserting two valves into a liquid-filled line, inserting a valve in the suction of pumps, or inserting a valve at the discharge of compressors (compressor speed or its equivalent compressor work should be manipulated).

__Equipment Sizing__ • For steady-state simulation, the size of the equipment is not needed, except for reactors. For dynamic simulation, the inventories of material contained in all the pieces of equipment affect the dynamic response, so the physical dimensions of all units must be known.

In distillation columns, the diameter of the column, the weir height, and the sizes of the reflux drum and the column base must be specified. Of course, before these can be calculated, the number of stages and the feed stage location must be set by some heuristic or rigorous optimization method. Perhaps

> *The convergence of steady-state simulations of flowsheets with recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method.*

the easiest heuristic approach is to fix the distillate and bottoms specifications (using the *Design Spec* and *Vary* tools in AspenPlus) and keep increasing the number of stages until the required reflux ratio stops decreasing—this gives the minimum reflux ratio. Then the actual reflux ratio is set at 1.2 times this minimum. Finally, the optimum feed stage can be determined by varying the feed stage until the minimum reboiler energy consumption is found.

The *Tray Sizing* section of a distillation column block in AspenPlus can be easily used to provide the column diameter. The default weir height of 0.05 m can be used. The volumetric flowrates of liquid into the reflux drum (Stage 1, the "condenser" in Aspen terminology) and the liquid into the base of the column (the last stage, or "sump" in Aspen terminology) can be used to size the two vessels by using the heuristic of a 10-minute holdup time. These volumetric flowrates are given in the *Hydraulics* page tab of the *Profiles* section of the column block. To have these results made available, you must go to the *Report* section of the column block, select the *Property Options* page tab and click the *Include Hydraulic Parameters* box before running the program.

For example, the liquid holdup in the reflux drum of a column with a total condenser is calculated from the volumetric flowrate of liquid leaving the drum (distillate plus reflux).

[Drum volume (m³)]

= [Liquid volumetric flowrate (m³/min)][10 minutes]

If an aspect ratio (length to diameter, L/D) of 2 is used, the diameter of the drum is

$$D = [2(\text{Volume})/\pi]^{1/3}$$

The same procedure can be used for flash tanks and vaporizers. Flash tank vapor velocity should also be checked.[2]

Heat exchanger tube-and-shell volumes can be calculated from the heat-transfer area, which is known from the steady-state design, if a tube diameter D (typically 0.0245 m) is selected.

Area = [number of tubes][πD][tube length L] = $N_{tube}(\pi DL)$

[Volume of tubes] = $[\pi D^2/4][L][N_{tube}]$
= $[\pi D^2/4][L][\text{Area}]/[\pi DL] = D[\text{Area}]/4$

Shell volume is approximately equal to tube volume in most tube-in-shell heat exchangers. If the process streams in the heat exchanger are gases, the dynamics are very fast and can usually be ignored (specify *Instantaneous* in the Dynamic section of the heat-exchanger block.

__Plantwide Control__ • When the file containing the flowsheet is opened in AspenDynamic, a default control scheme is al-

ready installed on some loops. For example, level and pressure controllers are inserted on all distillation columns and reactors in the flowsheet. This default control must be modified and supplemented with other control loops to incorporate a stable basic regulatory control structure.

• *Plantwide Control Structure* A simple heuristic method for development of an effective plantwide control structure is presented by Luyben, *et al.*[3] General principles and many examples are given in great detail. The proposed nine-step procedure has been successfully applied to a large number of realistically complex industrial processes. Some of the key concepts are: (1) the control structure should guarantee that all chemical components fed into the system are either reacted or can leave in some exiting stream; (2) a flow controller should be installed somewhere in all liquid recycle loops; and (3) all liquid levels must be controlled and pressures in gas systems, which can be multiple units connected together, must be controlled.

• *Controller Tuning* Most of the controllers are easily tuned by simply using heuristics. All liquid levels should use proportional-only controllers with a gain of 2. All flow controllers should use a gain of 0.5 and an integral time of 0.3 minutes (also enable filtering with a filter time of 0.1 minutes).

The default values in AspenDynamics for most pressure controllers seem to work reasonably well. Temperature controllers often need some adjustments. The default transmitter ranges are usually too large, and spans should be set at about 10% of the absolute temperature level (typically a span of 100 K for moderate-temperature processes).

Distillation columns are typically controlled by manipulating reboiler heat input to control the temperature on some selected tray. The heuristic procedure of finding a tray where the temperature changes from tray to tray are large is easy to use and provides effective composition control in most cases. Direct composition measurements can be used if temperature changes are too small. If very large temperature changes occur in the column (over 100 K), an average temperature can be used (measuring the temperatures at three or four trays, calculating the average, and using this for control).

It should be kept in mind that the objective at this point is not to come up with the "best" control structure or the optimum controller tuning. We only need a structure and tunings that drive the simulation to a steady state.

EXAMPLE ("DME" PROCESS)

To illustrate the use of a dynamic simulator to converge a flowsheet, we select the dimethyl ether (DME) process discussed by Turton, *et al.*[4] This design text gives a flowsheet and some preliminary design param-

eters. The chemistry is the exothermic reversible decomposition of methanol to form DME and water in an adiabatic, tubular, gas-phase reactor.

$$2 \text{ MeOH} \iff \text{DME} + \text{Water}$$
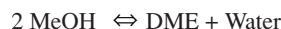
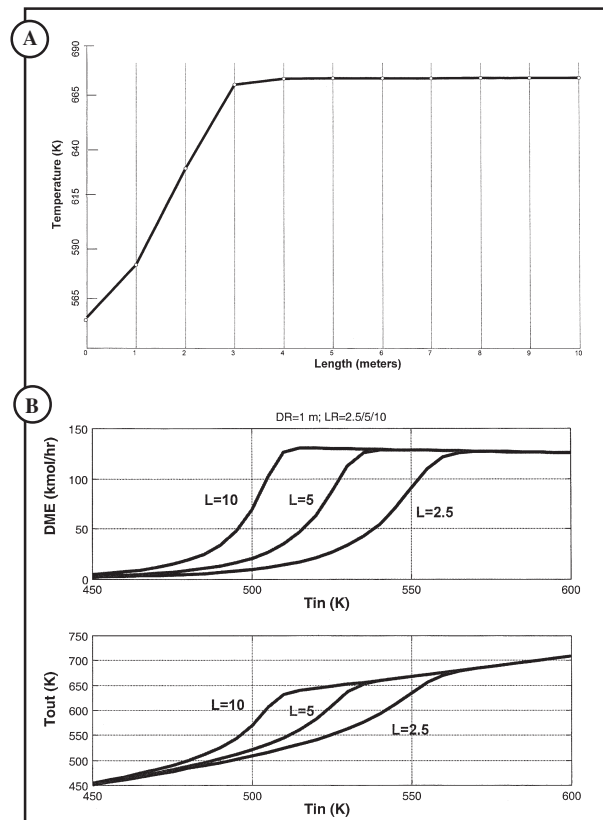The reaction is exothermic, and the adiabatic temperature

Figure 1.
(A) Adiabatic reactor temperature profile (10 meters length).
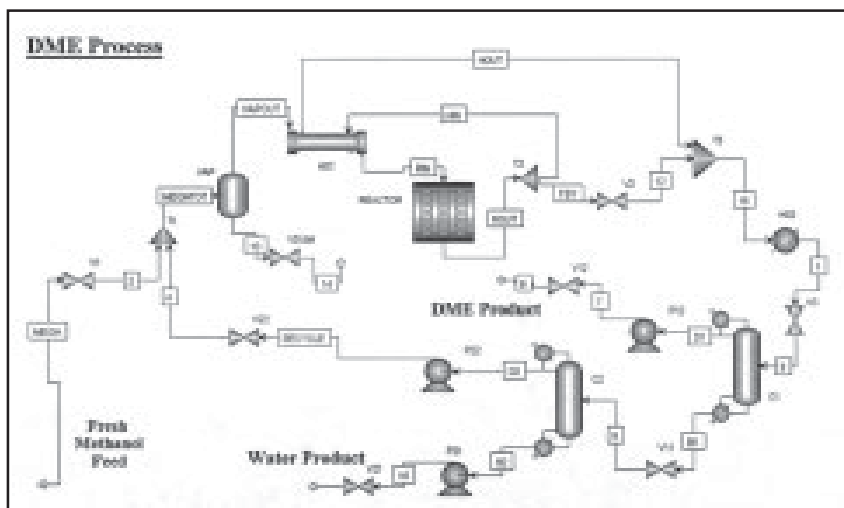*(B) Effect of inlet temperature for different reactor lengths.*

Figure 2. *DME flowsheet.*

rise is about 120 K. The temperature profile is shown in Figure 1A for a reactor that has a diameter of 0.72 m and is 10 m long. Figure 1B shows how reactor inlet temperature T_{in} affects the production of DME and the reactor exit temperature T_{out} for three different reactor lengths. The inlet temperature required to achieve maximum conversion decreases as the reactor is made bigger. Since the reaction is exothermic, the maximum conversion decreases slowly as temperatures increase.

The equilibrium constant is about 6 at a reactor temperature of about 600 K, so the per-pass conversion is about 80%. This requires a recycle of methanol back to the reactor from the separation section. Figure 2 gives the AspenPlus flowsheet, and Figure 3 gives stream conditions. The NRTL physical property package is used in the simulation.

Fresh methanol and recycle methanol are vaporized and heated to 555 K. The vapor-phase reaction occurs at about 15 atm. Reactor effluent is cooled and fed into a two-column separation section. The low-boiling DME is the distillate product in the first column C1, which operates at a pressure of 10 atm so that cooling water can be used in the condenser (reflux-drum temperature is 318 K with 99.9 mol% DME purity). The column has 32 stages, is fed on Stage 15, and is operated with a reflux ratio of 0.5.

The bottoms of Column C1 is fed to the second column C2 in which water is removed from the bottom and recycled methanol is removed from the top. This column operates at 1.1 atm and has a reflux-drum temperature of 340 K. It has 22 stages and a reflux ratio of 1.5.

Reaction Kinetics • One of the most difficult parts of developing a flowsheet is getting the reaction kinetic parameters correctly specified. Any errors in unit conversions are amplified by the exponential expressions.

Since the reaction is reversible, both the forward and the reverse reaction rates must be specified. Thurton, *et al.*,[2] provide a kinetic expression for the forward reaction rate

$$R_F\left(kmol/hr/m^3\right) = 1.21 \times 10^6\, e^{-80,480/RT} P_{MEOH} \qquad (1)$$

where P_{MEOH} has units of kPa and the activation energy has units of kJ/kmol. Aspen insists on expressing reaction rates in kmol/sec/m^3, so we must divide by 3600. More seriously, Aspen also insists that partial pressure be in Pa, not in kPa. A common error is to multiply by 1000 to convert the pressure in Eq. (1) from kPa to Pa. This is incorrect. The pressure in Eq. (1) is in kPa, and Aspen uses Pa, so the pre-exponential factor must be divided by 1000.

$$R_F\left(kmol/sec/m^3\right) = 1.21 \times 10^6\, e^{-80,480/RT}[P^{kPa}]/3600$$

$$= 1.21 \times 10^6\, e^{-80,480/RT}\left[\frac{P^{Pa}}{1000}\right]/3600$$

$$= 0.3361 e^{-80,480/RT} P^{Pa} \qquad (2)$$

Turton, *et al.*,[4] also give information about the equilibrium constant, but state that the published data does not seem to match the calculations using free energies. This was confirmed by running an *R-Gibbs* reactor in AspenPlus, which gave a much lower reactor conversion than would be predicted by the published data.

The heat of reaction is λ = -11,770 kJ/kmol. so we can estimate the activation energy of the reverse reaction from that of the forward reaction.

$$E_F - E_R = \lambda \Rightarrow E_R = 80,480 - \left(-11,770\right) = 92,250\ kJ/kmol$$

$$(3)$$

Figure 3. *DME stream data.*

To find a reasonable pre-exponential factor for the reverse reaction, the conversion data (reactor size; inlet flowrate, temperature, and composition; and exit composition) given Turton, *et al.,* were used to back-calculate this parameter by trial and error. The resulting kinetic expression is

$$R_R (kmol / sec/ m^3)$$
$$= 2.7 \times 10^{-6} e^{-92,250/RT} (P_{DME})(P_{Water}) \quad (4)$$

where P_{DME} and P_{Water} have units of Pa.

Thermal Recycle Loop • A feed-effluent heat exchanger (HX1) is used to preheat reactor feed, using a portion (201 kmol/hr) of the hot reactor effluent to heat the vapor from the vaporizer from 427 K to 555 K. Some of the reactor effluent (134 kmol/hr) is bypassed through valve V2 to control reactor inlet temperature.

Thus there is a thermal recycle loop in the process. Unless the reactor effluent stream is known, the HX1 equations cannot be solved. The conventional procedure to get started is to use a tear stream (see Figure 4). We specify a stream "HIN" and provide estimates of its flow (193 kmol/hr), temperature (672 K), pressure (14.4 atm), and composition (40 mol% DME, 20 mol% methanol, and 40 mol% water).

When this flowsheet is converged, the source of "HIN" is changed to the splitter T2 (deleting stream "5" in Figure 4). In the *Convergence* section of the *Data Browser*, we select *Tear* and specify *HIN* to be a tear stream. Then we rerun the program to get the converged flowsheet around the reactor and heat exchanger HX1.

Material Recycle Loop • Figure 5 shows the flowsheet with a tear stream *RECYCLE*, whose stream conditions have been estimated to be 72 kmol/hr, 345 K, 17 atm, 99 mol% methanol, and 1 mol% water. The calculated conditions for stream *RCALC* are only slightly different from those assumed for *RECYCLE* (73.2 kmol/hr, 342 K, 17 atm, 99.3 mol% methanol, and 0.1 mol% water).
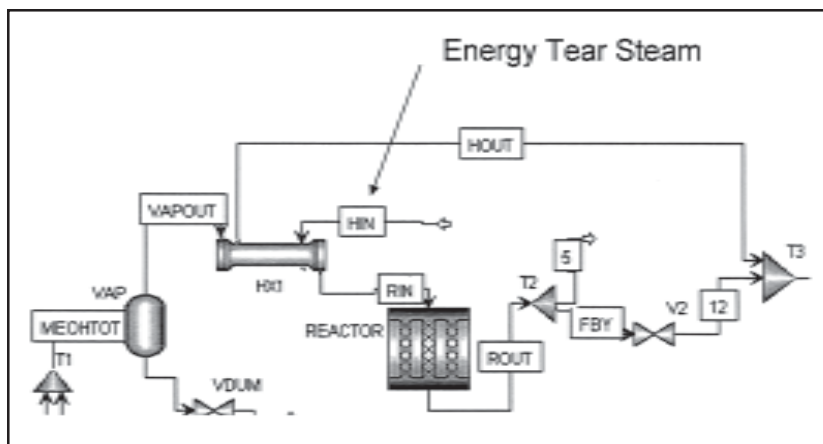
The default convergence method
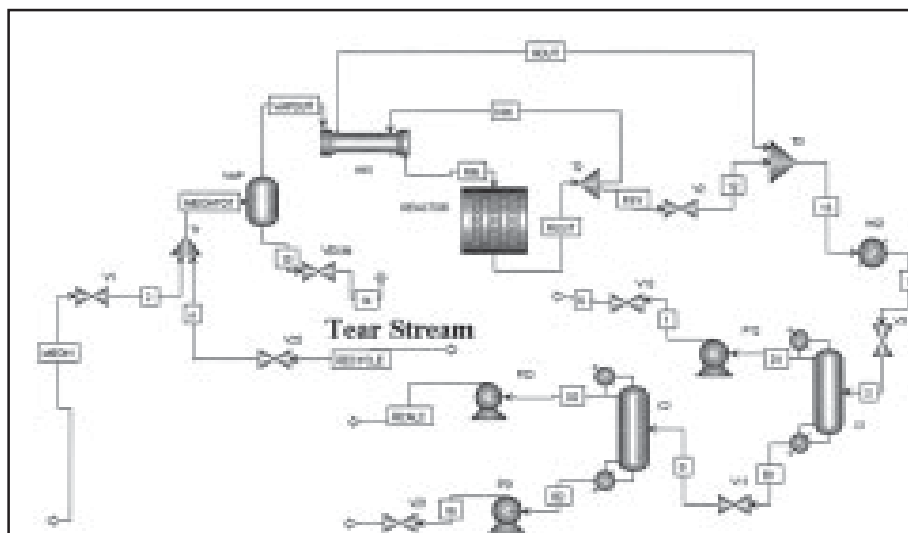

Figure 4. Flowsheet with energy tear stream.

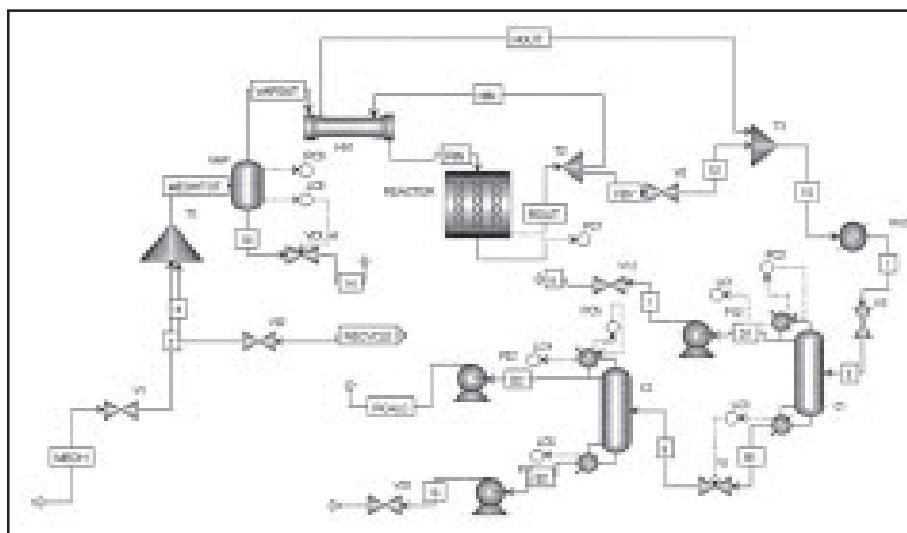*Figure 5. Flowsheet with material tear stream RECYCLE.*

Figure 6. Default control scheme; DME process.

Wegstein is used (with a limit of 30 iterations), the source of the *RECYCLE* stream is specified to be the discharge of pump P22 and it is specified as a *Tear* under the *Convergence Section* of the *Data Browser*. The program is run.

The convergence loop fails to converge.

This is a typical result in many cases. It should be noted that *Design Specs* and *Vary* features are used on both distillation columns. In Column C1, the distillate DME product purity is specified to be 99.9 mol% DME, and the distillate flowrate is varied. In Column C2, the bottoms water product purity is specified to be 99.9 mol% water, and the bottoms flowrate is varied. The reflux ratio is fixed in both columns.

Increasing the maximum iterations does not achieve convergence. Switching to the Broyden algorithm is equally unsuccessful.

This failure to converge certainly does not occur in all cases for all flowsheets, but it does occur in many cases. Senior students spend many frustrating hours trying to get recycle loops to converge.

Converting to Dynamic Simulation • The diameters of the two columns are calculated in the *Tray Sizing* section: 0.61 m for C1 and 0.94 m for C2. The liquid flowrates into the reflux drums of C1 and C2 are 0.242 and 0.131 m³/min, respectively, as found in the *Hydraulics* page tab. Reflux drum sizes (D x L) in the two columns are set at 1.2 x 2.4 m and 1 x 2 m, respectively, using an aspect ratio of 2. The liquid flowrates into the base (to the sump from the next-to-last stage in the column) of C1 and C2 are 0.213 and 0.0853 m³ min, respectively. Reboiler sizes in the two columns are set at 1.1 x 2.2 m and 0.82 x 1.64 m, respectively.

The heat exchangers are assumed to be "instantaneous" since they are gas phase. Reactor size is already specified for the steady-state simulation. The only other dynamic unit in the flowsheet is the vaporizer. Its liquid feed is 10,700 kg/hr with a density of 785 kg/m³, which gives a diameter of 1.1 m and a length of 2.2 m to provide ten minutes of holdup.

The file is pressure checked and exported into AspenDynamics. The default control scheme is shown in Figure 6. Note that each column has pressure and level controllers, some of which are fully connected and others without the controller output signal (OP) connected to a valve. This default control scheme must be modified to provide an effective regulatory control scheme.

Before doing anything, an *Initialization* run and a short *Dynamic* run should be made to confirm that all the plumbing is okay and the process is correctly configured.

Closing the Recycle Loop • The procedure for changing the process structure in AspenDynamics is the same as in AspenPlus. The stream *RECYCLE* is deleted. The destination of the stream *RCALC* is made the inlet to valve V22. Another set of *Initialization* and *Dynamic* runs should be made. Now the default control structure can be modified. It is a good idea to perform *Initialization* and *Dynamic* runs after each new change in the control structure so that any error in controller installation can be detected individually. The most common error is to have the wrong action in the controller (for example, specifying reverse action when it should be direct action).

An obvious alternative to deleting *RECYCLE* and reattaching *RCALC* is to delete *RCALC* and reattach *RECYCLE*. If this is attempted, the little green box at the bottom of the AspenDynamics screen turns red, indicating that something is wrong. Double-clicking the red box opens the window shown at the top of Figure 7, which states that the problem is overspecified. Clicking the *Analyze* button opens the window shown at the bottom of Figure 7, which says that the temperature and pressure of the *RECYCLE* stream must be changed from fixed to variable. Clicking the *ACCEPT* button turns the box green again. Then *Initiation* and *Dynamic* are again run to make sure all is okay. Now the default control scheme can be modified.

Plantwide Control Structure • Using the method proposed in Luyben, *et al.*,[3] a plantwide control scheme is developed that features the following loops:

- *The feed flow to the first column is flow controlled. This puts a flow controller in the liquid recycle loop. It also has the advantage of keeping a fixed steady flow to the column. Since the final DME product is produced in this column, product quality variability is minimized by not permitting disturbances to enter this column.*
- *The vaporizer level is controlled by manipulating the fresh methanol feed. This guarantees that only the amount of methanol that is being consumed in the reactor will be fed into the process. If more DME production is required, the setpoint of the flow controller on Column C1 feed can be increased. Using reactor inlet temperature to change production is not effective because of the reversibility of the reaction. For example, sometimes increasing reactor inlet*
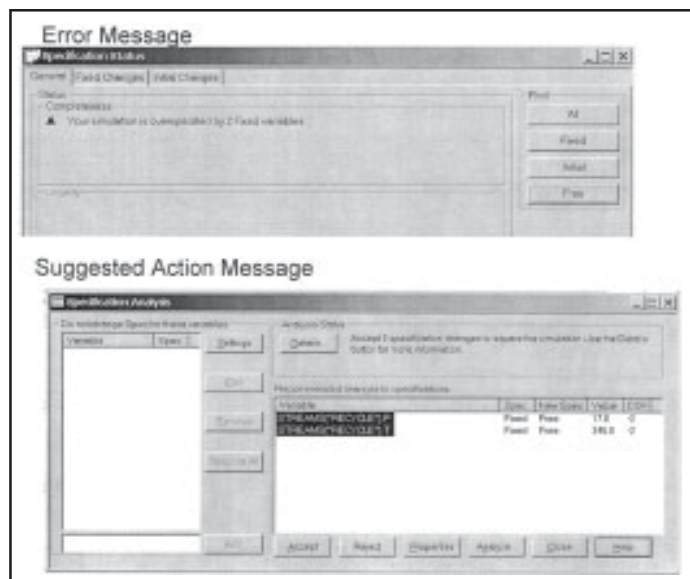

Figure 7. *Error message and suggested action message.*

temperature produces a decrease in the production of DME.

- *Vaporizer pressure is controlled by manipulating steam (heat input Q) to the vaporizer.*
- *Reactor inlet temperature is controlled by the HX1 heat exchanger bypass flow (valve V2).*
- *Condenser HX2 exit temperature is controlled by manipulating cooling water (heat removal Q).*
- *The pressure in each column is controlled by condenser heat removal.*
- *The reflux-drum level in each column is controlled by manipulating distillate flow.*
- *The base level in each column is controlled by manipulating bottoms product flow.*
- *A temperature in each column is controlled by manipulating reboiler heat input. The steep part of the temperature profile in C1 is at Stage 17 and in C2 at Stage 19, so these tray locations are selected. The temperature setpoint in C1 is 380 K and in C2 is 370 K.*
- *The reflux ratio in each column is controlled. The distillate flowrate is measured, multiplied by the desired reflux ratio (0.5 in C1 and 1.5 in C2) and this signal sets the flowrate of reflux.*

Figure 8 gives the

AspenDynamics flowsheet with this control structure installed. All level controllers are proportional with $K_c = 2$. Table 1 gives controller tuning parameters and transmitter spans. The dynamic simulation is run until it reaches a steady-state condition. This may take several "process hours" (several minutes of computer time), depending on the complexity of the flowsheet. When running the dynamic simulation out to a steady state, valve V22 in the recycle line went wide open and the reflux-drum level in Column C2 began to rise. The power to the pump P22 was increased to solve this valve saturation problem. The details of how this is done are given in Luyben.[1]
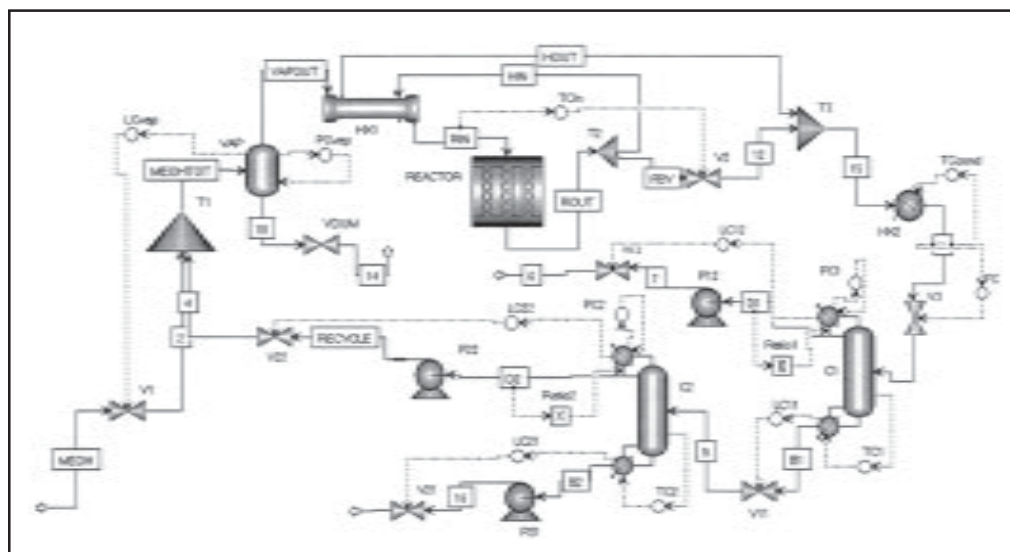
The same valve saturation problem occurred in V12 when the

***Figure 8.** Plantwide control structure: DME process.*

TABLE 1
DME Controller Parameters

| Controller (Action)	Transmitter Range min/max (units)	Valve Range min/max (Units)	K_c	Integral Time τ_I (min)
FC (Rev)	0/663 (kmol/hr)	0/100 (%)	0.5	0.3
TCin (Dir)	500/600 (K)	0/100 (%)	2	5
LCvap (Rev)	0/3.26 (m)	0/100 (%)	2	
TCcond (Rev)	300/400 (K)	-2030/0 (kcal.sec)	2	20
PCvap (Rev)	10/20 (atm)	0/1910 (kcal/sec)	5	12
TC1 (Rev)	300/400 (K)	0/690 (kcal/sec)	1	20
LC11 (Dir)	0/2.5 (m)	0/100 (%)	2	
LC12 (Dir)	0/3.4 (m)	0/100 (%)	2	
PC1 (Dir)	5/15 (atm)	-442/0 (kcal/sec)	5	12
TC2 (Rev)	300/400 (K)	0/688 (kcal/sec)	1	20
LC21 (Dir)	0/2 (m)	0/100 (%)	2	
LC22 (Dir)	0/2.52 (m)	0/100 (%)	2	
PC2 (Dir)	0/2.2 (atm)	-860/0 (kcal/sec)	20	5
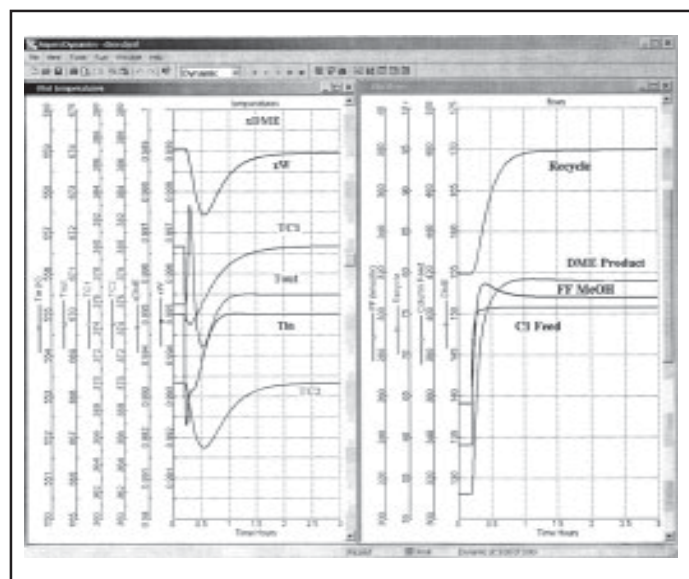
***Figure 9.** Dynamic responses to 20% increase in feed to column C1.*

setpoint of the C1 column feed flow controller was increased 20% (from 236 to 402 kmol/hr). The power to pump P12 was increased. Notice that the steady-state signals to valves V22 and V12 are 20% and 29%, respectively, instead of the normal 50%, because of the higher valve pressure drops.

Figure 9 shows the dynamic response of the system to a 20% increase in column C1 feed. The initial condition is the steady-state condition. The fresh feed of methanol increases from 262 to 308 kmol/hr and DME product increased from 131 to 154 kmol/hr (17.5% increase in production rate). The purities of both the DME and the water products are maintained for this large disturbance. The system takes about two process hours to come to the new steady state.

The one-recycle process illustrates how easily the flowsheet can be converged by using dynamic simulation. Figures 10 and 11 give an example of a process with two recycles. The methyl acetate and butanol reactants not consumed in the reactor are separated in a three-column separation section and recycled in two different streams. More details of this example are available from the author.

CONCLUSION

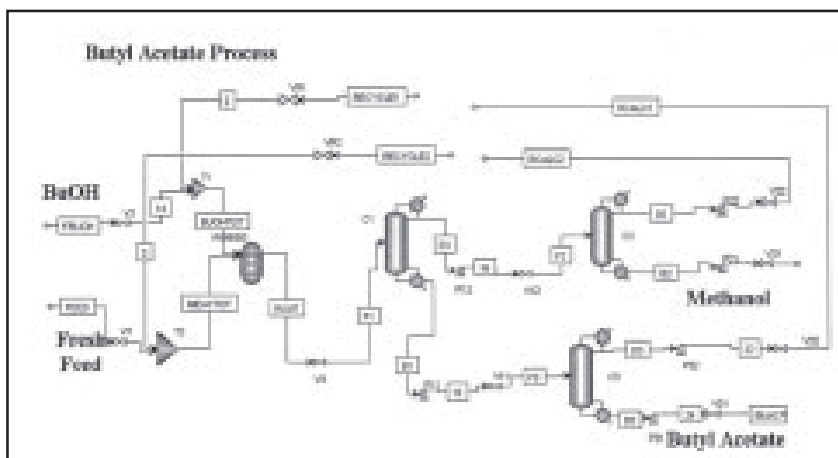The convergence of steady-state simulations of flowsheets with recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method. The steady-state simulation is converted into a dynamic simulation, and the recycle loops are converged by letting the dynamic simulation run to steady-state conditions.

The method depends on the development of a base-level regulatory plantwide control structure, which can be obtained by following a simple heuristic design procedure. Simple controller tuning rules can be applied to eliminate detailed and lengthy controller tuning efforts.

There is, of course, an additional benefit for this approach. The dynamic simulation can also be used to look at the dynamic effects of alternative design conditions (flowsheet structure, operating conditions, equipment sizes, etc.). This approach, which is called "simultaneous design," is a design philosophy in which both the steady state and the dynamic performances of a process are considered at all stages of the development of a process. The book by Seider, *et al.*,[5] discusses this approach in more detail.

Figure 10. Flowsheet for two-recycle butyl acetate process.
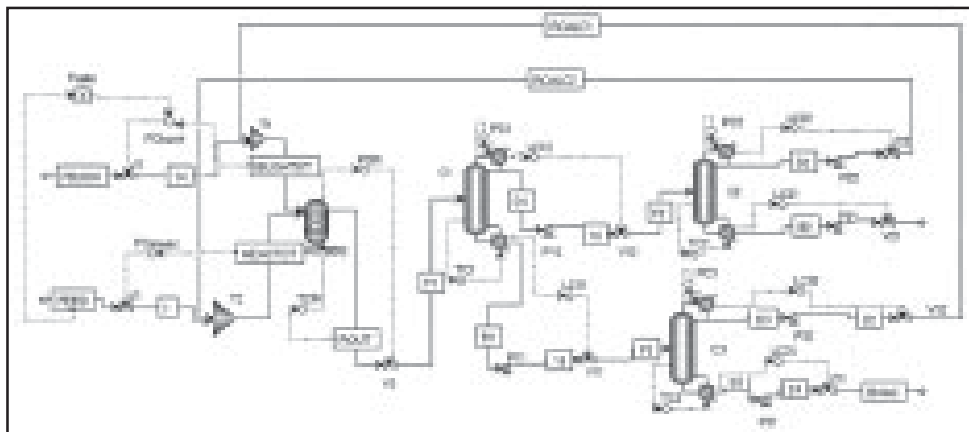
Figure 11. Plantwide control structure for two-recycle process.

NOMENCLATURE

D	diameter
DME	dimethyl ether
E	activation energy
FF	fresh feed
K_c	controller gain
L	length
P_j	partial pressure of component j
TCn	tray temperature controller in column n
Tin	reactor inlet temperature
Tout	reactor exit temperature
τ_I	integral time constant in PI controller (minutes)
λ	heat of reaction

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