The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. We request problems that can be used to motivate student learning by presenting a particular principle in a new light, can be assigned as novel home problems, are suited for a collaborative learning environment, or demonstrate a cutting-edge application or principle. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Dr. Daina Briedis (e-mail: briedis@egr.msu.edu), Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI 48824-1226.

SEMI-BATCH STEAM DISTILLATION OF A BINARY ORGANIC MIXTURE
a Demonstration of Advanced Problem-Solving Techniques and Tools

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Mathematical software packages such as Excel®, MAPLE™, MATHCAD®, MATLAB®, Mathematica®, and POLYMATH™ are currently routinely used for numerical problem solving in engineering education.[1-3] It is equally essential, however, to follow the continuing development of new tools and techniques in this field. These new tools may enable effective and efficient solution of more complex and realistic problems while presenting clear and precise documentation of the problem and its solution.

In this paper a problem is presented that demonstrates the use of the following new tools and techniques:

1. *A new interface from Polymath Software to the DIPPR® physical property database[4] that enables transference of the data and the correlations directly into computer code for POLYMATH, Excel, or MATLAB.*

2. *A new technique for grouping the equations and data according to their role in problem solving, that provides clear and precise documentation of the model. The use of this technique is best implemented when software*

packages are used that allow documentation prior to the automatic reordering of the code during the generation of the numerical solution.

3. *A demonstration of new tools available for solution of two-point boundary-value problems and systems of differential-algebraic equations.*

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PROBLEM BACKGROUND

Semi-Batch Steam Distillation of a Binary Organic Mixture

This illustrative example involves semi-batch steam distillation of binary mixture. A schematic plot of the steam distillation apparatus is shown in Figure 1. The organic mixture is charged into the still initially, and then steam is bubbled through continuously until the desired degree of separation has been reached. There are two different periods in the operation of the still: the heating period, until the boiling point temperature of the organic mixture is reached, and the distillation period. A brief description of the mathematical models for the two periods follows.

Heating Period

A simple mass balance on the water phase yields

$$\frac{dm_w}{dt} = W_s \qquad (1)$$

where W_s is the steam flow-rate in kmol/s and m_w is the mass of water in the still in kmol. It is assumed that all the steam condenses in the distillation vessel and that the organic phase masses remain constant during the heating period.

An energy balance on the still provides the equation for the change of the temperature T in °C

$$\frac{dT}{dt} = \frac{W_s(H_s - H_{Lw}) - Q}{m_w c_{pLw} + m(x_1 c_{pL1} + x_2 c_{pL2})} \qquad (2)$$

where H_s is the enthalpy of the steam in J/kmol, H_{Lw} is the enthalpy of liquid water in J/kmol, Q is the rate of heat transfer to the surroundings in J/s, c_{pLw} is the molar specific heat of the water in J/kmol·K, m is the mass of the organic phase in the still in kmol, x_1 and x_2 are the mole fractions, and c_{pL1} and c_{pL2} are the molar specific heats of organic compounds No. 1 and 2, respectively, in J/kmol·K. The heat transfer rate to the surroundings is calculated from Eq. (3)

$$Q = UA(T - T_a) \qquad (3)$$

where UA is the product of the overall heat transfer coefficient U and the contact area A with the surroundings in J/s·K, T_a is the ambient temperature in K, and T is the temperature of the liquid in the still in K.

Assuming ideal liquid behavior, Raoult's law can be used to calculate the vapor mole fraction of the components in the organic phase

$$y_1 = \frac{x_1 P_1}{P} \qquad y_2 = \frac{x_2 P_2}{P} \qquad (4)$$

where P is the total pressure in Pa and P_1 and P_2 are the vapor pressures of the organic compounds in Pa. The mole fraction of the water which is immiscible in the organic phase is given by $y_w = P_w/P$. The heating period continues until the sum of vapor pressures of the organic compounds and the water is

equal to the total pressure. Thus, the "bubble point" equation to be satisfied can be expressed as

$$f(T) = 1 - (y_1 + y_2 + y_w) = 0 \qquad (5)$$

Distillation Period

During the distillation period, there is output of water vapor from the still. Thus Eq. (1) must be modified to

$$\frac{dm_w}{dt} = W_s - Vy_w \qquad (6)$$

where V is the outlet vapor flow rate. Material balances on the two organic compounds yield two additional differential equations

$$\frac{d(mx_1)}{dt} = -Vy_1 \qquad \frac{d(mx_2)}{dt} = -Vy_2 \qquad (7)$$

The organic mass in the still at any time is given by: $m = mx_1 + mx_2$. The temperature in the still changes in a manner so that the bubble point equation [Eq. (5)] is satisfied. The energy balance at a particular temperature yields the momentary vapor flow rate

$$V = \frac{W_s(H_s - H_{Lw}) - Q}{H_V - [y_w h_{Lw} + (y_1 h_{L1} + y_2 h_{L2})]} \qquad (8)$$

where H_V is the molar enthalpy of the vapor phase; h_{Lw}, h_{L1}, and h_{L2} are the liquid phase molar enthalpies of water, n-octane and n-decane, respectively. Material balances on the water and organic phases in the still can provide the amount and the mole fractions of the various components in the distillate.

PROBLEM STATEMENT

Prenosil[5] and Ingham et al.[6] have considered the semi-batch steam distillation of an n-octane (comp. 1) and n-decane (comp. 2) mixture. The data provided by Ingham et al.[6] are the following. Initially M = 0.015 kmol of organics with composition x_1 = 0.725 is charged into the still. The initial temperature in the still is T_0 = 25 °C. Starting at time t = 0,
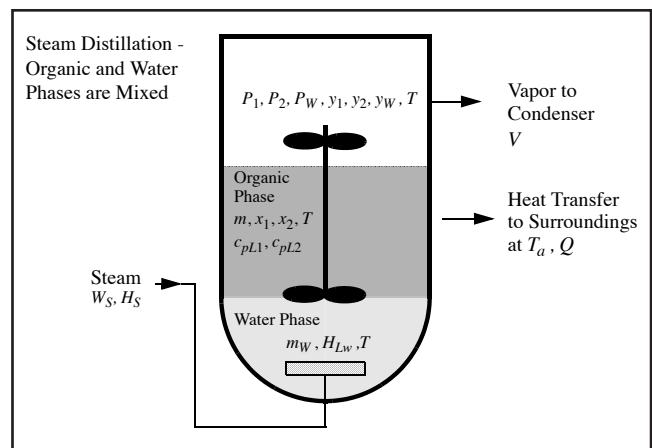

Figure 1. *Schematic plot of steam distillation.*

steam at a temperature $T_{steam} = 99.2$ °C is bubbled continuously through the organic phase at the rate of $M_S = 3.85e\text{-}5$ kmol/s. All the steam is assumed to condense during the heating period. The ambient temperature is $T_E = 25$ °C and the heat transfer coefficient between the still and the surrounding is $UA = 1.05$ J/s-K. The ambient pressure is $P = 9.839E{+}04$ Pa.

Assumptions: 1) Ideal behavior of all components in pure state or mixture; 2) complete immiscibility of the water and the organic phases; 3) ideal mixing in the boiler; and 4) equilibrium between the organic vapor and its liquid at all times. The standard state for enthalpy calculations pure liquids at 0 °C and 1 atm. can be used.

> a) Calculate and plot the still temperature (T), component mole fractions inside the still (x_1, x_2, y_1, and y_2), and the component mole fractions in the distillate (x_{1dist} and x_{2dist}) using the data and the initial values provided.
>
> b) Determine the lowest n-octane mole fraction in the feed that can yield a distillate concentration of 90% of n-octane. Compute the percent recovery of n-octane in the distillate as function of its concentration in the feed. Vary the feed concentration in the range where the requirement for the n-octane concentration in the distillate is attainable.

PROBLEM SOLUTION

Physical Property Data and Equations for the Steam Distillation Problem

In addition to the mathematical models presented in Eqs. (1) through (8), physical property data is required for all three components involved in the steam distillation process. The data include liquid vapor pressure and heat capacity, heat of vaporization, and ideal gas heat capacity. These data should be provided in the form of equations (correlations) that enable

calculation of the pure component properties as function of the temperature.

In the past various handbooks were used as sources of physical property correlation. Prenosil,[5] for example, describes the sources of the correlations and data he used for solving this problem: "The constants of the Antoine equations for the vapor pressures of n-octane and n-decane were taken from *The Handbook of Chemistry and Physics*[7] and for water they were obtained by non-linear regression from steam tables (Perry[8]). The C_p values of the liquid components were also found in Perry[8] and their temperature dependence was neglected. The C_p data for the vapor components were calculated as functions of temperature from the equation $C_p = A + BT + CT^2$ with the constants taken from Balshiser et al.[9] The latent heats of evaporation for the organic material came from Cox and Pilcher[10] and that of water from Landolt-Börnstein.[11]"

Currently, most of the needed properties can be found in available databases. The database used in this work is the DIPPR® database.[4] In order to simplify the transfer of the data from the database to computer code and thus minimize the probability of the introduction of errors during the process, we have developed a Polymath Database Interface (PDI). The PDI enables searching the database for a particular compound, marking the desired properties, and obtaining as output the necessary data and correlations in a format that can be copied and pasted directly into a computer code. The formats that are currently supported are for POLYMATH,[12] Excel, and MATLAB.[13]

The information that is provided by the PDI for the POLYMATH solution format is demonstrated in Table 1 for the properties of n-octane that are required for the steam distillation problem. This table shows most of the information as provided by the PDI when the POLYMATH format is

TABLE 1
Physical properties of n-OCTANE as obtained from the DIPPR database by the Polymath Software Interface for use in POLYMATH

No.	Equation/ # Comment
1	# Liquid Vapor Pressure of n-OCTANE (C8H18)
2	# Uncertainty < 1%; Min_T=216.38, Max_T=568.7, Min_Val=2.1083, Max_Val=2467300 0 [K ; Pa]
3	VP_C8H18 = exp(96.084 - 7900.2 / T - 11.003 * ln(T) + 7.1802E-06 * T ^ 2) # Pa
4	# Liquid heat Capacity (at 1 atm below normal boiling point, saturation pressure at and above) of n-OCTANE (C8H18)
5	# Uncertainty < 1%; Min_T=216.38, Max_T=460, Min_Val=229340, Max_Val=341890 0 [K ; J/kmol*K]
6	LCP_C8H18=0-186.63*T+0.95891*T^2+224830#J/kmol*K
7	# Ideal Gas Heat Capacity of n-OCTANE (C8H18)
8	# Uncertainty < 1%; Min_T=200, Max_T=1500, Min_Val=145290, Max_Val=497640
9	#HIG_C8H18 = 135540*T + 443100 *1635.6* (coth(1635.6 / T)) - 305400 *746.4* (tanh(746.4 / T))+HCON_C8H18 # J/kmol
10	ICP_C8H18 = 135540 + 443100 * (1635.6 / T / sinh(1635.6 / T)) ^ 2 + 305400 * (746.4 / T / cosh(746.4 / T)) ^ 2 # J/kmol*K
11	# Heat of Vaporization of n-OCTANE (C8H18)
12	# Uncertainty < 3%; Min_T=216.38, Max_T=568.7, Min_Val=45898000, Max_Val=0 [K ; J/kmol]
13	HVP_C8H18 = 55180000 * (1 - T / 568.7) ^ 0.38467 # J/kmol

TABLE 2
Calculation of HCON_C8H18 for n-Octane (reference state for enthalpy: pure liquid at 273.15 K)

No.	Equation/ # Comment
1	T0 = 273.15 #K
2	HIG_C8H18 = 135540*T0 + 443100 *1635.6* (coth(1635.6 / T0)) - 305400 *746.4* (tanh(746.4 / T0)) # J/kmol
3	HVP_C8H18 = 55180000 * (1 - T0 / 568.7) ^ 0.38467 # J/kmol
4	HCON_C8H18 = HVP_C8H18-HIG_C8H18 # J/kmol

specified. The code that is generated by the interface program includes correlation equations, definition of constant values, and comments (text that starts with the "#" sign and ends with the end of the line). The row numbers shown in Table 1 are not part of the output generated by the interface program; they were added as references for the explanations that follow. Lines 1-13 can be generated at once by selecting the desired "Temperature-dependent Properties" and then "Generating Report" at the "Basic Report" level. The "Report Level" determines the amount of information that is to be included as comments.

Lines 1 through 3 contain the information related to the vapor pressure of n-octane. In line 1 the full name of the property, the full name of the compound, and its formula are shown (as a comment). In line 2, the uncertainty (error) in the calculated property (vapor pressure) is shown as < 1%. The additional details given in this line include the range of validity of the correlation equation. "Min_T" is the lower temperature limit of the range of validity, "Max_T" is the upper temperature limit, "Min_Val" is the property value (vapor pressure, in this case) at the lower temperature limit and "Max_Val" is the property value at the upper temperature limit. The units of the temperature (K) and the property (Pa) are shown at the end of line 2.

In line 3, the property correlation is shown. The variable into which the calculated value of the vapor pressure is entered is made up from the symbol of the property (VP in this case) and the chemical formula of the compound involved. The Riedel equation is used to model the change of the vapor pressure with the temperature. The units of the property (vapor pressure in this case) are included in a "comment" in the same line with the equation. Similar information is provided for liquid heat capacity (lines 4 through 6) and heat of vaporization (lines 11 through 13).

The ideal gas heat capacity for n-octane (lines 7 through 10) deserves special discussion. The DIPPR Database provides the coefficients for the Aly and Lee[14] equation that utilizes transcendental hyperbolic functions. The integrated form of this transcendental equation for calculating ideal gas enthalpy is considerably different than the heat capacity equation. The integrated form of the enthalpy calculation when the ideal gas heat capacity is a polynomial expression is uncomplicated. For the benefit of the users, the PDI provides the equation for ideal gas enthalpy whenever the ideal gas heat capacity requested by the user involves transcendental functions. This is also included as a comment as shown in line 9. Note that the enthalpy equation includes an integration constant HCON_C8H18. This constant depends on the standard state selected for the enthalpy calculation. For example, selecting as standard state pure liquid component at 0 ˚C (273.15 K) yields HCON_C8H18 as ideal gas enthalpy at 273.15 K subtracted from the heat of vaporization of the component at the same temperature. The equations for calculating HCON_C8H18 for n-octane are shown in Table 2. This set of equations yields: HCON_C8H18 = -4.928E+08 J/kmol. Similar calculations for n-decane and water yield: HCON_C10H22 = -5.791E+08 J/kmol and HCON_H2O = -4.471E+07 J/kmol.

Modeling the Heating Period with POLYMATH

The POLYMATH program for modeling the heating period of the semi-batch distiller is shown in Table 3. The equations are grouped according to similarity in their roles in order to provide clear and concise documentation of the model and the pertinent data. Note that POLYMATH automatically reorders the equations, as needed, before starting the computations and this allows structuring the program for clarity rather than requirements of programming syntax. The first group of statements (lines 1 through 10) contains the model equations, mostly the ones that were introduced already as Eqs. (1) through (5). The pure compound property equations are grouped in lines 12 through 22. The heat capacity of the liquid phase and the enthalpy of the organic liquid are calculated in lines 25 and 26. Problem-specific data and initial values, as provided by Ingham et al.[6] are included in lines 29 through 39.

The determination of the final time (t_f) for the heating period requires some trial and error until the bubble point condition of Eq. (5) is satisfied. Linear interpolation can be conveniently used for determining the correct value of t_f. Assigning t_f = 180 s yields a final still temperature of T = 90.14 ˚C with f(T) = 0.01903 [Eq. (5)]. A higher value of t_f (= 190 s) yields a final still temperature of T = 93.12 ˚C with f(T) = - 0.09490. Linear interpolation between the two t_f and f(T) values yields t_f = 181.67 s. Additional trials give t_f = 181.72 s. This value is accurate up to four digits, yielding temperature value of T = 90.66 ˚C which is accurate up to three decimal digits.

No.	Equation/ # Comment
	TABLE 3 **POLYMATH program for simulating the "heating period" in the steam distiller**
1	# Heating period model equations
2	d(T)/d(t) = (MS * (HS - HL_H2O) -Q)/ CpL # Eq. 1. Still temperature from heat balance
3	d(MW)/d(t) = MS # Eq. 2. Mass of water in the still (kmol) from mass balance
4	Q = U* (T - Ta) # Eq. 3. Heat transferred from the still to the surroundings (J/s)
5	Y1= VP_C8H18* x1 / P # Eq. 4. n-octane vapor mole fraction
6	Y2 = VP_C10H22* x2 / P # Eq. 4. n-decane vapor mole fraction
7	YW =VP_H2O / P # Water vapor mole fraction
8	fT = 1 - (Y1 + Y2 + YW) # Eq. 5. Stop the integration when fT=~0.
9	x2=1-x1 #Mole Fraction of n-decane
10	TK = T + 273.15 # Absolute temperature (K)
11	#
12	# Pure compound property equations
13	VP_C8H18 = exp(96.084 - 7900.2 / TK - 11.003 * ln(TK) + 7.1802E-06 * TK ^ 2) # Pa
14	VP_C10H22 = exp(112.73 - 9749.6 / TK - 13.245 * ln(TK) + 7.1266E-06 * TK ^ 2) # Pa
15	VP_H2O = exp(73.649 - 7258.2 / TK - 7.3037 * ln(TK) + 4.1653E-06 * TK ^ 2) # Pa
16	LCP_C8H18 = (0 - 186.63 * TK + 0.95891 * TK ^ 2 + 224830) # J/kmol*K
17	LCP_C10H22 = (0 - 197.91 * TK + 1.0737 * TK^ 2 + 278620) # J/kmol*K
18	LCP_H2O=(276370-2090.1*TK+8.125*TK^2-0.014116*TK^3+9.3701E-06*TK^4)#J/kmol*K
19	HS = (33363*TSK + 26790 *2610.5* (coth(2610.5 / TSK)) ^ 2 + 8896 * 1169*(tanh(1169 / TSK)) -4.471E+07)# Steam Enthalpy (J/kmol)
20	HL_C8H18 = (224830*(TK-T0) - 186.63 *(TK^2-T0^2)/2 + 0.95891 * (TK ^ 3-T0^3)/3) # J/kmol
21	HL_C10H22 = (278620*(TK-T0) - 197.91 * (TK^2-T0^2)/2 + 1.0737 *(TK ^ 3-T0^3)/3)# J/kmol
22	HL_H2O = (276370*(TK-T0) - 2090.1 * (TK^2-T0^2)/2 + 8.125 * (TK ^ 3-T0^3)/3 - 0.014116 * (TK ^ 4-T0^4)/4 + 9.3701E-06 * (TK ^ 5-T0^5)/5)# J/kmol)
23	#
24	#Mixture property equations
25	CpL = MW * LCP_H2O + M * (x1 * LCP_C8H18 + x2 * LCP_C10H22) # Heat capacity of the liquid phase J/kmol*K
26	HL= x1*HL_C8H18+x2*HL_C10H22 # Enthalpy of the liquid organic phase (J/kmol)
27	#
28	#Problem specific data, initial and final values
29	T0=273.15 # Enthalpy reference temperature (K)
30	TSK = 99.2 + 273.15 # Steam temperature (K)
31	P = 9.839E+04 # Ambient Pressure (Pa)
32	MS = 3.85e-5 # Steam flow rate (kmol/s)
33	U = 1.05 # Heat transfer coeff (J/s-K)
34	Ta = 25 # Ambient temperature (deg C)
35	x1=0.725 #Mole Fraction of n-octane
36	M=0.015 # Initial amount of organics, kmol
37	T(0) = 25 # Temperature in the still (deg. C)
38	MW(0) = 0 # Mass of water in the still (kmol)
39	t(0)=0
40	t(f) = 181.72 # s

Modeling the Distillation Period with POLYMATH

A specific challenge in the solution for the distillation period is the need to follow the bubble point temperature curve [Eq. (5)] during the time of the integration. This requires solving a nonlinear algebraic equation for each and every integration step. (This is basically a differential-algebraic or DAE problem.) A simple method that can be used within POLYMATH for this purpose is the "controlled integration" technique of Shacham and Brauner.[15] Using this method, Eq. (5) is rewritten

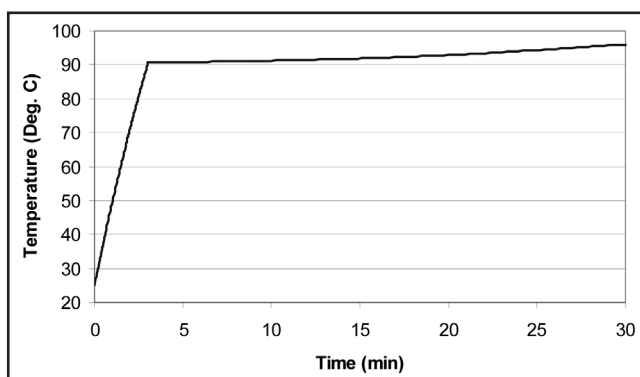$$\varepsilon = 1 - (y_1 + y_2 + y_w) \qquad (5A)$$

Figure 2. Temperature change during semi-batch steam distillation (POLYMATH results).
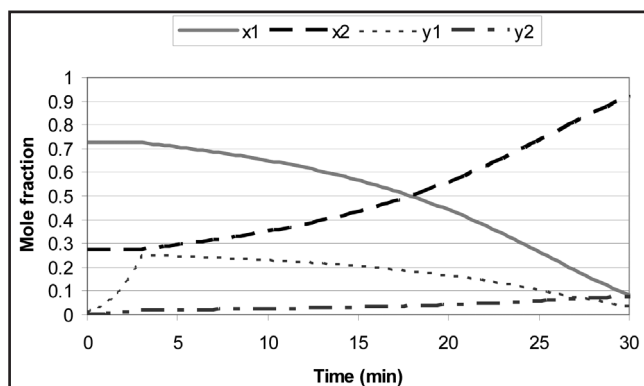

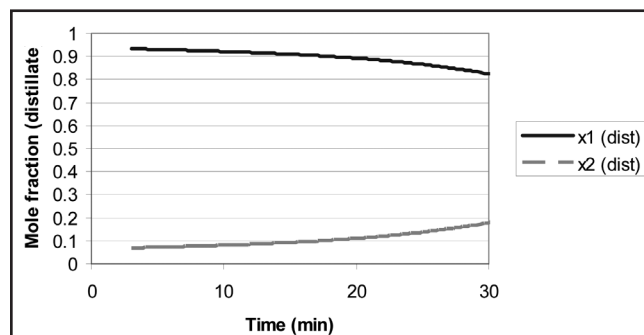*Figure 3. Change of organic phase composition during semi-batch steam distillation (POLYMATH results).*

Figure 4. Change of organic phase distillate composition during semi-batch steam distillation (POLYMATH results).

and a "proportional controller" is added to the system of equations for changing the temperature:

$$\frac{dT}{dt} = K_c \varepsilon \qquad (9)$$

The proportional gain, K_c, is selected large enough so as to keep ε below a pre-specified tolerance. Setting K_c at a large positive value will often lead to a "stiff" system of differential equations which has to be solved using specific stiff integration algorithms.

Part of the POLYMATH program for modeling the distillation period of the semi-batch distiller is shown in Table 4. Most of the equations that remain the same as in Table 3 were omitted here, for brevity. The model equations for this period (see lines 1 to 21 in Table 4) include the mass balance equations [Eqs. (6)-(8)], the equations used for changing the temperature using the controlled integration technique [Eqs. (8) and (9)], and supporting equations for calculating the amount and composition of the liquid in the still, vapor composition, and the amount and composition of the distillate. The value of the proportional gain K_c ($K_c = 1000$) was selected to keep the deviation of Eq. (5A) below the value of 10^{-5} ($\varepsilon < 10^{-5}$).

The equations for calculating the vapor phase enthalpy are added to the "pure compound" and "mixture" property sections. The initial values used for t, T, and m_w are the final values that were obtained in the "heating period." The final time for integration is set at 2000 s.

Results for the Case where $x_{10} = 0.725$

The calculated temperature profile in the steam distiller is shown in Figure 2. There is a rapid increase within the first three minutes during which the temperature increases from the initial value of 25 ˚C to the boiling temperature of 90.65 ˚C. During the distillation period there is a more gradual increase of the temperature because of the depletion of the more volatile n-octane in the still. After 30 min of distillation the temperature reaches 96 ˚C.

The variation of the concentration of the organic compounds in the still (liquid and vapor phases) is shown in Figure 3. At the beginning of the distillation period, there is a steady decrease in the liquid mole fraction of the more volatile component and a steady increase in the mole fraction of the less volatile component. After 30 minutes, the concentration of n-octane reaches the value of $x_1 = 0.085$ while the concentration of n-decane reaches: $x_2 = 0.915$. During the heating period a rapid increase in the concentration n-octane occurs in the vapor phase. After distillation starts, however, the vapor phase concentration follows the same trend as the liquid phase.

Figure 4 shows the concentration of the organic compounds in the distillate. The mole fraction of the n-octane at the start of the distillation is $x_{1dist} = 93\%$ and after 30 minutes it is reduced to $x_{1dist} = 82\%$. If the desired n-octane concentration is $x_{1dist} = 90\%$, the distillation should be stopped after 18 min.

	TABLE 4
	POLYMATH program for simulating the "distillation period" in the steam distiller
No.	**Equation/ # Comment**
1	# Distillation period model equations
2	d(MW)/d(t) = MS - V * YW # Eq. 6. Mass of water in the still (kmol) from mass balance
3	d(Mx1)/d(t) = -V * Y1 # Eq. 7. Mass of n-octane in the still (kmol) from mass balance
4	d(Mx2)/d(t) = -V * Y2 # Eq. 7. Mass of n-decane in the still (kmol) from mass balance
5	V =(MS*(HS-HL_H2O)+ Q) / (HV - (HL_H2O * YW + (Y1 * HL_C8H18 + Y2 * HL_C10H22))) # Eq. 8. Vapor flow rate (kmol/s)
6	d(T)/d(t) = 1000 * eps # Eq. 9. Still temperature by controlled integration
7	M = Mx1 + Mx2 # Organic mass in the still (kmol)
8	x1 = Mx1 / M # n-octane organic liquid mole fraction
9	x2 = Mx2 / M # n-decane organic liquid mole fraction
10	Q = U* (T - Ta) # Eq. 3. Heat transferred from the still to the surroundings (J/s)
11	Y1= VP_C8H18* x1 / P # Eq. 4. n-octane vapor mole fraction
12	Y2 = VP_C10H22* x2 / P # Eq. 4. n-decane vapor mole fraction
13	YW =VP_H2O / P # Water vapor mole fraction
14	eps = 1 - (Y1 + Y2 + YW) # Eq. 5A. Error used in controlled integration
15	M1dist = M0 * x01 - Mx1 # Mass of n-octane in the distillate (kmol)
16	M2dist = M0 * x02 - Mx2 # Mass of n-decane in the distillate (kmol)
17	MWdist = MS * t - MW # Mass of water in the distillate (kmol)
18	Mdist = M1dist + M2dist # Distilled organic phase (kmol)
19	x1dist = If (Mdist > 0) Then (M1dist / Mdist) Else (0) # n-octane distillate mole fraction
20	x2dist = If (Mdist > 0) Then (M2dist / Mdist) Else (0) # n-decane distillate mole fraction
21	TK = T + 273.15 # Absolute temperature (K)
22	#
23	*#Pure compound property equations*
-	*lines13-22inTable3*
24	HIG_C8H18 = (135540*TK + 443100 *1635.6* (coth(1635.6 / TK)) - 305400 *746.4* (tanh(746.4 / TK))-4.928E+08) # n-octane vapor enthalpy (J/kmol)
25	HIG_C10H22= (167200*TK+ 535300 * 1614.1*(coth(1614.1 / TK)) - 378200 *742* (tanh(742 / TK)) -5.791E+08) # n-decane vapor enthalpy (J/kmol)
26	HIG_H2O = (33363*TK + 26790 *2610.5* (coth(2610.5 / TK)) ^ 2 + 8896 * 1169*(tanh(1169 / TK)) -4.471E+07) # Water vapor enthalpy (J/kmol)
27	#
28	#Mixture property equations
-	*line 26 in Table 3*
29	HV = YW * HIG_H2O + Y1 * HIG_C8H18 + Y2 * HIG_C10H22 # Vapor phase enthalpy (J/kmol)
30	#
31	*#Problem specific data, initial and final values*
-	*lines 29 -34 in Table 3*
32	x01 = 0.725 # Initial n-octane organic liquid mole fraction
33	x02 = 0.275 # Initial n-decane organic liquid mole fraction
34	M0 = 0.015 # Initial amount of organics, kmol
35	T(0) = 90.66 # Temperature in the still (deg. C)
36	Mx1(0) = 0.010875 # Mass of n-octane in the still (kmol)
37	Mx2(0) = 0.004125 # Mass of n-decane in the still (kmol)
38	MW(0) = 0.0069955 # Mass of water in the still (kmol)
39	t(0) = 181.72
40	t(f) =2000

MATLAB Implementation of the Program for Parametric Runs

Parametric runs, requested in the second part of the assignment, can be carried out with POLYMATH by manually changing the parameter values. This approach, however, is inefficient and somewhat cumbersome. A more efficient approach involves derivation of an algorithm for repetitive solution of the problem with the various parameter values and using a programming language to implement the algorithm. One option is to use MATLAB for implementing the solution algorithm. The MATLAB functions for modeling the heating and distillation periods of the steam distiller can be automatically generated by POLYMATH, as demonstrated, for example, by Cutlip et al.[16]

The key steps of an algorithm that can efficiently solve the second part of the assignment are 1) Stop the integration at the heating period when the bubble point condition [Eq. (5)] is satisfied; 2) Solve the DAE system that represents the distillation period; and 3) Stop the integration of the distillation period model when the n-octane concentration in the distillate gets down to 90%.

Stopping the integration when a condition is satisfied (as in items 1 and 4) can be considered as a "two-point boundary value" problem. Such a problem can be solved using the "secant" method as demonstrated, for example, in Example 6.4 of the textbook by Cutlip and Shacham.[17] MATLAB provides library functions *decic.m* and *ode15i.m* for solving DAEs. The function *decic.m* provides consistent initial conditions that satisfy the DAE system at the starting point. The function *ode15i.m* solves fully implicit DAEs of index 1.

The MATLAB program steam_dist.m, which implements these principles and provides the solution for second part of the assignment, is available at: <ftp://ftp.bgu.ac.il/shacham/SteamDist>. Feed with initial n-octane mole fraction of x_{10} = 0.635 yields distillate with 90% concentration of n-octane. The recovery of the n-octane is 3.7% in this case. The n-octane

recovery vs. its feed concentration is shown in Figure 5. A rapid increase of recovery is achieved for higher values of x_{10}, reaching close to 100% for x_{10} = 0.85. The time period of the distillation increases as well, from ~ 4 min for x_{10} = 0.635 to 29 min for x_{10} = 0.89.

CONCLUSIONS

The example presented here provides an opportunity to practice effective use of advanced problem-solving tools and techniques:

- *Use of consistent physical property data with documented uncertainty and range of applicability values, extracted from reliable property databases.*

- *Grouping the equations and data for solution according to their role in the model: 1. Model equations characteristic to the problem type; 2. Physical property data and equations characteristic of the compounds involved; and 3. Problem-specific data and initial and final values.*

- *Constructing and testing the components of the general model using a user-friendly software package that requires minimal programming effort.*

- *Combining the various components of the model and carrying out parametric studies by deriving an efficient algorithm for carrying out these tasks and implementing the algorithm using a programming language.*

- *Using advanced tools available for solving two-point boundary value problems and differential algebraic systems of equations.*

Such a combination of the latest tools and techniques enables the solution of problems of increasing complexity in the educational setting. The example presented is suitable for courses in thermodynamics, separation processes, process simulation, and numerical methods.

The POLYMATH and MATLAB programs used in this study are available at the site: <ftp://ftp.bgu.ac.il/shacham/SteamDist/>.

Figure 5. Percent recovery of n-octane as function of its initial mole fraction in the feed (MATLAB results).
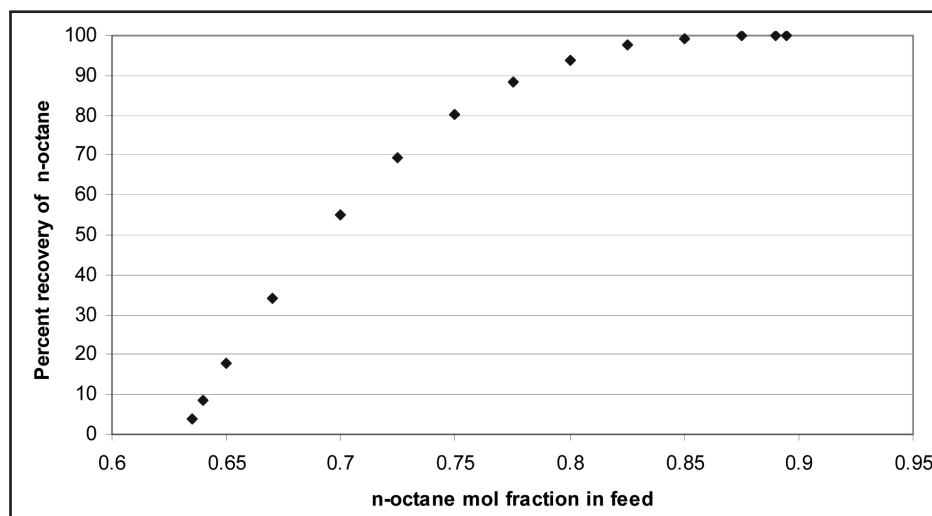
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