A Real Time, Dynamic, Binary Distillation Simulation for WEB Based Instruction

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Abstract

Simulation of complex processes in real time is essential for web-based instruction. Dynamic distillation has unique problems because of the large number of differential equations that must be solved simultaneously. This paper describes a simplified model that simulates the dynamic operation of the distillation of isopropanol/water. The model simulates all aspects of batch operation; beginning from cold startup, through the startup, total reflux operation, production of product, through shutdown. The control scheme is included so that users can operate and tune controllers. In spite of numerous simplifications, the model preserves the essential features for a real time simulation. The entire applet is only approximately 70K and is used for Internet based laboratory instruction. This paper focuses on the derivation of the model. A more complete discussion of the results will be presented at some other time.

Background

A process simulation of a binary batch distillation column was desired for a portion of the on line Virtual Chemical Engineering Laboratory (VCEL) being developed at Widener University. The model was to be used to acquaint students with the operation of an existing seven-stage distillation column and had to simulate the operation from cold startup, through operation and shut down. Therefore, it was necessary to simulate the entire behavior of the unit. Still feed is a mixture isopropanol/water at a composition of approximately 3 mole% isopropanol (an azeotrope exists at ~76 mole % isopropanol). Additionally, the finished model would be part of an interactive JAVA applet that would run at least at real time speed. The use of JAVA applets reduces the load to the web server by shifting the computational work to the client computer. However, this mode of operation places severe restrictions both on the size of the model (because the applet containing the entire model and associated graphical user interface must be sent across the web) and the speed of calculation. The calculations must be done on the client computer quickly enough so that the applet has adequate time to update screen graphics and scan the user’s keyboard and pointing device. The design criteria was that the finished applet be able to run on a Pentium 1 100 MHz machine, which was judged to be the slowest machine likely to be used by a student. Therefore, the model was made as simple as possible while still preserving behaviors of the unit essential to familiarize students with its operation.
Prototype description

The distillation unit being modeled is a seven stage Technovate column with electrically heated reboiler and total condenser. Condensate enters an accumulator from which reflux can be pumped through a preheater back to the column and product can be sent to a receiving tank. The unit is equipped with an OPTO LCSX programmable logic controller (PLC), product and reflux flows can be measured and controlled by the PLC. Power to the reboiler and reflux preheater is controlled manually.

The startup of the batch still consists of heating the charged reboiler with liquid at ambient temperature. The column is heated by air and vapor rising from the reboiler. Once condensate fills the accumulator level to a specified level, a PID control using accumulator level as input and reflux flow as output is switched to automatic. When the flow has stabilized, the reflux preheater is switched on and the unit is run at total reflux for several minutes. Product can be removed using one of two standard control schemes; either 1) constant temperature (representing composition) or 2) constant reflux flow. Constant temperature control is achieved by using a PID controller to control temperature using reflux flow. Constant flow is achieved by setting the reflux valve to a constant setting. In either method a PID controller uses liquid level in the accumulator to regulate product flow. This method of product takeoff allows the product flow to be measured. Vapor flow is calculated from the sum of the product and reflux flows. A plot of temperatures during a typical startup is shown in figure 1.

Figure 1

![Typical Startup](image-url)
Literature

A dynamic model of continuous binary distillation is included in Luyben\textsuperscript{2}, however this model is designed for systems with constant relative volatility and therefore, could not be used. Additionally, this model does not include startup. There are several complete models of distillation available. Of particular interest here the work of Yue and Billing\textsuperscript{3}, who used a dynamic simulation as part of a training course. Giani, Ruiz and Cameron\textsuperscript{4,5} presented a complete and detailed model of multicomponent distillation in a lengthy series of articles. This model was then used to simulate startup and shutdown (29, 30). A binary model was developed to minimize the applet size and maximize computational speed.

Mathematical development.

Distillation simulation requires the solution of a stiff system of differential equations normally consisting of a heat balance, total material balance and k-1 component material balances (where k is the number of chemical species present) for each tray. Additional energy and material balances are required for the reboiler and condenser. Thermodynamic data, together with other column properties such as liquid levels, column pressure, etc. are evaluated for each tray at every integration step.

Therefore, it is essential that the thermodynamic calculations be extremely fast. The distillation column is run under atmospheric pressure using a mixture of isopropanol and water. This mixture has an azeotrope at 76 mole\% 2 propanol and one atmosphere. The total pressure difference between the condenser and reboiler is small compared to atmospheric pressure. Therefore, for thermodynamic calculations, the column can be assumed to be at one atmosphere. The program contains Txy data from Perry’s Handbook in a tabular form. Linear interpolation is used to provide intermediate values to minimize calculation time. Additional thermodynamic properties (molar heat capacity, density, etc.) are estimated by linear interpolation of pure component values.

Reboiler

When the reboiler is below the boiling point, the reboiler heat balance is described by:

\[ n_c C_p \frac{dT_r}{dt} = Q \] (1)

where \( C_p \) = the molar heat of the material in the reboiler (joule/gmoleK)
\( n_c \) = the moles in the reboiler (gmole)
\( Q \) = heat input, taken to be the power input to reboiler (W)
\( T_r \) = reboiler temperature (K)
\( t \) = time (sec)
When the liquid is at the boiling point, the rate of vapor formation is \( V \) given by
\[
V = \frac{Q}{\Delta H_v} \tag{2}
\]
where \( V \) = vapor from the reboiler (gmole/sec)
\( \Delta H_v \) = molar heart of vaporization (joule/sec)

Tray Heat Balance

The rise in temperature of the lower stages prior to the onset of full boiling (figure 1) is assumed to be due primarily to free convection from the reboiler, during this stage air is in the column and little condensation occurs, consequently, the plates contain no liquid. The equation describing heating in this stage is
\[
m_i C_i \frac{dT_i}{dt} = U_i (T_i - T_r) \tag{3a}
\]
where \( C_i \) = the mean heat capacity of the tray itself (the same for each tray)
(joule/gm K)
\( m_i \) = the mass of the tray (the same for each tray) (gm)
\( T_i \) = the temperature of the tray (K)
\( U_i \) = the heat transfer coefficient between the i-th stage and the reboiler
due to free convection of air

The overall heat transfer coefficient between the reboiler and a tray rather than between the tray and the next lower one is used for computation simplicity. Note that \( U_i \) is a strong function of temperature for free convection between vertical surfaces. Linearizing \( U_i \) yields
\[
m_i C_i \frac{dT_i}{dt} = (U_i T_r + \bar{U}_i)(T_i - T_r) \tag{3b}
\]
where \( U_i \) and \( \bar{U}_i \) are experimentally measured for the first two plates and assumed 0 for the remaining ones.

During the second portion of startup, tray heating is the result of condensation of vapors heating the column. During this portion vapor from the reboiler is rising at a rate \( V \) from equation 2. Following the approach used by ___ and ___, negligible vapor hold up is assumed. Therefore vapor rise through trays already at the boiling temperature until reaching a tray below its boiling point. All the vapor condenses at this tray until its temperature reaches the boiling point. The differential equation describing tray temperature during this phase is:
\[
\frac{d(n_i C_i + n_i C_p)T_i}{dt} = \Delta H_v V_{i-1} \tag{4}
\]
where \( n_i \) = the moles of liquid on the i-th tray determined from a material balance described below.(gmole)
\( V_{i-1} \) = the vapor flow rate from the next lower column (gmole/sec)
As a result, the vapor flow from all trays at their boiling points is taken to be the same. The vapor flow from any tray below its boiling point is 0 (all the vapor is assumed to condense). Once a tray has achieved the boiling point, the heat balance is neglected (MacCabe-Thiele assumptions) and tray temperature is taken to be the boiling point at the tray composition. This assumption is reasonable because the molar heats of vaporization of isopropanol and water are similar (39.9 kJ/gmol vs 40.7 kJ/gmole)

Tray Material balances

Liquid Total material balance

The material balance for a tray is given by equation 5:

\[
\frac{dn_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i
\]  
(5)

where \(L_i\) = the liquid flow from the i-th tray (\(L_{N+1}\) = the reflux flow) (gmole/sec)  
\(V_i\) = the vapor flow from the i-th tray (\(V_0\) = the reboiler flow) (gmole/sec)  
\(n_i\) = the moles on the i-th tray (gmole)

The liquid flow from the i-th tray is given by

\[
L_i = k(h_i - h_w)^{2/3}
\]  
(6)

where \(k\) = the wier constant (empirically determined) (gmole/m \(^{3/2}\) sec)  
\(h_i\) = the height of liquid in the i-th tray (m)  
\(h_w\) = the wier height (m)

The constant \(k\) normally includes a term to account for increase in liquid height associated with vapor flow. Foaming is included in the model by setting \(h_w\) to an empirically determined value that is lower than the actual value.

The mole fraction of isopropanol in the liquid phase is determined from a component material balance assuming perfect mixing of liquid on the tray. This yields equation 7a

\[
\frac{dx_i n_i}{dt} = x_{i+1} L_{i+1} - x_i L_i + V_{i-1} y_{i-1} - V_i y_i
\]  
(7a)

where \(x_i\) = the mole fraction of isopropanol in the liquid phase of the i-th tray  
\(y_i\) = the mole fraction of isopropanol in the vapor phase of the i-th tray

Differentiating the left hand of 7a and substituting the value of dni/dt from equation 5 yields equation 7b

\[
\frac{dx_i}{dt} = \frac{(x_{i+1} - x_i)L_{i+1} + V_{i-1}(y_{i-1} - x_i) - V_i(y_i - x_i)}{n_i}
\]  
(7b)

Accumulator
Perfect mixing is also assumed in the accumulator because the pump for the reflux and product is oversized so that a large stream recirculates back to the accumulator. The overall material balance for the accumulator is

$$\frac{dn_a}{dt} = V_N - R - D$$

(8)

where $n_a$ = the moles of liquid in the accumulator (gmole)
$D$ = the product (distillate) flow rate (gmole/sec)
$h_a$ = the height of liquid in the accumulator (m)

The derivative of the mole fraction of isopropanol in the accumulator is given by a component material balance (equation 9a)

$$\frac{dx_a n_a}{dt} = y_N V_N - x_a (R - D)$$

(9a)

After differentiating the left hand side and replacing $dn_a/dt$ with the right hand side of equation 8, equation 9 upon substitution and rearrangement yields.

$$\frac{dx_a}{dt} = \left( \frac{y_N - x_a}{n_a} \right) V_N$$

(9b)

where $x_a$ = the mole fraction of isopropanol in the accumulator

The total condenser is oversized and the condensate enters the accumulator at ~ 30C. Because of this fact, and the presence of the reflux preheater, a heat balance around the condenser is unnecessary for this model. However, the reflux preheater must be modeled to provide the temperature of the reflux, and hence the temperature profile of the column.

Reflux preheater

The reflux preheater exhibits a second order response and therefore, must be modeled in more detail than the reboiler. The preheater consists of an electric heater immersed in the reflux stream. The reflux is never raised above boiling in ordinary operation, so phase changes are neglected to simplify computation. The temperature of the electric heating element is calculated from an energy balance assuming the heating element is at uniform temperature

$$m_e C_e \frac{dT_e}{dt} = Q_e - h_r A_r (T_e - T_r)$$

(10)

where $A_r$ = the area of the reflux heater
$C_e$ = the mean heat capacity of the heating element (joule/gm K)
$h_r$ = the heat transfer coefficient between the reflux and the heating element (joule/m2 sec)
$m_e$ = the mass of the heating element (gm)
$T_e$ = the temperature of the heating element (K)
$T_r$ = the temperature of the reflux (K)
Note that it would be more appropriate to use the log mean temperature difference in equation 10, however the $T_e - T_r$ is used for computational simplicity. The second term represents the heat delivered to the reflux. The equation used to determine $dT_r/dt$ is

$$n_rC_p\frac{dT_r}{dt} = h_rA_r(T_e - T_r) + (T_{in} - T_r)V_N$$

(11)

where $n_r$ = the moles of reflux in the heater (gmole)

$T_{in}$ = the inlet temperature (assumed to be 25°C)

PID Controllers

The PID controllers are simulated using the control algorithm used by the OPTO LCSX itself and given by equation 12

$$\Delta O = P\left(e - e_{\text{last}}\right) + T_I e_{\text{last}} + T_D \frac{e_{\text{last}} - e_{\text{last-1}}}{\Delta t}$$

(12)

where $e$ = the most recently measured difference between the measured variable and the set point

$e_{\text{last}}$ = the deviation measured at the last time interval

$e_{\text{last-1}}$ = the deviation measured at the second last time interval

$P$ = the controller gain

$T_I$ = the controller constant for integral action

$T_D$ = the controller constant for derivative action

Tray Efficiency

The Murphree tray efficiency is assumed constant at 30% over the entire range of conditions. Thus the vapor phase composition is given by

$$y_i = [Y(x_i) - y_{i-1}]\varepsilon + y_{i-1}$$

(13)

where $Y(x_i)$ = the theoretical vapor phase composition determined from the xy diagram

$\varepsilon$ = the Murphree efficiency (assumed to be constant throughout the process)

Shutdown

Shutdown of distillation can be modeled simply. The applet in which the model runs automatically ends after user turns off the power, process air, and cooling water are turned off. Liquid drains from the trays following equations 5 and 6. Heat loss from the surroundings is assumed to follow a first order equation with a small value of $k’$.

$$\frac{dT_d}{dt} = h_sA_s(T_s - T_d)$$

where $k’ = a constant related to$

$T_d$ = the ambient temperature (20°C)
Solution of the differential equations

The differential equations for liquid flows and compositions are coupled and therefore must be integrated carefully. A semi implicit Runge Kutta algorithm (SIRK) described by Holland and Liapis is used for the accumulator and those trays having achieved thermal equilibrium. This approach requires the simultaneous evaluation of all coupled derivatives in the system. An important consideration is minimizing the size of the \( n \times n \) Jacobean that must be inverted at each step. To reduce the size of the Jacobean (thereby speeding computation) the derivatives for temperature during start up (eqns. 1 and 3b), and the equations for the reflux preheater (eqns. 10 and 11) are integrated separately using Euler integration after the SIRK calculation of flows and liquid compositions.

Tests

The accountability of the simulation was found to be within 0.2% of isopropanol and 0.005% on total material balance after a simulated hour of operation.

A simulation of the startup is shown Figure 2. This simplified model preserves the general shape of the temperature curve.
Bibliography


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Prof. Nippert has been on the faculty of the Chemical Engineering Department of Widener University, Chester Pa. since 1980. He is a graduate of Lehigh University and worked for several years at Kawecki-Berylco (now Cabot Specialty Metals). His current interests include the development of web-based instructional materials for use in a variety of engineering courses. The material is contained in "The Virtual Chemical Engineering Laboratory", found at www2.widener.edu/~crn0001/VirtualLab.html. The site is open to all for examination and use. He is married and has two children.