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Decanter Anomaly

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A counter-intuitive decanter level control structure was reported in an earlier article which the aqueous level controller had to use reverse action for stable control. The Aspen model used in this study was the simple Decanter model, which assumes that there are only two liquid phases and pressure remains constant. This article presents results when the alternative Flash3 model is used. The aqueous level controller with direct action works well.
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Introduction

Decanters are used in distillation processes that feature heterogeneous azeotropes. The strong repulsive nonlinearity of the phase equilibrium produces two liquid phases over a range of temperatures. The addition of a light entrainer can modify the volatilities in some binary azeotropic systems such that the entrainer carries one of the components overhead in the distillation column, where it condenses and forms two liquid phases. One of the earliest examples is the use of benzene or cyclohexane to break the ethanol/water azeotrope.

In modeling these systems using Aspen Technology software, we have two decanter models from which to choose. The more simple model is the "Decanter model" in which only the two liquid phases are assumed to be present. The decanter pressure is assumed to be constant at the value specified in the design. This means that decanter pressure is not a function of temperature or composition. The alternative model is the "Flash3 model" that considers all three phases: two liquids and a vapor. The pressure in the vessel varies with temperature and composition.

In an earlier article,[1] the simple Decanter model was used, and some counter-intuitive behavior was observed. The expected control structure for the decanter would be to use two direct-acting level controllers on the two liquid levels (the aqueous/organic interface and the organic level) that manipulate the exiting flow rates of the two liquid streams. However, in the previous article, the action of the aqueous level controller had to be changed to reverse to achieve a stable control system.

In this article, we again illustrate this unexpected anomaly and demonstrate that the use of the alternative Flash3 model eliminates this counter-intuitive response.

Process Studied

The phase equilibrium of the ethanol/water/benzene system is quite complex, as Figure 1 illustrates. The UNIQUAC physical property model is used in this study. There are three binary azeotropes (two homogeneous and one heterogeneous) and one heterogeneous ternary azeotrope. The ternary diagram is split into three regions by distillation boundaries.

Figure 2 shows the two-column distillation system used to produce high-purity ethanol out the bottom of the first column and high-purity water out the bottom of the second column. Fresh ethanol/water feed is fed to the first Column C1. The distillate stream from the second Column C2 is also fed to C1. Benzene is recycled from the organic phase of the decanter back to the top of C1 as reflux. A very small benzene make-up stream is added to account for the small losses of benzene in the two product streams. The bottoms stream from C1 is high-purity ethanol.

The overhead vapor is condensed and fed to a decanter. The decanter aqueous phase is fed to C2, which produces a bottoms stream of high-purity water and a distillate that is recycled back to C1.

Design with Decanter model

There are two degrees of freedom in the model. The pressure and the heat duty are normally specified. The heat should be zero, because the decanter is typically a simple vessel with no heat-transfer capability. The decanter temperature (313 K) is then determined by the temperature specified in the upstream heat exchanger (condenser). In this design, the pressure is specified to be 1 atm. Note that Figure 2 shows a pressure of 0.367 atm, which is the real pressure found in the Flash3 model discussed in the next section.

The single design specification for Column C1 is a low concentration of benzene in the bottoms (0.49 mol %). It has only one design degree of freedom because the column model is a reboiled stripper with no condenser and no reflux. In the Aspen Plus simulation, this specification is achieved by using a "Design spec/Vary" function that adjusts the flow rate of the organic reflux to the top of C1. In Column C2, one of the two design specifications is a low ethanol concentration in the bottoms (0.1 mol %) and is achieved by manipulating the bottoms flow rate. The separation is quite easy, so the second specification is a reflux ratio of 0.2.

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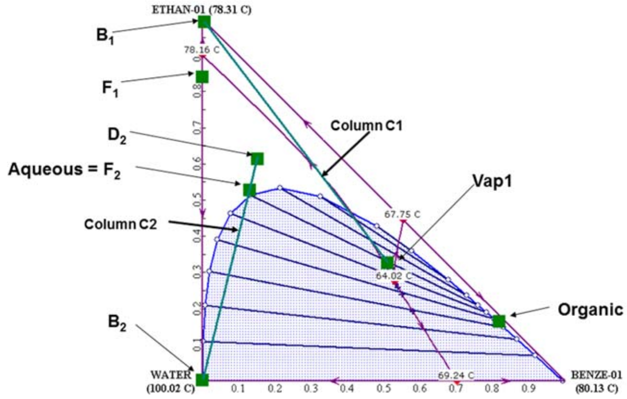

Figure 1. Ethanol/water/benzene ternary diagram with streams located.

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

Design with Flash3 model

The Flash3 Aspen model requires that there must be a vapor stream. The system is designed so that a very small amount of vapor is formed, but later in the dynamic simulations, the valve on the vapor line is completely closed.

One way to achieve these design conditions is to specify the heat removal (adiabatic) and the pressure in the flash3 block. Then, the heat duty in the upstream condenser is adjusted to give a very small vapor flow rate. Note that the decanter temperature is not specified. However, in the dynamic simulation with the vapor valve closed, a decanter temperature controller is used to manipulate the condenser duty to drive the temperature to 313 K.

The designs of the two columns are exactly the same as discussed earlier. So the only difference between the two cases is the decanter model being used. The columns are identical.

Control Structure

The sizes of the column bases and the C2 reflux drum are calculated to provide 5 min of liquid holdup when half full. The size of decanter is calculated to give 20 min of holdup to provide adequate time for phase separation. The file is exported into Aspen Dynamics, and controllers are added. Base levels are held by bottoms flow rates. Reflux drum level in Column C2 is held by the distillate flow rate (the recycle stream back to C1). The reflux flow rate in C2 is ratioed to its feed flow rate (the aqueous stream from the decanter).

Temperatures

Figure 3A shows that Stage 28 in Column C1 is the only location with a significant break. Temperature controller TC1 controls Stage 28 temperature by manipulating reboiler duty QR1.

The tray with the sharpest temperature change in Column C2 is Stage 19 as shown in Figure 3B. The temperature controller TC2 manipulates reboiler heat input QR2. A third temperature controller is added on the heat exchanger before the decanter to control the temperature of the stream entering the decanter at 313 K.

A deadtime of 1 min is included in both column temperature controllers, and relay-feedback tests are run to find controller settings. In TC1, they are $K_C = 0.98$ and $\tau_I = 9.2$ min (using a temperature range of 300–400 K and an output range of 0–27.8 MW). In TC2, the controller settings are $K_C = 0.84$ and $\tau_I = 10.6$ min (using a temperature range of 300–400 K and an output range of 0–9.26 MW).

Organic reflux

Another very important variable is the flow rate of organic reflux to the top of Column C1. If there is too little benzene, water will drop out the bottom. If there is too much benzene in the column, benzene will drop out the bottom. The amount of benzene required depends on the feed flow rate and also the flow rate of recycle from Column C2 back to

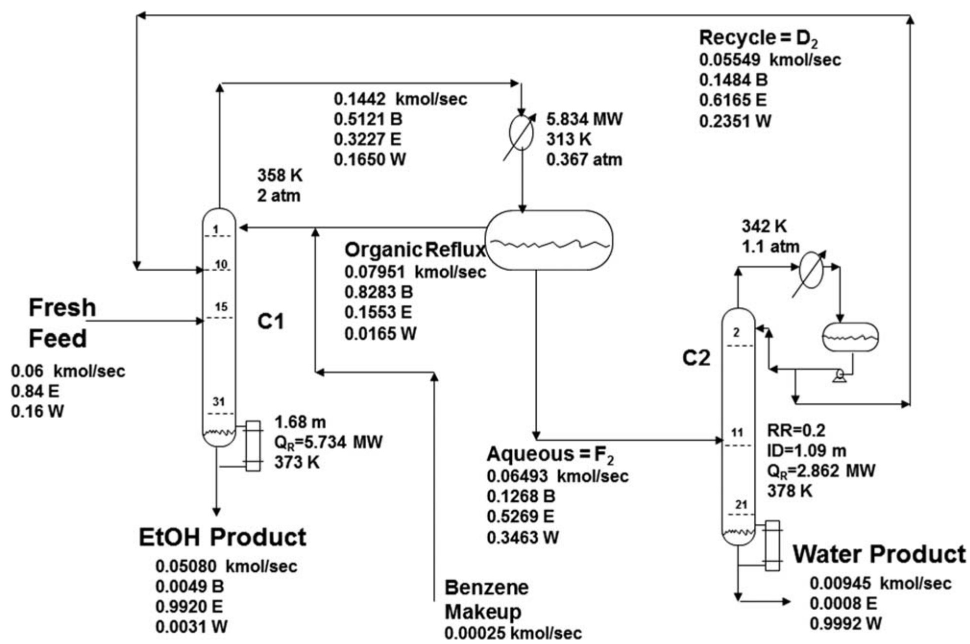

Figure 2. Heterogeneous azeotropic distillation flowsheet.

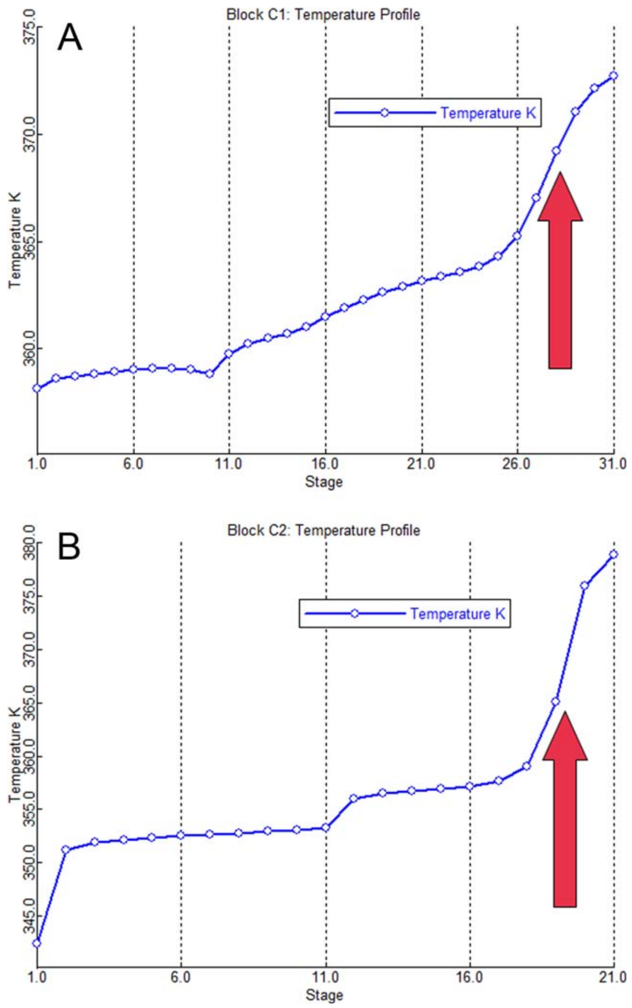

Figure 3. (A) C1 temperature profile and (B) C2 temperature profile.

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

Column C1. The control structure selected adds these two flow rates and sends this signal to a multiplier whose other input is the ratio of organic reflux flow rate at design to the sum of the design feed and recycle flow rates (molar flow rates are used in this example). The output of the multiplier adjusts the setpoint of a flow controller on the organic reflux. The entire control structure is shown in Figure 4.

Decanter levels

The control of the two liquid inventories in the decanter is critical. As only a very small amount of benzene is lost, the organic level basically floats up and down as changes occur in the reflux flow rate. An organic-phase level controller adjusts the benzene make-up stream, but it is so small that the level changes are significant. This does not hurt anything, as long as the decanter does not overfill or the organic level is lost.

The control of the aqueous level would appear to be straight forward. A level controller would manipulate the valve "V5" in the aqueous line feeding C2. Conventional logic says that this controller should be "direct" acting. If the level goes up, the flow rate of the aqueous stream should be increased and more fed to Column C2. Very surprisingly, this set-up was found to not work when the simple Decanter model is used. The system shuts down. However, making the controller "reverse" acting produced a stable control structure. We demonstrate this in the next section.

Figure 5 gives the flow sheet when the Flash3 model is used for the decanter. The control structure is identical, except that the aqueous level controller uses direct action.

Figure 6 shows the Aspen Dynamics controller faceplates and the variables in the summer block "sum" used to add together the flow rates of the fresh feed and the recycle D2. Note that the flow controller on the organic reflux is on cascade with its setpoint coming from a multiplier whose two input signals are the output of the summer and the desired ratio of organic reflux to this sum.

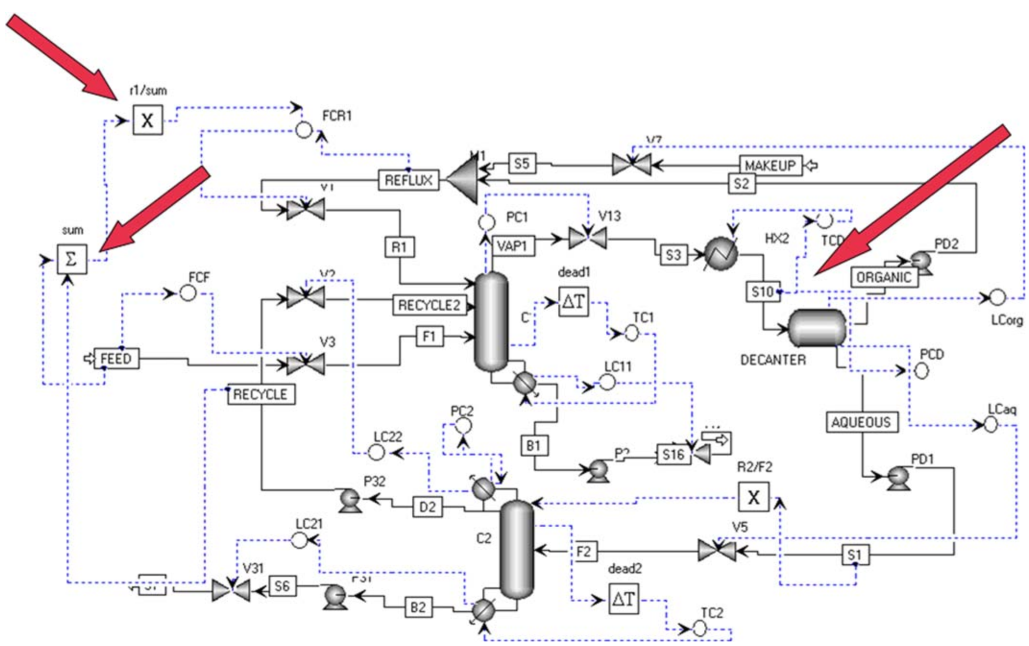

Figure 4. Control structure with Decanter model.

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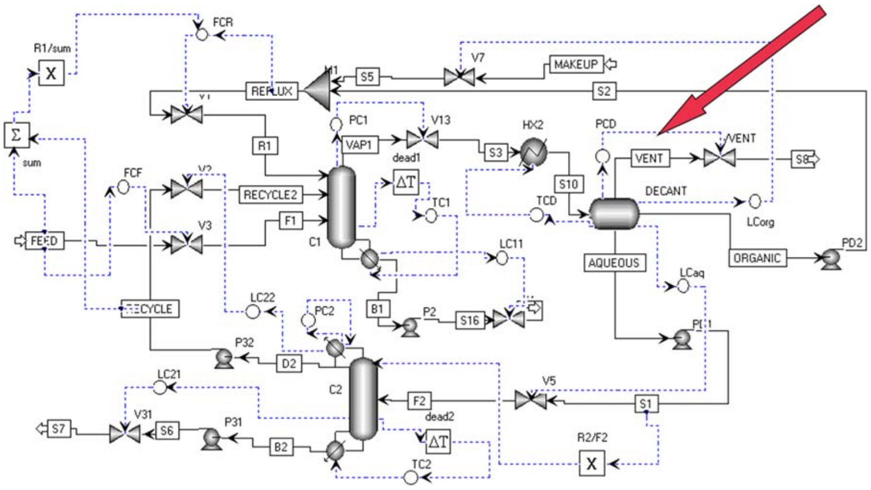

Figure 5. Control structure with Flash3 model.

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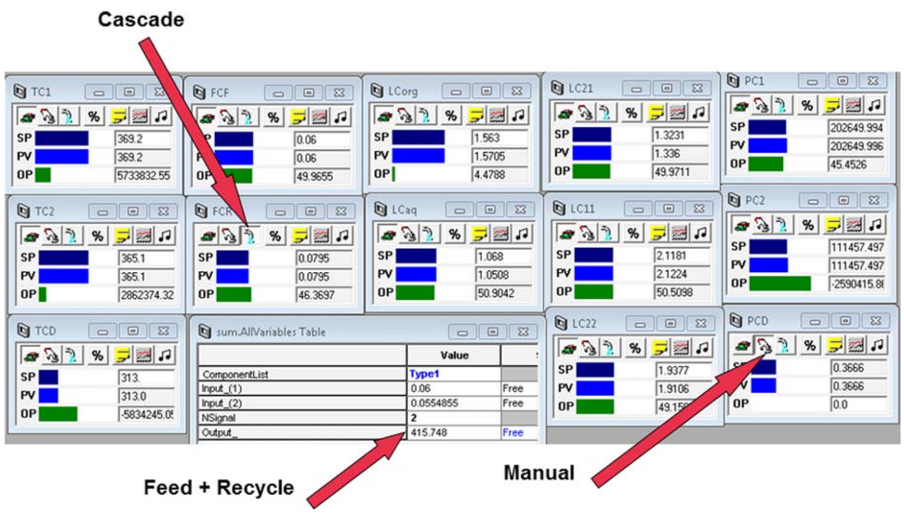

Figure 6. Controller faceplate with Flash3 model.

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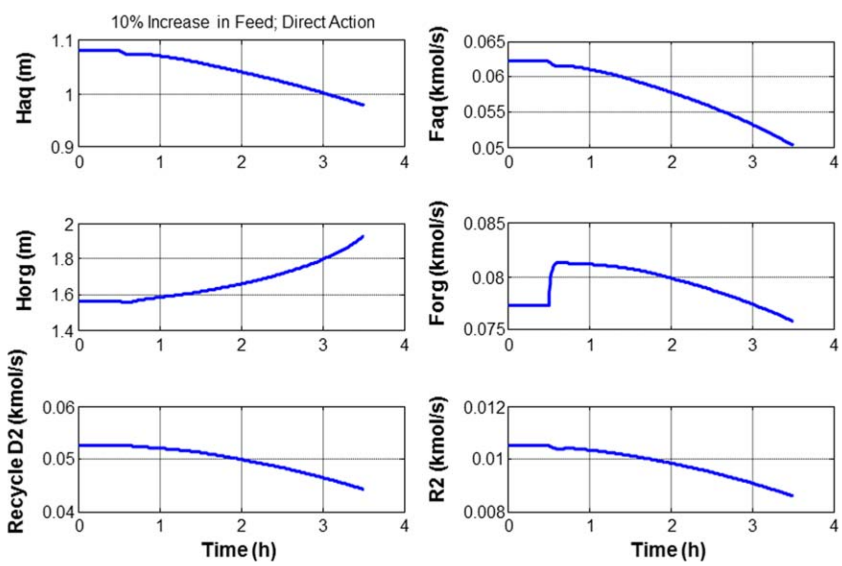

Figure 7. Direct-acting aqueous level controller: Decanter model.

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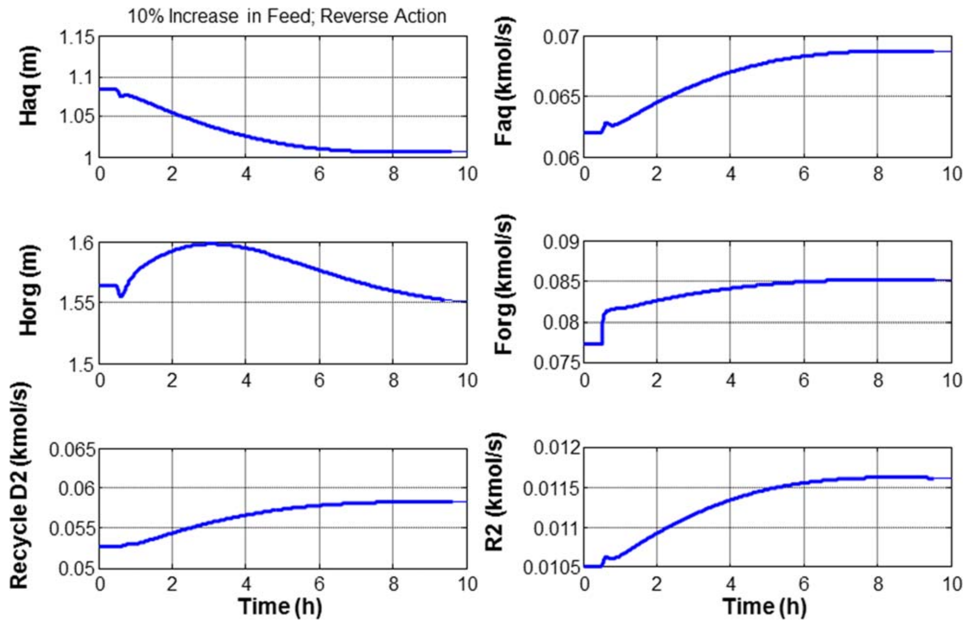

Figure 8. Reverse-acting aqueous level controller: Decanter model.

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Performance

Figure 7 gives responses of several decanter variables when a 10% increase in feed flow rate is made at time equal to 0.5 h. The Decanter model is used, and the aqueous level controller has conventional direct action. The height of the organic level is "Horg," and the flow rate of the organic liquid is "Forg." The height of the aqueous interface level is "Haq," and the flow rate of the aqueous liquid is "Faq."

The middle right graph in Figure 7 shows the instantaneous increase in the flow rate of the organic stream Forg from the decanter because the organic reflux is ratioed to the sum of the feed and the recycle D2 streams. The aqueous level goes down, and the direct-acting controller decreases the aqueous flow rate. The reduced feed to Column C2 reduces its distillate flow rate "D2" (and reflux flow rate "R2"). The reduction in the recycle stream to Column C1 produces an addition decrease in the organic reflux flow rate through the action of the summer. Eventually, in about 3.5 h, the organic level exceeds the high limit, and the simulation shuts down (liquid is vented from the decanter in the Aspen Dynamics simulation).

Figure 8 gives results when the aqueous level controller is switched to reverse action. As the aqueous level drops, the flow rate of the aqueous stream increases. The larger feed to Column C2 results in an increase in the flow rate of the recycle, which increases the organic reflux even more (Forg

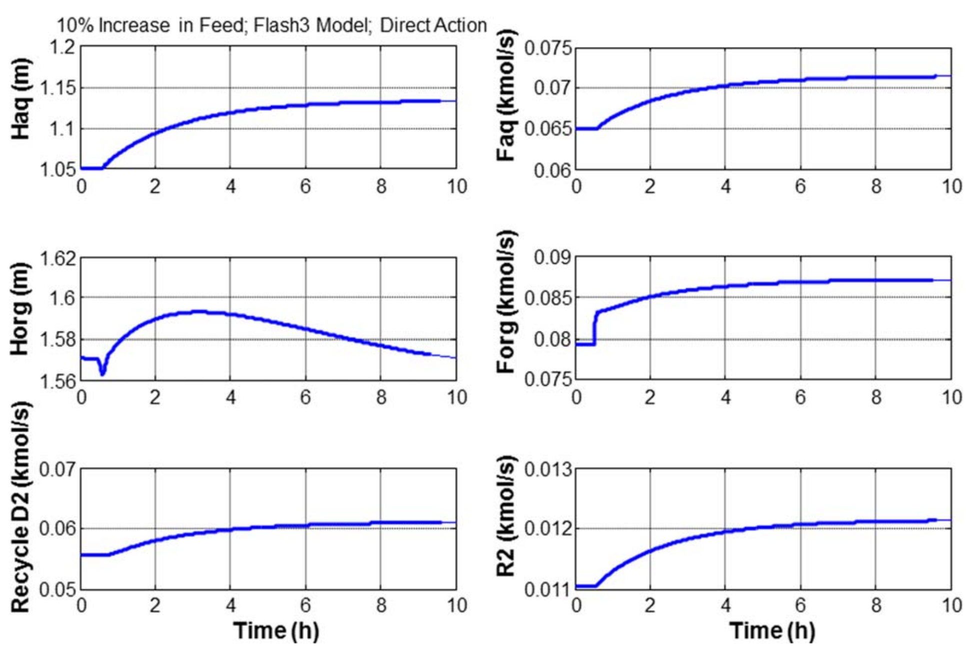

Figure 9. Flash3 model: direct-acting aqueous level controller.

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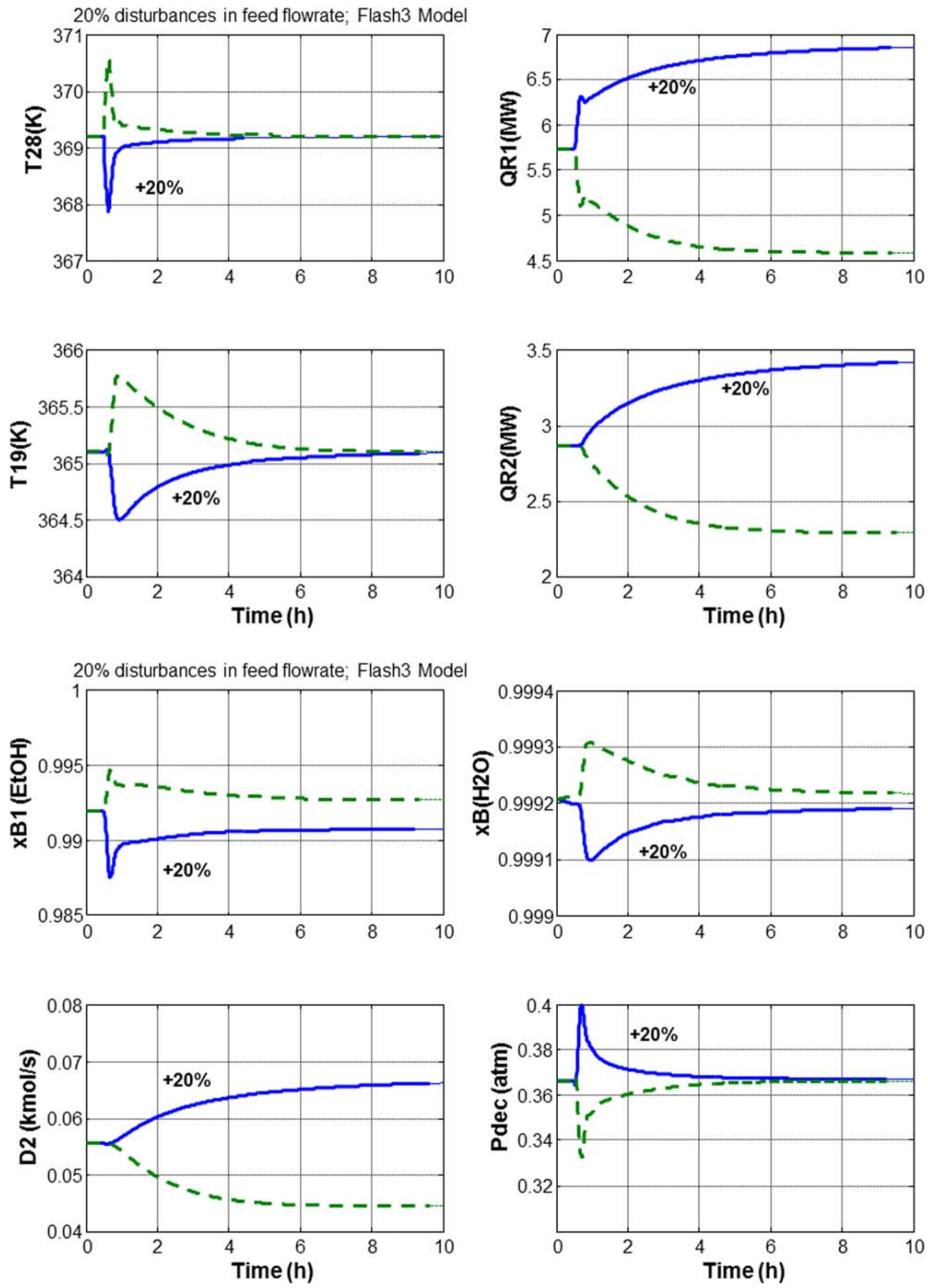

Figure 10. 20% feed flow rate disturbances.

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in the middle right graph in Figure 8). Thus, the organic level does not continue to climb. It increases for a while but eventually lines out at a steady-state level.

Figure 9 gives results when the Flash3 decanter model is used with a direct-acting aqueous level controller. A comparison of the upper left graphs in Figure 8 (Decanter model) and Figure 9 (Flash3 model) reveals the basic difference between these two models. The 10% increase in feed to the process causes the aqueous level Haq to go down in the former case, while in the latter case it increases, which makes sense physically.

Why the Decanter model behaves in this way is unclear. Other workers have not reported this problem. Chien and coworkers[2] apparently did not see this problem in the isopropanol/water/cyclohexane heterogeneous azeotropic distillation process, which has similar phase equilibrium properties. The problem could be physical (due to the constant pressure assumption), or it could be numerical (due to the solution method for minimizing free energy). Any attempt to explain the problem at this point would be speculation.

Figure 10 shows the responses of the system with the Flash3 decanter using a direct-acting aqueous level controller. The disturbances are positive and negative 20% step changes in the setpoint of the feed flow controller. Stable regulatory control of the highly nonideal distillation system is achieved. Both the ethanol and the water products are kept close to their desired purity levels. Note that the

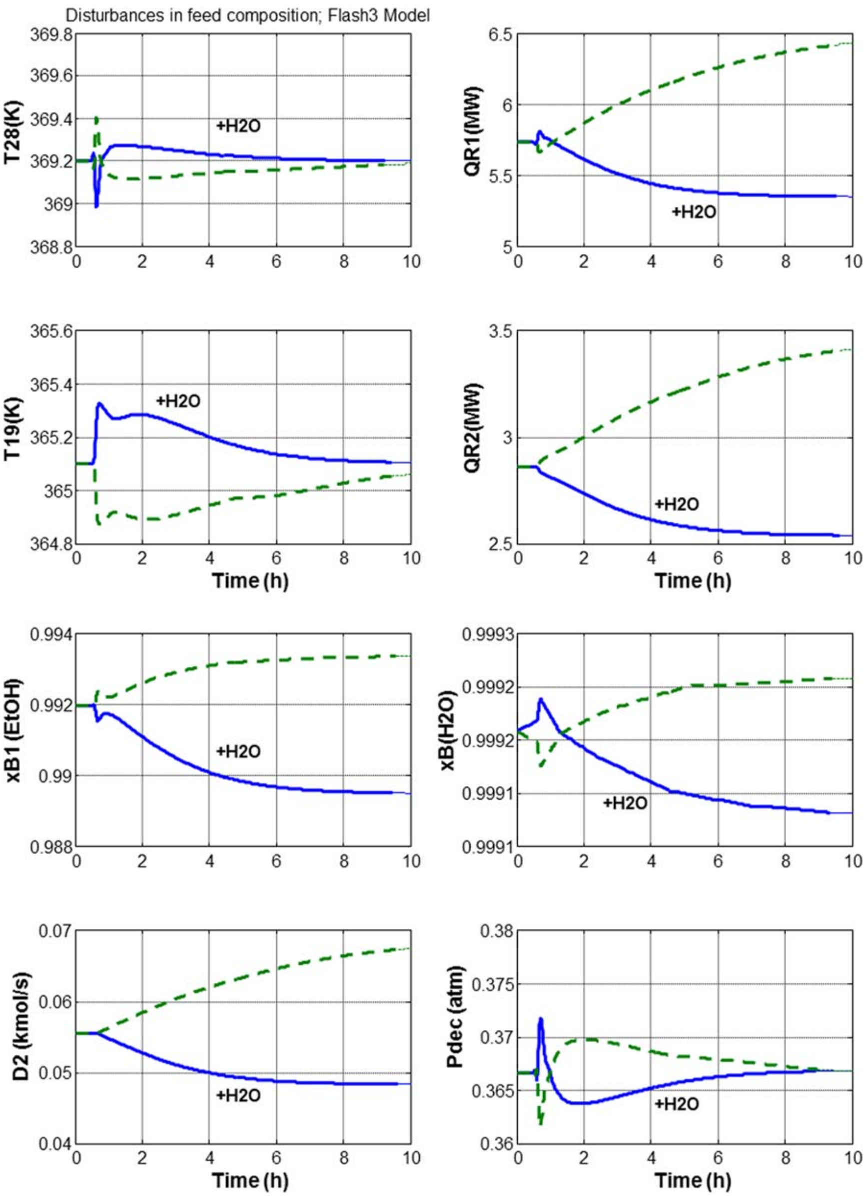

Figure 11. Feed composition disturbances.

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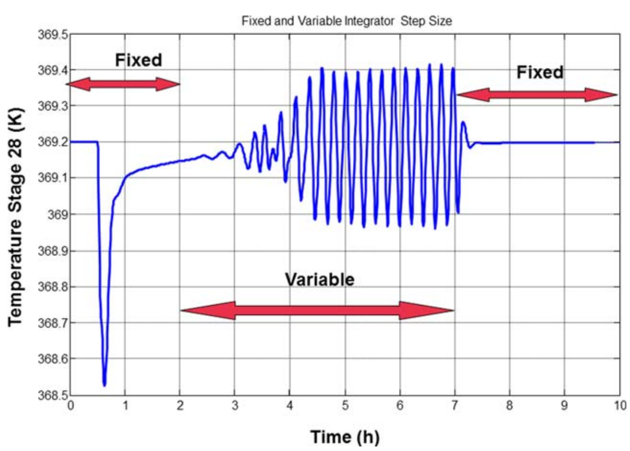

Figure 12. Effect of integrator step.

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pressure in the decanter Pdec is not constant but varies with temperature and composition.

Figure 11 gives responses to changes in feed composition from 16 to 20 mol % water (solid lines) and from 16 to 12 mol % water (dashed lines), with the corresponding changes in ethanol. Both the ethanol and the water products are kept close to their desired purity levels. More water in the feed requires less reboiler heat input to both reboilers since the recycle flow rate D2 is smaller.

Numerical Simulation Issues

During the development of several simulation studies using the current Aspen Version 7.3, a strange low-amplitude oscillation has been experienced, which is not affected by controller tuning. The solution to the problem was found to be a modification in the integrator.

The default numerical integration algorithm uses a variable step size. Switching to a fixed step size eliminated the oscillation problem. To achieve this, go to "run" on the upper toolbar in Aspen Dynamics, select "solver options" and click the "integrator" page tab. The step size can be changed to "fixed" on the window that opens.

The problem is illustrated in Figure 12 where the temperature on Stage 28 in Column C1 is plotted. The step size is specified to be fixed, and a 10% increase in feed flow rate is made at time equal 0.5 h. At time equal 2 h, the simulation is paused, and the step size is changed to variable. An oscillation occurs, until the step size is changed back to fixed at time equal 7 h. Aspen users should be aware of this problem.

Conclusions

The anomalous behavior of one of the Aspen decanter models has been demonstrated. The use of the Flash3 is highly recommended since the predicted results are more realistic and believable.

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