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Aspen Dynamics simulation of a middle-vessel batch distillation process

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ABSTRACT

Aspen Dynamics is a powerful dynamic simulator that is widely used to explore the dynamics and control of continuous processes around some steady-state design operating point. This paper explores its use to study the dynamics of a batch process. The example studied is a middle-vessel batch distillation system for separating a ternary mixture. The batch system is operated by adjusting the two reflux flowrates (one from the reflux drum to the top of the upper column and the second from the middle vessel to the top of the lower column). The liquid inventories in the three drums vary with time. This paper shows how this batch operation can be conveniently simulated by first using the steady-state simulator Aspen Plus to correctly size the equipment. Then the file is exported into Aspen Dynamics where a rigorous dynamic simulation can explore alternative control strategies by using the large library of control functions.

1. Introduction

Control studies of both batch and continuous chemical processes have been widely used for many decades. Dynamic models of all the units and accurate physical property relationships are required as well as numerical methods for solving the large set of nonlinear algebraic and dynamic differential equations. Early studies required the engineer to develop the required dynamic equations from fundamental models (energy and component balances with appropriate phase equilibrium and reaction kinetics relationships). Then numerical integration methods were used to obtain dynamic responses.

In recent years, commercial steady-state and dynamic simulators have been developed that provide built-in quite rigorous models of many unit operations. They also provide a large library of physical property data and a reliable selection of numerical integration algorithms. They have an extensive array of realistic control models (controllers, multipliers, selectors, deadtimes, etc.), which permit dynamic simulations capable of accurately predicting the dynamics of quite sophisticated control structures.

The vast majority of studies have considered the dynamics and control of continuous processes. The process operates around a design steady-state condition. Alternative process designs and control structures can be quickly and easily evaluated.

Most studies of batch processes have used user-developed models and solution methods. The pioneering middle-vessel control paper by Skogestad et al. [1] is a good example. The model for a hypothetical chemical system was developed and implemented using SPEEDUP. A more recent study of the middle-vessel batch process by Rao and Barik [2] used a first-principles model for the ethanol/propanol/butanol separation.

Gruetzmann and Fieg [3] presented both simulation and experimental results for a middle-vessel batch distillation column for the hexanol/octanol/decanol separation. Aspen Custom Modeler was used for the simulations. They considered the detailed startup procedure from a cold start (column filled with nitrogen). It took 41 min for the vapor coming from the reboiler to reach the top of the column and begin building liquid in the reflux drum. When an adequate level was obtained, reflux to the top of the column was initiated (at 79 min). When the liquid reached the middle vessel and its level rose to an adequate level, reflux to the lower section of the column was begun. It took 180 min for the counter-current flow of vapor and liquid to be established so that fractionation could develop composition and temperature profiles under total reflux operation. Then various control strategies were explored for manipulating the two reflux flowrates to achieve the desired purities in the three vessels.

It is important to note that developing dynamic simulations in SPEEDUP or in Aspen Custom Modeler is a daunting task. The programming is complex and non-intuitive (at least to this author). A level of expertise is required that is well above that of the normal control engineer. This paper demonstrates that the more common

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and much more easily used (than user-developed models) software of Aspen Plus and Aspen Dynamics can be effectively used for the task of studying batch processes.

A number of simulators have been developed over the years for handling batch processes: BATCHFRAC, Aspen Batch Modeler, Aspen BatchSep, etc. All these require learning a different simulation language. Some studies [4] of batch processes have used hybrid systems combining Aspen Plus and Matlab. A study [5] using Aspen Plus and Aspen Dynamics developed a very complex simulation involving multiple steps and "Scripts" in a very lengthy design and analysis procedure. The method presented in this paper is much more straightforward and easy to implement.

Chien et al. [6,7] combined the steady-state simulator Aspen Plus with the dynamic simulator Aspen Dynamics for the simulation of two batch processes: batch extractive distillation and batch heterogeneous distillation. No details are provided in these papers of the required procedure in setting up the initial steady-state simulation in Aspen Plus and then converting it into a batch dynamic simulation in Aspen Dynamics.

There are a number of significant advantages in being able use the many capabilities of a rigorous but simple-to-use simulator to study batch processes. These advantages include extensive physical property libraries, built-in models of many process units, rigorous numerical integration algorithms and rigorous models of control elements (valves, controllers, deadtime, selectors, etc.). The Aspen *Radfrac* distillation column model is quite rigorous and gives realistic predictions of column hydraulics during dynamic changes (tray holdup and pressure drop). These are often ignored in simple simulations but can be significant in dynamic batch distillation.

The purpose of this paper is to provide the important step-by-step details ("the devil is in the details") of starting with steady-state Aspen Plus to size equipment and then performing the dynamic batch simulation in Aspen Dynamics. The important batch middle-vessel process is used as a realistic example to demonstrate how the widely used and user-friendly Aspen software can be conveniently applied for studying a batch process.

The middle-vessel configuration has some distinct advantages over more conventional batch processes. The major advantage is that there are no "slop cuts" (material that is off specification) that have to be managed (determine when to produce) and have to be further processed (e.g. recycle back to the next batch). See Ref. [8].

2. Process studied and design procedure

The numerical example studied has a ternary feed of benzene, toluene and o-xylene. The NRTL physical properties are used in the Aspen Plus and Aspen Dynamics simulations. The number of stages in each column section (upper and lower) is set at 16 since the separation is fairly easy with the minimum number of trays well below 16. A *Radfrac* rectifier model (condenser but no reboiler) is used for the upper column. A *Radfrac* stripper model (reboiler but no condenser) is used for the lower column. Operating pressure in the reflux drum is 1.1 bar since operation at about atmospheric pressure eliminates issue with vacuum columns.

2.1. Setup of continuous process in steady-state Aspen Plus

The first step is to set up a simulation in Aspen Plus that has the required pieces of equipment and to size the columns and vessels for the desired capacity (vapor boilup) and batch size (volume of initial charge to the sump of the lower column). Remember that in Aspen Plus the flowsheet must be a continuous process with feed and product streams. These will be eliminated (valves shut) in the dynamic simulation.

The most critical design parameter is to set the vapor and liquid load in the column to be approximately equal to what is desired for the batch operation. This is necessary so that the column diameter is appropriately sized. For example, in the numerical example we assume that a vapor boilup rate of 100 kmol/h is going to be used in the batch process. To achieve this objective, the vapor stream from the lower section into the upper section is "torn" as shown in Fig. 1. The stream "VUPPER" is specified to be 100 kmol/h with an

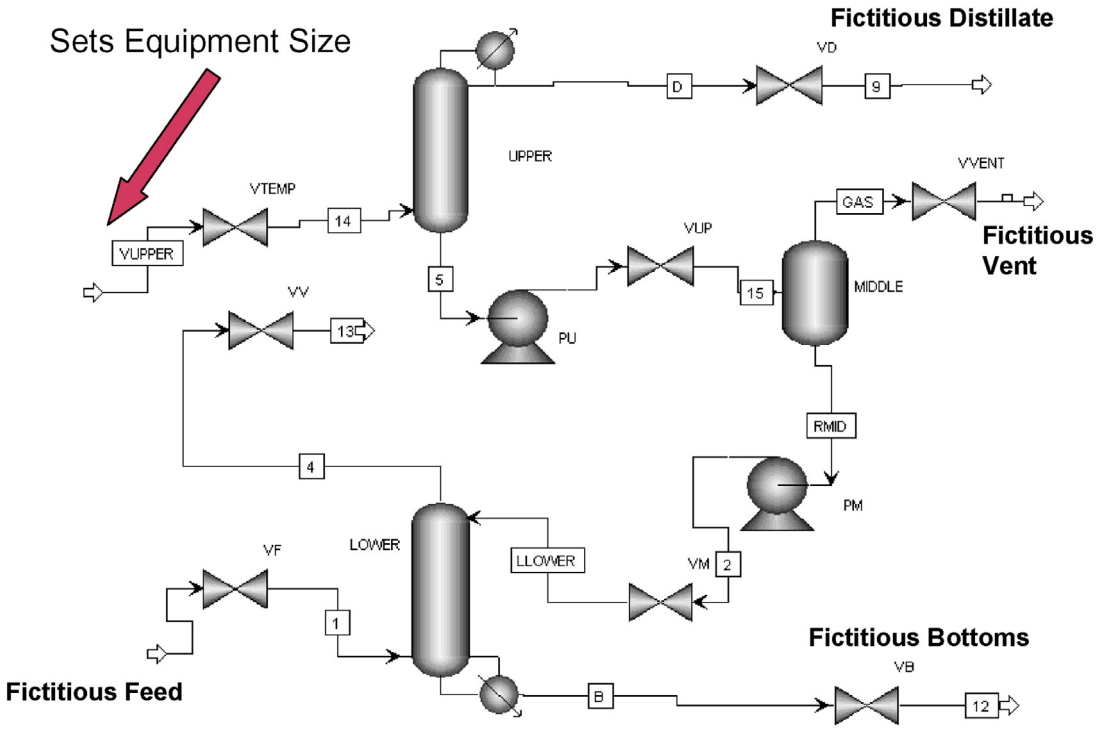

Fig. 1. Aspen Plus PDF showing fictitious streams.

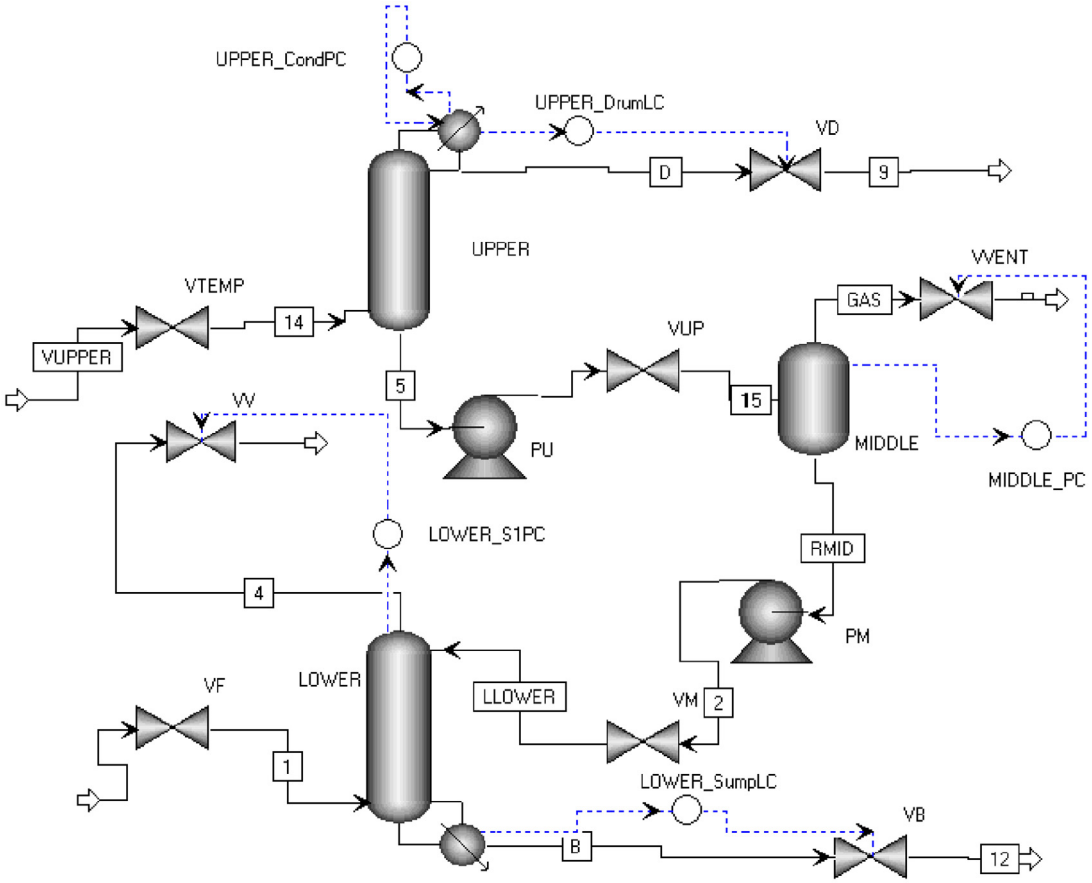

Fig. 2. Initial Aspen Dynamics flowsheet after exporting.

approximate composition of 99 mol% benzene and 1 mol% toluene. This torn stream will be connected after the file is exported into Aspen Dynamics.

A fictitious and large fresh feed stream (1000 kmol/h) with composition 30 mol% benzene, 30 mol% toluene and 40 mol% xylene is fed into the sump of the lower column through valve "VF." A small (and fictitious) distillate flowrate (1 kmol/h) is specified to be removed through valve "VD." Specifying these three streams (VUPPER, FEED and D) completely specifies the steady-state simulation since there are three design degrees of freedom in the system once pressure and the number of stages have been fixed. Now the simulation can be run to give all the vapor and liquid flowrates and compositions. The resulting bottoms stream from the base of the lower column is large (and fictitious).

Column diameters are calculated using the Aspen *Tray Sizing* function to be 0.81 and 0.79 m in the upper and lower sections, respectively, for the specified vapor flowrate to the base of the upper column. Weir height is assumed to be 0.025 m. Tray pressure drop is 0.01 bar per tray.

Before exporting into Aspen Dynamics, the sizes and the initial liquid levels of the three final-product vessels must be specified. These depend on the desired initial charge to the sump. At the end of the batch run, the reflux drum should contain essentially all of the benzene. The middle vessel should contain essentially all of the toluene. The sump in the base of the lower section should contain essentially all of the xylene. For the numerical case, the initial holdup in the sump is assumed to be about 800 kmol (with a composition of 30 mol% benzene, 30 mol% toluene and 40 mol% xylene). The sump in the lower column is sized to have a diameter of 4 m and a length of 8 m, giving a total volume of 100 m^3. The molar density is 8.35 kmol/m^3, so the sump could hold about 800 kmol. We specify in Aspen Plus that it is initially 80% full of liquid.

The reflux drum is sized to have a diameter of 3 m and a length of 6 m, which gives a total volume of 43 m^3, so it could hold about 350 kmol. This should be large enough to hold all of the lightest component at the end of the batch. We specify that this vessel is initially only 5% full of liquid. The middle vessel is sized in the same way. These sizes can be easily changed for different compositions of the initial feed charge to the sump of the lower column.

The sump of the upper column holds liquid to be pumped into the middle vessel. Its holdup should be small and should not change significantly during the batch. The conventional level sizing heuristic [9] is used to give 5 min of holdup when 50% full at the maximum liquid flowrate of 99 kmol/h (diameter 1 m, length 2 m).

The Aspen model used for the middle vessel is a *Flash2* separator model so that realistic pressures will be predicted during the dynamic simulation. The design pressure in the vessel is adjusted in Aspen Plus so that vapor flowrate is very small. The valve in the vapor line will be completely closed during the dynamic simulation.

The rest of the plumbing (pumps and control valves) is set up to give reasonable pressure drops over valves. Note that when we get into the dynamic simulation, a number of valves will be completely closed so as to simulate the batch operation. The feed valve, the distillate valve, the bottoms valve and the gas valve from the middle vessel will all be completely closed. It is important to note that pumps are not installed on the feed, distillate or bottoms streams as we would in a normal continuous design. Pumps are not used on the streams whose flowrates will be set to zero because error messages will appear in Aspen Dynamics when the flow through a pump is zero.

The file is now ready to be pressure checked so a realistic pressure-driven dynamic simulation can be studied. If the plumbing is correctly designed, the file is ready to export into Aspen Dynamics to generate the "dynf" file.

2.2. Initial setup of Aspen Dynamics

When the "dynf" file is opened in Aspen Dynamics, the first thing to do is to see if the integrator is running okay. A common problem is that error messages occur such as "Failure to Initialize." These are usually caused by plumbing errors, so appropriate corrections in the Aspen Plus file must be made. Some common errors are discussed by Luyben [10].

The initial flowsheet that opens up in Aspen Dynamics is shown in Fig. 2. Some default controllers are automatically installed. All of these initial controller blocks and control signals should be deleted. Next the "torn" vapor stream from the lower to the upper column is connected by deleting the stream "VUPPER" and the stream leaving the valve "VV." The valve "VTEMP" is also deleted. Finally the stream "14" is reconnected to the exit of valve "VV." The simulation is run for short period to make sure it is still running okay (no numerical integration error messages). The recycle between the two columns is now connected.

Then the positions of the valves to be closed are set to 0% by going to *Forms* and *All Variables* and scrolling down to *Pos* and entering zero. We want nothing coming in or going out of this batch process. The valves (see Fig. 2) are VF, VB, VVENT and VD.

Three level controllers are now installed. The level controller "LCtop" holds the liquid level in the reflux drum by manipulating the reflux flowrate. The input PV signal to this controller is the level on Stage 1 of the upper column. The output OP signal is the mass flowrate of the reflux to the top of the upper column (see Fig. 3).

A second level controller "LCbase" holds the liquid level in the sump of the upper column by manipulating the position of the valve "VUP" in the line to the middle vessel. The input PV signal is the liquid level in the sump of the upper column.

A third level controller "LCmid" holds the liquid level in the middle vessel by manipulating the position of the valve "VM" in the line to the top of the lower column.

The liquid levels in the reflux drum and the middle vessels are initially as low as possible and still provide sufficient NPSH to the pumps. A specification of 5% full was used in the original design. This corresponds to about 25 kmol of liquid in each of these two vessels. The control action should be PI because we initially want to maintain these two levels at their low level as we drive the process to a reasonable initial condition (to be discussed in the next section).

2.3. Establishing initial conditions of the batch distillation

The startup of distillation columns, both batch and continuous, has been the subject of many papers. In particular, the procedure for the batch middle-vessel process has been extensively discussed by Gruetzmann and Fieg [3] who begin with a cold column filled with nitrogen.

The startup of this type of distillation column is fairly straightforward in actual practice. Liquid is fed into the base of the lower column to establish a liquid level. Then steam is slowly introduced into the reboiler. This is done slowly to avoid thermal stresses as equipment heats up and expands. When the liquid in the base reaches it bubble-point temperature, vapor begins to move up the column. This vapor is rich in the lightest component. During this period the reboiler steam flowrate is slowly increased until it is about 50% of its maximum.

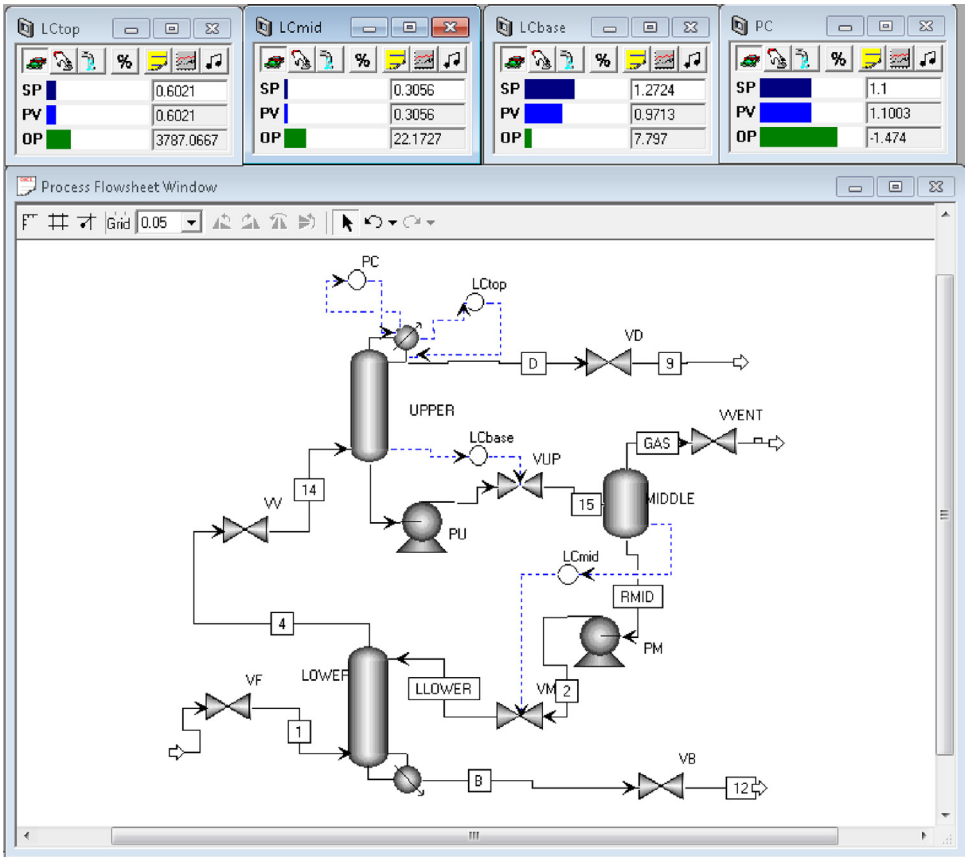

Fig. 3. Three level controllers; QR = 50% of design.

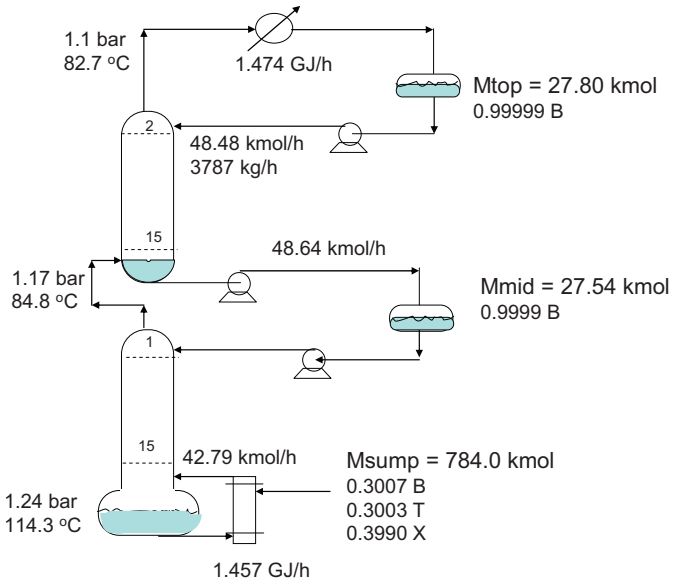

Fig. 4. Initial conditions at total reflux; QR = 50% of design.

The time it takes for the vapor to heat up the metal of the trays and shell depends on the number of stages (trays or packing). There is essentially no fractionation since the flowrate of the liquid formed by the condensing vapor is small. It should be noted that this heat-up time is fairly independent of the diameter of the column because all variables scale directly with cross-sectional area, which scales with the square of the diameter. The only exceptions are the shell metal and heat losses, which scale linearly with the diameter. In industrial size columns, heat losses are typically quite small on a relative basis. As a real example, in the 8-inch diameter column with 14 trays in the Lehigh Process Laboratory, it takes

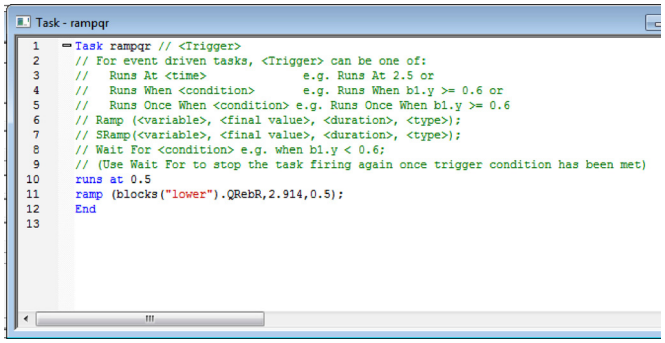

Fig. 6. Task to ramp QR to 100% of design at 0.5 h.

about 20 min for the vapor to reach the top of the column. A larger-diameter column with the same number of trays would take about the same time to send vapor overhead.

Once the vapor gets to the top of the upper column, it is condensed and liquid begins to fill the reflux drum. As soon as sufficient liquid level is built up to satisfy pump NPSH requirements, the reflux to the top of the upper column is begun and the liquid level in the reflux drum is maintained at a low level. The liquid flows down through the upper column and begins to build up a liquid in the sump of the upper column. When this level is sufficiently high, the pump "PU" is started and the sump level is controlled at a normal level by feeding liquid into the middle vessel.

The liquid entering the middle vessel builds up a liquid level. When the level is sufficiently high, the pump "PM" is started, and the level in the middle vessel is controlled at a low level.

At this point there are vapor flowing up the column and liquid flowing down through all the stages in the two columns. Fractionation begins and the concentration of the lightest component builds up on all the trays in the two column sections and in the two drums (reflux and middle vessel). The vapor flowrate (and

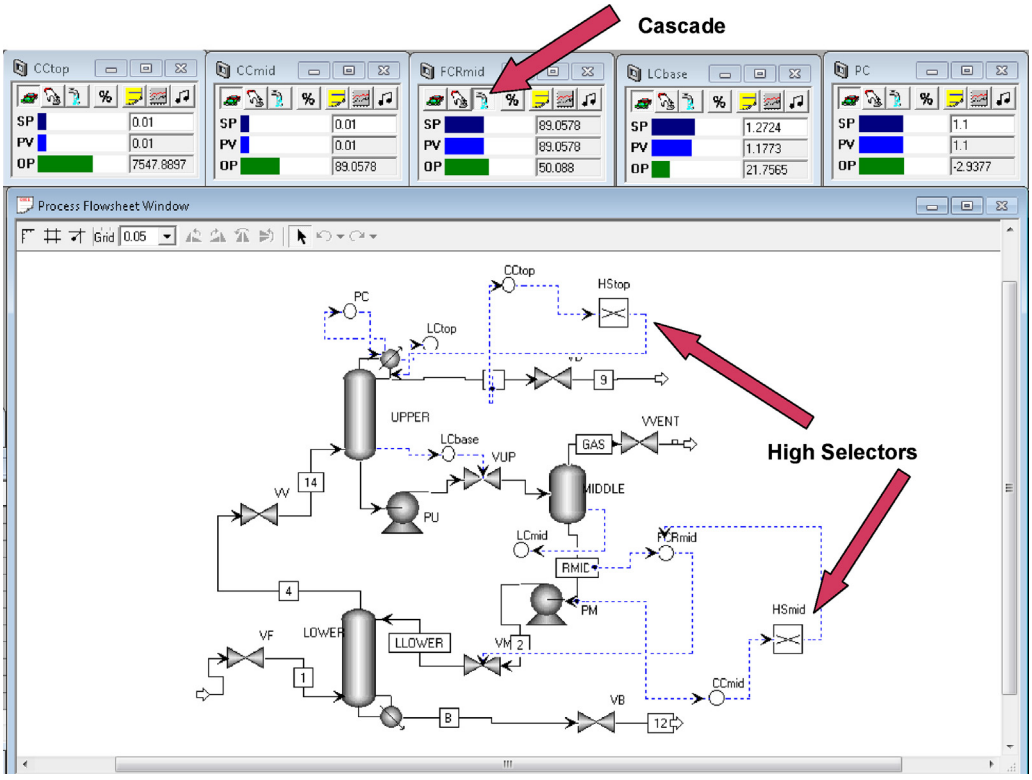

Fig. 5. Two CC and high selectors: QR = 100% of design.

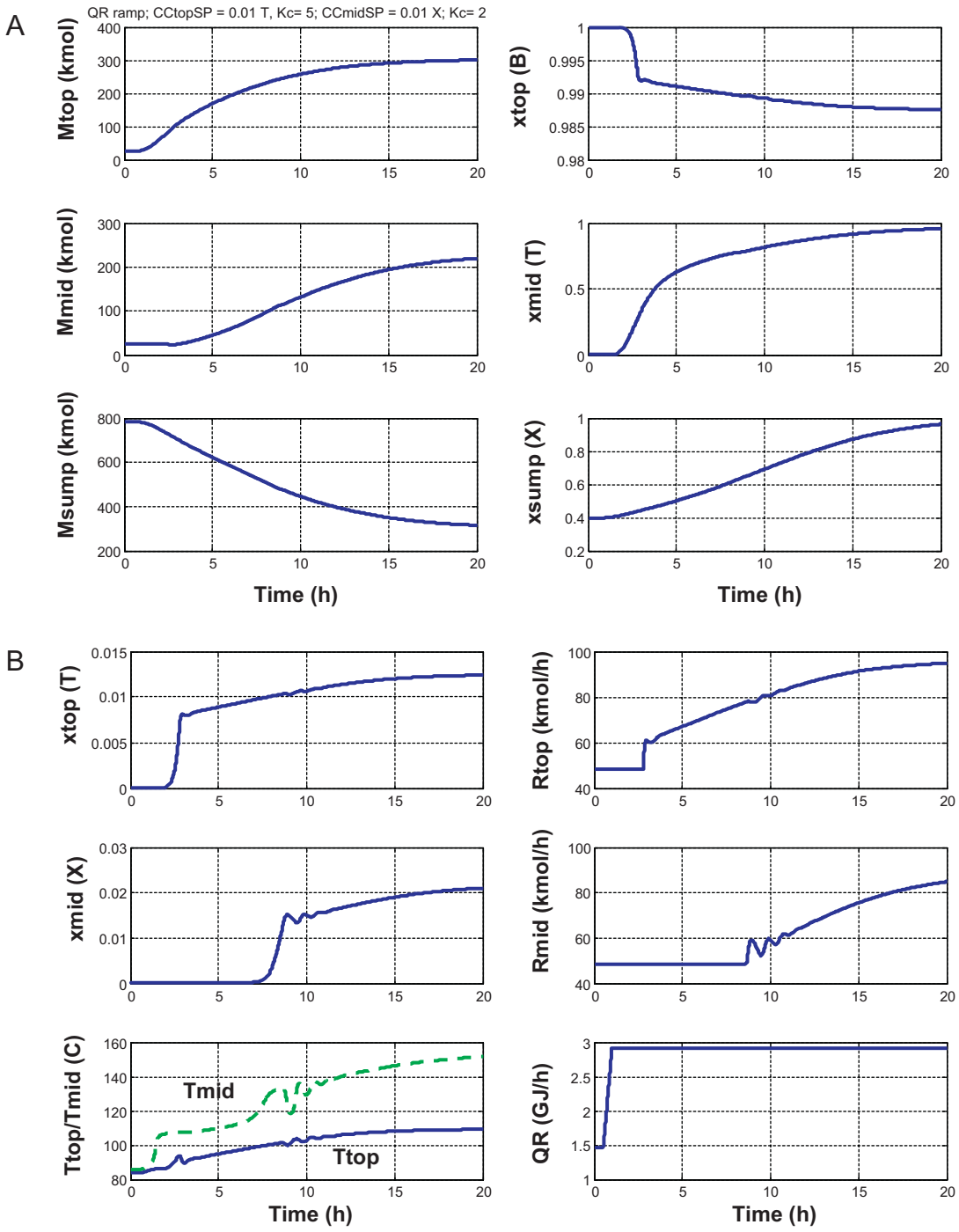

Fig. 7. (A) Composition control; P only; SP = 1 mol%; K_C = 5 and 2. (B) Control loop results with P composition control.

the corresponding reboiler duty) is perhaps 50% of design. The flowrates of the top reflux and middle reflux are about 50% of their design values.

We assume that the startup procedure described above is used for the middle-vessel process. The initial conditions are established by fixing the reboiler heat input at 1.457 GJ/h, which is half of the design reboiler duty (2.914 GJ/h) used in the original steady-state design back in Aspen Plus to give the design vapor flowrate of 100 kmol/h. Thus the initial conditions are established with a vapor boilup in the reboiler of 42.70 kmol/h. The reflux to the top of the upper column (Rtop) is 48.48 kmol/h (3787 kg/h). The reflux to the top of the lower column from the middle vessel (Rmid) is 48.65 kmol/h.

Fig. 4 gives the conditions at this initial steady state when liquid and vapor flows have been established and compositions and holdups are essentially constant. Now we are ready to begin the batch distillation.

3. Batch dynamics and control structure

The initial conditions have now been established with the liquid levels in the reflux drum and the middle vessel controlled at low values. The material in these drums is essentially the light component benzene. To operate the batch unit, we must modify the control structure such that the two reflux flowrates are controlled

to drive the compositions in the product tanks to their desired purities.

First, the two level controllers LCtop and LCmid are put on manual. Then two composition controllers are installed that will eventually manipulate the two reflux flowrates. In a later section of this paper, we will explore the use of temperature controllers instead of composition controllers.

3.1. Top Composition controller manipulating top reflux

The first controller CCtop measures the toluene impurity of the material in the reflux drum and manipulates the reflux to the top of the upper column (Rtop). The setpoint signal is 1 mol% toluene. Of course the initial composition is almost pure benzene, so the direct-acting controller tries to reduce the reflux flowrate. A high-selector block is used to prevent the reflux flowrate from being any smaller than the startup value (3787 kg/h). The high selector has two inputs. The first is a fixed value (3783). The second input is the CCtop controller output signal. The initial value of the output is set equal to zero. To prevent reset windup, proportional-only action is used with $K_C = 5$. Later in the batch cycle, integral action will be added to drive the composition to the desired value of 1 mol% toluene impurity.

This control structure is shown in Fig. 5.

3.2. Middle composition controller manipulating middle reflux

The second controller CCmid measures the xylene impurity of the material in the middle vessel and manipulates liquid flowrate from the middle vessel to the top of the lower column (Rmid). The setpoint signal is 1 mol% xylene. Of course the initial composition of xylene in the middle vessel is much smaller than 1%, so the direct-acting controller tries to reduce the flowrate of Rmid. But a second high-selector block is used to prevent the flowrate from being any smaller than the startup value (48.64 kmol/h). The high selector has two inputs. The first is a fixed value (48.64). The second input is the CCmid controller output signal. To prevent reset windup, proportional-only action is used with $K_C = 2$. Later in the batch cycle, integral action will be added to drive the composition to the desired value of 1 mol% xylene impurity.

Note that a flow controller has been installed on the liquid line from the middle vessel, and the output signal from the high selector is the setpoint signal of the FCRmid controller, which must be on "cascade" with its remote setpoint coming from the high selector. A common error is to send the signal directly to the control valve. In the upper loop, the Aspen simulation assumes the mass flowrate of the reflux can be set directly. In a real physical system, a flow controller on cascade for the reflux flow would be used.

An *Initialization* run is made, and the *Rewind* button is clicked to set time equal to zero. Saving the file provides the startup conditions for further control structure studies.

3.3. Ramp up reboiler heat input

The heat input to the reboiler of the lower column is ramped up at time equal 0.5 h from the initial value (50% of design) to the full design value (2.914 GJ/h) in 0.5 h by using an Aspen Dynamics *Task* (see Fig. 6). The slow ramp is used so as to not cause column flooding problems.

The vapor entering the reflux drum increases, and the composition of toluene impurity begins to increase. As it approaches the setpoint of 1% toluene, the output signal from the CCtop controller increases and eventually becomes larger than the minimum flowrate signal fed to the top high selector. Then the reflux flowrate is increased so as to maintain the composition close to the specified value.

Similar events occur when the xylene impurity in the middle vessel begins to approach the 1% setpoint. The CCmid controller output signal increases so as to maintain the composition close to the specified value.

4. Performance with alternative control structures

Several control structures have been proposed for the batch distillation process. Skogestad et al. [1] proposed controlling two temperatures in the two column sections by manipulating the two reflux flowrates. These authors used controllers with only proportional action, claiming that integral action was not needed because the process itself was an integrator. Gruetzmann and Fieg [3] discussed determining optimum trajectories of the two reflux flowrates to drive the three compositions to their specifications in the minimum batch time.

In this paper, we initially look at composition control, first with proportional-only controllers and then with PI action. Then the use of temperature control is explored.

4.1. Proportional composition control

Fig. 7 shows the batch trajectories for this control structure. Fig. 7A gives holdups and compositions in the three vessels. Fig. 7B shows how the composition loops perform.

A time equal 0.5 h, the reboiler heat input is increased from 1.457 to 2.914 GJ/h (QR in bottom right graph in Fig. 7B). The increase in vapor boilup sends more vapor to the condenser. More liquid enters the reflux drum. The liquid holdup in the reflux drum (Mtop in the top left graph in Fig. 7A) increases because the liquid flowrate out of the drum remains constant. However, the toluene impurity in the reflux drum begins to rise (xtopT in the top left graph in Fig. 7B). As it approaches the setpoint of the CCtop controller, the controller output signal begins to increase. At about 3 h, this output signal becomes larger than the fixed signal going into the high selector, so the top reflux flowrate increases (Rtop in the top right graph in Fig. 7B). The liquid holdup still increases but less quickly and eventually rises asymptotically to a final steady-stage value in about 20 h. Note that the composition in the reflux drum is not exactly at its specification because the controller is proportional only.

Similar events occur in the middle vessel. Its holdup does not start to change until the top reflux is increased. The flowrate out of

Task - topreset

```
1  Task topreset // <Trigger>
2    // For event driven tasks, <Trigger> can be one of:
3    //   Runs At <time>              e.g. Runs At 2.5 or
4    //   Runs When <condition>       e.g. Runs When bl.y >= 0.6 or
5    //   Runs Once When <condition> e.g. Runs Once When bl.y >= 0.6
6    // Ramp (<variable>, <final value>, <duration>, <type>);
7    // SRamp(<variable>, <final value>, <duration>, <type>);
8    // Wait For <condition> e.g. when bl.y < 0.6;
9    // (Use Wait For to stop the task firing again once trigger conditi
10   runs once when streams("D").zn("T") > .01
11   ramp(blocks("CCtop").IntegralTime,50,.1);
12   End
13
```

Task - midreset

```
1  Task midreset // <Trigger>
2    // For event driven tasks, <Trigger> can be one of:
3    //   Runs At <time>              e.g. Runs At 2.5 or
4    //   Runs When <condition>       e.g. Runs When bl.y >= 0.6 or
5    //   Runs Once When <condition> e.g. Runs Once When bl.y >= 0.6
6    // Ramp (<variable>, <final value>, <duration>, <type>);
7    // SRamp(<variable>, <final value>, <duration>, <type>);
8    // Wait For <condition> e.g. when bl.y < 0.6;
9    // (Use Wait For to stop the task firing again once trigger conditic
10   runs once when streams("RMID").zn("X") > .01;
11   ramp(blocks("CCmid").IntegralTime,50,.1);
12   End
13
```

Fig. 8. Tasks to add integral action.

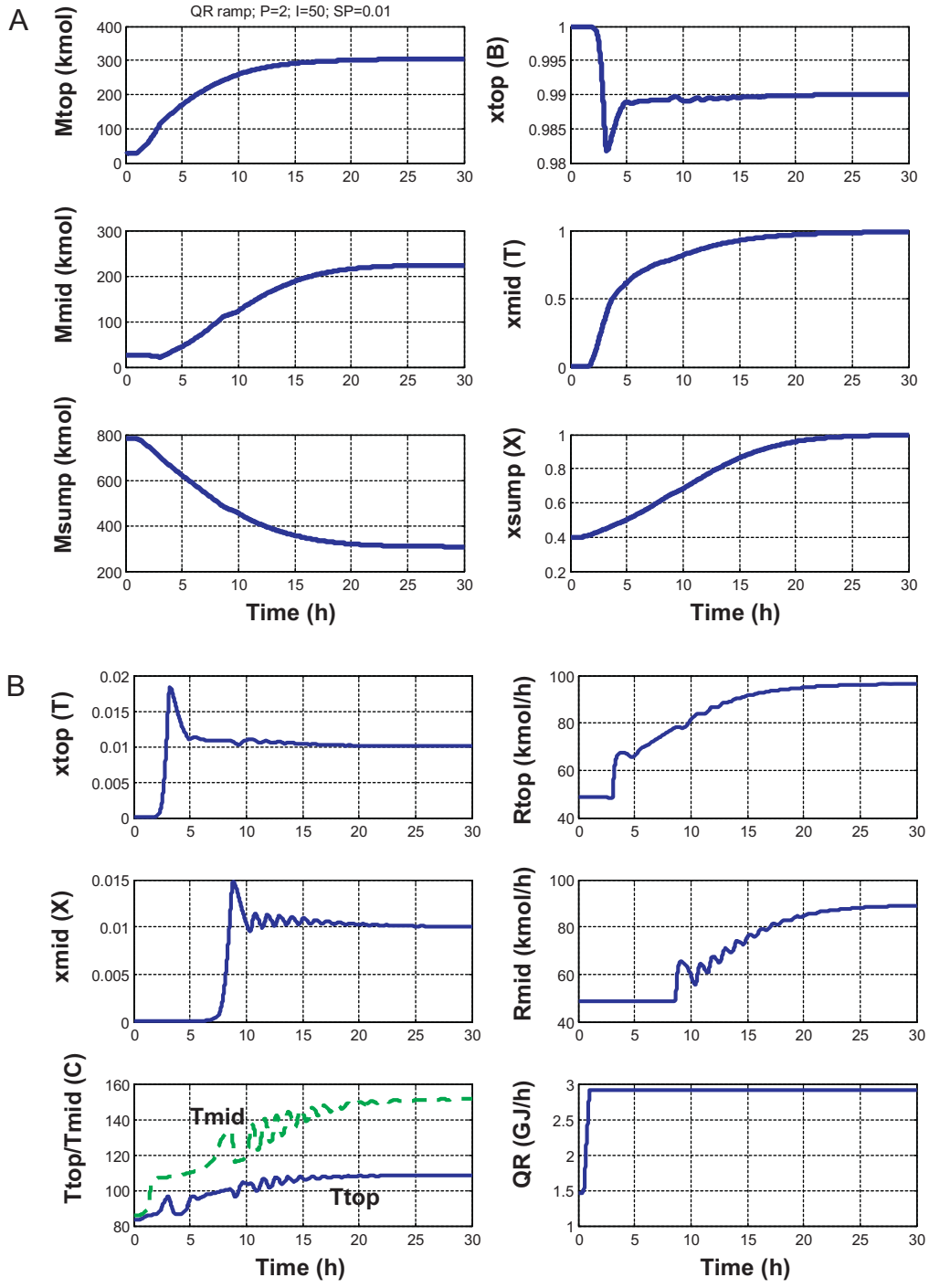

Fig. 9. (A) Composition PI control; SP = 1 mol%; $K_C = 2$; $\tau_I = 50$. (B) Control loop results with PI composition control.

the middle vessel xylene stays constant until the xylene impurity in the middle vessel begins to climb (xmidX in the middle left graph in Fig. 7B) at about 7 h. Then the output signal from the CCmid controller begins to climb and eventually increases the setpoint of the flow controller on the middle reflux (Rmid in the middle right graph in Fig. 7B) at about 8 h. The variables Tmid and Ttop are the temperatures on Stage 8 in the two column sections. The reboiler duty is QR.

The liquid holdup in the middle vessel still increases but less quickly and eventually rises asymptotically to a final steady-stage value in about 20 h. Note that the impurity of xylene in the middle vessel ends up at about twice its specification because the controller is proportional only. A higher controller gain would reduce this steady-state error (offset), but the loop becomes more oscillatory. In the next section we demonstrate how integral action can be added to eliminate the steady-state errors in both composition controllers.

4.2. Proportional-integral composition control

Proportional controllers were used in the previous section to avoid reset–windup issues during the startup period when the

composition controllers do not set the reflux flowrates. During this initial period, the high selector output signal is the low flowrates that were set when the liquid levels in the drums were first established.

Integral action in a controller can cause its output to saturate, which is called reset windup. There are several methods for handling reset windup. In continuous processes the use of external reset feedback is effective. In a batch process the most simple method is to turn on integral when the controller starts to take over control.

In our example, the integral tuning constants in the two composition controllers are set at 9999 min (proportional-only control in Aspen Dynamics convention). During the batch run when the controller input signal PV climbs up to the setpoint signal SP, an Aspen *Task* is run to switch the integral time to 50 min. Fig. 8 shows the tasks for the two composition controllers. Note that the trigger to run the task is "*runs once when*." Once the event has occurred, the integral time stays at 50.

Fig. 9 gives batch trajectories with PI action switched on once activated. The impurities in the reflux drum and middle vessel are driven to their specified values at the end of the 30-h batch. Remember that the reboiler heat input is constant during all this period once it has been ramped up to its design value at 0.5 h.

The final conditions in the reflux drum are 304.7 kmol of liquid with a composition of 99.50 mol% benzene and 0.41 mol% toluene. The reflux flowrate Rtop to the upper column is 96.45 kmol/h (7548 kg/h).

The final conditions in the middle vessel are 224.3 kmol of liquid with a composition of 0.62 mol% benzene, 98.97 mol% toluene and 0.41 mol% xylene. The reflux flowrate Rmid to the lower column is 89.06 kmol/h.

The final conditions in the sump of the lower column are 306.8 kmol of liquid with a composition of 0.24 mol% toluene and 99.76 mol% xylene. The reboiler duty is 2.914 GJ/h, which gives a vapor boilup rate of 81.48 kmol/h at the base of the lower column.

The base of the upper column contains material that is mostly toluene and can be recovered as product. The liquid holdup is 7.187 kmol with a composition of 0.15 mol% benzene, 98.85 mol% toluene and 0.33 mol% xylene.

It is interesting compare the distribution of liquid holdup at the beginning of the batch with the distribution at the end. As shown in Fig. 4, the total liquid holdup in the three drums is 839.3 kmol with 784 kmol in the sump, 27.8 kmol in the reflux drum and 27.5 kmol in the middle vessel. At the end of the batch the total in the three vessels is 835.8 kmol with the distribution described above. This difference (839.3–835.8 kmol) is due to the small increase in the holdup on all the trays in the column and in the base of upper column. The larger vapor and liquid flowrates result in higher tray pressure drop and larger tray holdups.

4.3. Temperature control

The composition control structure develop in previous sections provide effective control of the batch middle-vessel process. However, on-line composition measurements can be expensive and require high maintenance. Therefore a temperature control structure that can infer compositions from temperature measurement would be desirable. In this section we explore this possibility.

Fig. 10 gives the temperature profiles in the two columns at the end of the batch when PI composition controllers are used. There are significant temperature changes in the middle parts of both columns. The temperature on Stage 8 in the upper column is 108.5 °C. The temperature on Stage 8 in the lower column is 151.3 °C. These are used as the setpoints for two temperature controllers TCtop and TCmid. Temperature transmitter spans are 100 °C. Controller output spans are 0–12,000 kg/h for TCtop and 0–200 kmol/h for TCmid. Both controllers are proportional-only with $K_C = 4$ in TCtop and $K_C = 1$ in TCmid.

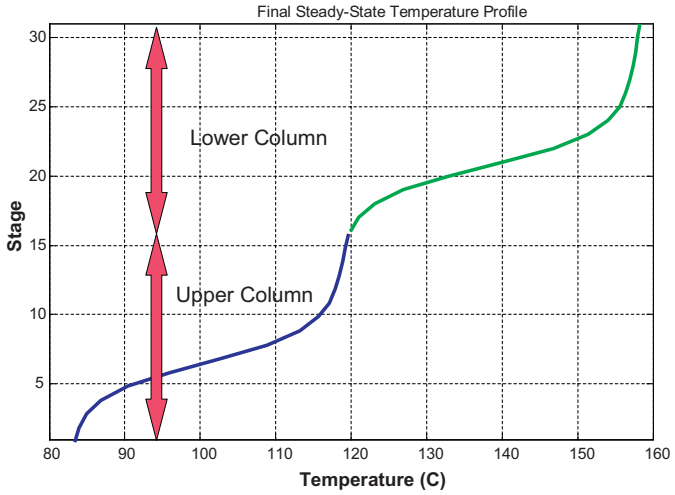

Fig. 10. Temperature profile at end of batch.

Fig. 11 shows the performance of the temperature control structure, which uses the same basic scheme with temperature controllers and high selectors. Reboiler duty is ramped up in the same way. The results are similar to those with the composition control structure. Since the temperature controllers have only proportional action, the tray temperatures are not driven to their setpoints. There are temperature offsets in both loops, 7.2 °C below the setpoint in TCtop and 3.7 °C below the setpoint in TCmid. This contradicts the findings of Skogestad et al. [1] who found that proportional-only controllers drove the temperatures to the setpoints. The reason for this difference is probably the higher rigor of the Aspen Dynamics model used in this work in which temperatures are affected by tray pressures changes as vapor and liquid flowrates change.

However, the compositions of the liquids in the three product vessels are almost the same as those using PI composition controllers. The final flowrates of the two reflux streams are also essentially the same for the two structures. Table 1 compares the final steady-state conditions for the PI composition control structure and the P temperature control structure.

The slight shift in the temperature profile appears to have little effect on final product compositions, so there is no need for integral action.

Table 1
Final conditions at end of batch using alternative control structures.

		CC	TC
Mtop	kmol	304.7	302.2
Rtop	kg/h	7548	7549
xtop	mf B	0.9959	0.9965
	mf T	0.0041	0.0035
Ttop (8)	°C	108.5	101.3
Mmid	kmol	224.3	225.3
Rmid	kmol/h	89.06	89.18
xmid	mf B	0.0062	0.0037
	mf T	0.9897	0.9917
	mf X	0.0041	0.0046
Tmid (8)	°C	151.5	147.8
Msump	kmol	306.8	308.3
QR	GJ/h	2.914	2.914
	mf T	0.0024	0.0025
	mf X	0.9976	0.9975

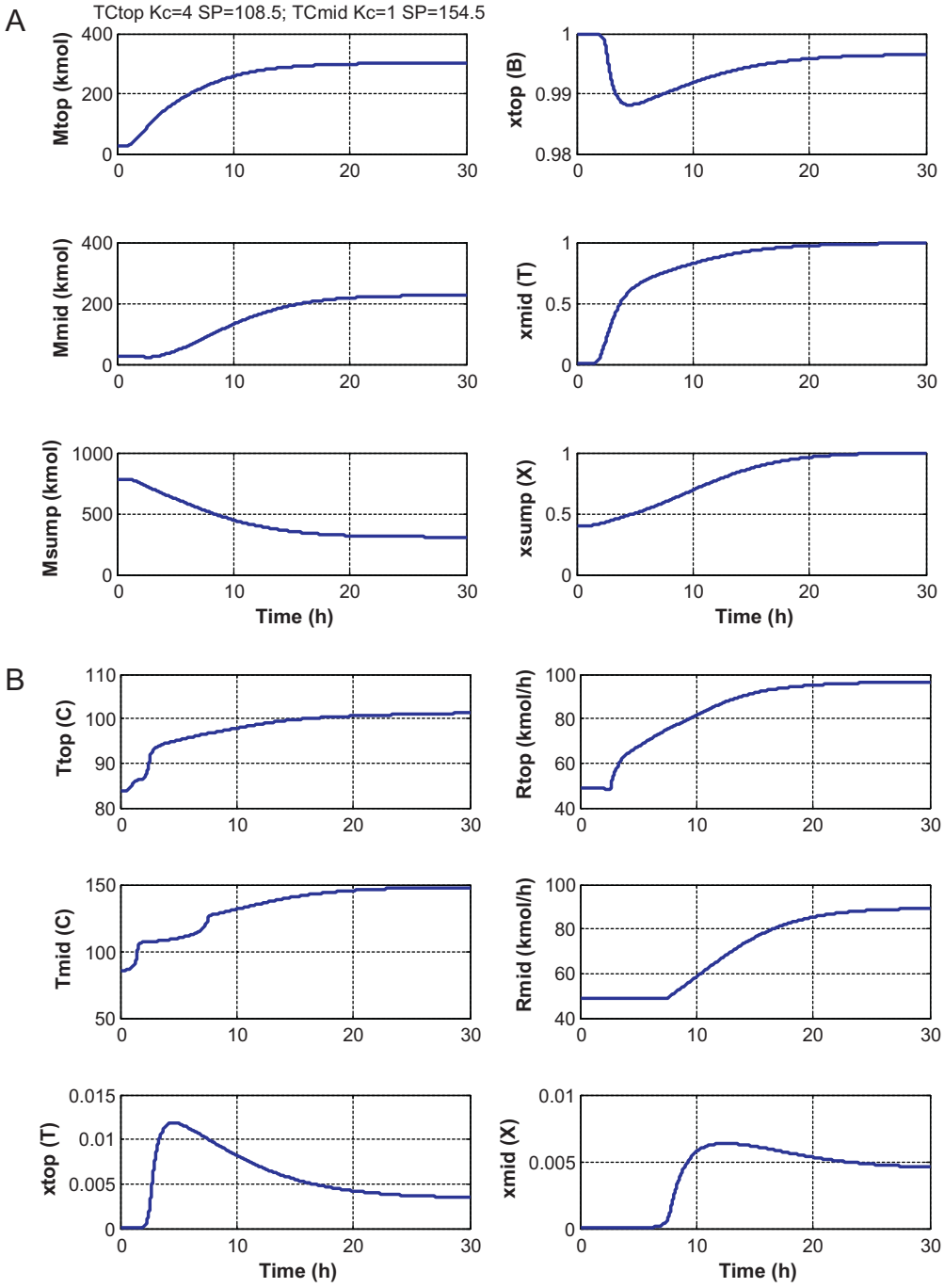

Fig. 11. (A) Temperature P control. (B) Control loop results with P temperature control.

5. Conclusion

The widely used Aspen Plus and Aspen Dynamics simulators can be applied to batch processes in a simple and straightforward way by minor modifications to the flowsheet generated in Aspen Plus. The rigorous models (particularly in terms of hydraulics) provide realistic dynamic responses.

The batch middle-vessel distillation provides an important illustrative example of the techniques to set up a fictitious steady-state continuous process in Aspen Plus to obtain the desired equipment sizes. The process structure is modified in the dynamic simulation be closing feed and product valves. Then an appropriate control structure with whatever complexity is required can draw elements from the Aspen Dynamics control model library to construct a realistic control scheme that matches physical reality.

References

[1] S. Skogestad, B. Wittgens, R. Litto, E. Sorensen, Multivessel batch distillation, AIChE J. 43 (4) (1997) 971–978.
[2] C.S. Rao, K. Barik, Modeling, simulation and control of middle vessel batch distillation column, Procedia Eng 38 (2012) 2383–2397.
[3] S. Gruetzmann, G. Fieg, Startup operation of middle-vessel batch distillation: modeling and simulation, Ind. Eng. Chem. Res. 47 (2008) 813–824.
[4] http://10.16.16.16/InternalPublicCgi/SolutionDisplay_view_google.cgi?key=115731

[5] http://xa.yimg.com/kq/groups/31024744/. . ./name/ASPEN+DYNAMICS.pptx
[6] J. Yao, S. Lin, I. Chien, Operation and control of batch extractive distillation for the separation of mixtures with minimum-boiling azeotropes, J. Chin. Inst. Chem. Eng. 38 (2007) 371–383.
[7] H.J. Huang, I. Chien, Choice of suitable entrainer in heterogeneous batch distillation system for acetic acid dehydration, J. Chin. Inst. Chem. Eng. 39 (2008) 503–517.
[8] E. Quintero-Marmol, W.L. Luyben, Multicomponent batch distillation: part 2 – alternative operating strategies for handling slop cuts in ternary systems, Ind. Eng. Chem. Res. 29 (1990) 1915.
[9] W.L. Luyben, Design and Control of Distillation Columns Using Aspen Simulation, second ed., Wiley, 2013.
[10] W.L. Luyben, Common plumbing and control errors in plantwide flowsheets, Chem. Eng. Educ. 39 (2005) 3.