

Selecting the Appropriate Numerical Software for a Chemical Engineering Course

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Abstract

Criteria for evaluating mathematical software packages and the results of a recent comparison of such packages are briefly reviewed. A benchmark problem that was developed based on the results of this comparison is presented. This problem can be used in various courses, representing various levels of knowledge in chemical process analysis, mathematical modeling and numerical methods where the solution is achieved using the software most appropriate to the objectives of the particular course. This work demonstrates and illustrates the conclusion that the most educational benefits can be gained by using several packages throughout the chemical engineering curriculum. The software that is most appropriate for a particular course must be determined according to the course objectives and the previous exposure of the students to mathematical models, numerical algorithms and computer programming.

Keywords. Mathematical software, Numerical methods, Modeling, Chemical engineering, Problem solving

INTRODUCTION

Numerical software is routinely and extensively used for problem solving in recent years in some of the core chemical engineering courses (the “process dynamics and control” and “chemical reaction engineering” courses, for example), but in many of the courses the use of computers is still disappointingly low. This may contribute to the finding that the number of practicing engineers who use numerical software for process design is below 10% as was found in a recent survey (Davis et al., 1994).

This underutilization of computers and numerical solution packages in some of the ChE courses has been attributed to the following (Shacham et al., 1996): The examples and homework problems given in many of the textbooks are retained from the pre-computer era, and thus they can be solved either with or without a computer. These problems do not encourage educators and students to use numerical software. Furthermore, most departments typically select one numerical computation package to be used by their students, and this package may be inappropriate for use in a particular course. It may even be too difficult to be used by the less computer-literate students.

The departmental computer expert typically does the identification of a package for general departmental use. Often this expert will select the package that is the most powerful, most flexible, and gives the user the widest range of options. Typically some research usage has been given strong emphasis. However, other attributes of the package may be more important for educational use by undergraduates. The package must have enough capabilities to solve most problems encountered in a particular course and it should serve properly the objective of the course. Serving the objective of the course means that the effort spent in learning to use and using the package

for achieving the course objectives should be minimized. This requirement puts more emphasis on user friendliness and shorter learning curve than on the power and the options provided by the software.

Cutlip and Shacham (1999) have published recently a book entitled *Problem Solving in Chemical Engineering with Numerical Methods* that contains examples and homework assignments that require the use of computer for their solution for most required chemical engineering courses. The examples and assignments in this book demonstrate for the students and instructors the benefits of the use of the software packages in solving realistic engineering problems.

Criteria for comparing mathematical software for educational use has been developed (Shacham et al., 1998, Shacham and Cutlip, 1998). Ten representative problems from various required Chemical Engineering courses were selected and this set of problems was solved using six numerical software packages including Excel, MAPLE, MATHCAD, MATLAB, MATHEMATICA, and POLYMATH. Details of some comparisons are given by Shacham and Cutlip, 1998.

The main conclusion from this comparison was that there is no single package which is the best for all the courses, but the most appropriate package must be selected according to the objectives of the course and the students previous exposure to mathematical models, numerical algorithms and computer programming.

This paper reviews the set of benchmark problems and the software evaluation criteria used by Cutlip et al. (1998) and Shacham and Cutlip (1998) for comparison of mathematical software packages. A benchmark problem, which was developed based on the results of the comparison conducted by Cutlip et al. (1998), is presented. This problem can be used in various courses, representing various levels of

knowledge in chemical process analysis, mathematical modeling and numerical methods where the solution is achieved using the most appropriate software so as to attain the objectives of the particular course.

A BENCHMARK PROBLEM SET FOR SOFTWARE PACKAGE EVALUATION

The set of benchmark problems of Cutlip et al. (1998), which was developed for evaluation of software packages, is shown in Table 1. Within this set there are representative problems from almost every required course in a typical chemical engineering curriculum. This problem set has been solved with six software packages. The CACHE Corporation provides this problem set as well as the individual package write-ups and problem solutions files for downloading from the Internet at

<http://www.che.utexas.edu/cache/>.

Table 1 – Benchmark Problem Set

Problem	Title
1	Molar Volume and Compressibility Factor from Van Der Waal's Equation
2	Steady State Material Balances on a Separation Train
3	Vapor Pressure Data Representation by Polynomials and Equations
4	Reaction Equilibrium for Multiple Gas Phase Reactions
5	Terminal Velocity of Falling Particles
6	Unsteady State Heat Exchange in a Series of Agitated Tanks
7	Diffusion with Chemical Reaction in a One Dimensional Slab
8	Binary Batch Distillation
9	Reversible, Exothermic, Gas Phase Reaction in a Catalytic Reactor
10	Dynamics of a Heated Tank with PI Temperature Control

CRITERIA FOR SOFTWARE EVALUATION

Shacham et al. (1998) and Shacham and Cutlip (1998) have suggested the following criteria for software evaluation and comparison:

1. Numerical Performance
 - 1.1. Ability to solve all typical benchmark problems
2. User Friendliness
 - 2.1. Menu versus command based program control
 - 2.2. Notation and format used in equation entry
 - 2.3. Debugging aids (syntax errors, undefined or not initialized variables, etc.)
 - 2.4. Equation ordering and detection of implicit relationships
 - 2.5. Solution verification
3. Technical effort required for:
 - 3.1. Preparation of the model
 - 3.2. Documentation of the model
 - 3.3. Setting up the solution algorithm
 - 3.4. Presentation of the results

3.5. Documentation of the results

3.6. Alteration of the model for parametric studies

Most of the above criteria are self-explanatory. More detailed discussions of the various criteria are provided in the references.

SELECTING THE APPROPRIATE SOFTWARE BASED ON COURSE OBJECTIVES

Our work and experience with mathematical software, as well as the results of the comparison that was described in the previous sections, has lead us to conclude that the most educational benefit can be gained by using several packages throughout the curriculum. The software that is most appropriate for a particular course must be determined according to the course objectives and the students previous exposure to mathematical models, numerical algorithms and computer programming. The software selection procedure will be demonstrated in reference to a homework assignment that is outlined below. The complete paper including the problem statement and detailed solutions are available on the Internet at

<http://www.polymath-software.com/papers/>.

RIGOROUS DISTILLATION CALCULATIONS BY THE WANG AND HENKE METHOD - PROBLEM DEFINITION

Numerical Methods. Solution of a single nonlinear algebraic equation, solution of systems of linear algebraic equations.

Concepts used. Calculation of bubble point temperature for a multicomponent mixture. Material and energy balance on an equilibrium stage. Use of the Wang and Henke method for rigorous distillation calculation.

Course (and Software) Usage. (I) Basic Principles and Calculations (Excel, POLYMATH), (II) Separation Processes (Excel, POLYMATH, HYSIS), (III) Process Modeling and Simulation (Matlab, HYSIS)

Problem Statement. A simple distillation column with three theoretical stages is used to separate n-hexane (1) and n-octane (2). Feed with flow rate of F (kgmol/hr) and composition of z_1 and z_2 (mole fractions) enters the column at its bubble point on tray No. 2. The column's operating pressure is P (mmHg). A total condenser is used and the amount of heat added to the reboiler is Q (kcal/hr). Distillate is removed at the rate of D (kgmol/hr).

The vapor-liquid equilibrium ratios (k_j) can be calculated assuming ideal solutions, thus $k_j = P_j/P$, where P_j is the vapor pressure of component j. The vapor pressure of a pure component is calculated from the Antoine equation:

$$\log(P_j) = A_j + B_j / (t + C_j) \quad (1)$$

where P_j is the vapor pressure (mmHg), t is the temperature ($^{\circ}\text{C}$) and A_j , B_j and C_j are constants characteristic for component j. The molar enthalpies of pure liquid (h_j , kcal/mol) and pure vapor (H_j , kcal/mol) can be calculated from equations (2) and (3)

$$h_j = a_j * t \quad (2)$$

$$H_j = a_j + b_j * t + c_j * t^2 \quad (3)$$

where t is the temperature ($^{\circ}\text{C}$) and a_i , av_i , bv_i , and cv_i are constant.

Problem Questions

1a. Use the specified data and the estimates for vapor, liquid flow rates, and liquid compositions (Tables 1A¹ to 5A¹) to calculate the bubble point temperatures of the feed, condenser, and stages 1, 2, and 3. Carry out enthalpy balances on stages 1, 2, and 3.

1b. Repeat the calculations using the estimates for vapor and liquid flow rates, and liquid compositions that are given. Explain the differences in the enthalpy balance discrepancies between 1a and 1b.

2. Carry out one iteration of the Wang and Henke method using the given data and the initial estimates for vapor flow rates and the stage temperatures that are provided.

3. Solve the distillation column problem using the Wang and Henke method using the given data and initial estimates. The criteria for stopping the iterations: $\|\mathbf{V}_{k+1} - \mathbf{V}_k\| < 1e-5$ and $\|\mathbf{t}_{k+1} - \mathbf{t}_k\| < 1e-5$, where k is the number of the iteration, \mathbf{V} is the vector of the flow rates and $\|\cdot\|$ indicates Euclidean norm.

4. Investigate the effects of changing the column pressure and the heat added in the reboiler on the n-hexane recovery.

This assignment involves calculation of the flow rates and compositions of the various streams as well as stage temperatures for a simple three-stage distillation column, for a binary mixture using the Wang and Henke method. This method essentially involves the following steps:

Step 1. Assume temperatures (T_j) and vapor flow rates (V_j) for the various stages of the column.

Step 2. Calculate liquid flow rates and liquid compositions (x_j) based on the current T_j and V_j values using material balance equations. Normalize x_j .

Step 3. Calculate bubble point temperatures for the various stages using the normalized x_j values and calculate the enthalpies of the various streams using these temperatures.

Step 4. Carry out enthalpy balance on the various stages. Change the vapor flow rates to eliminate discrepancy in the enthalpy balances.

Step 5. Use the calculated bubble point temperatures as new T_j estimates and the calculated vapor flow rates as new estimates for V_j . Return to step (2) if the discrepancy between the estimated and calculated values is too large.

This assignment can be used in several courses including *Basic Principles and Calculations*, *Separation Processes* and *Process Modeling and Simulation*. The objectives of these courses vary, and consequently the assignments and the recommended software must be carefully considered.

I. Basic Principles and Calculations Course

This is a basic course in which the students first learn material and energy balances, and they probably do not have any previous exposure to mathematical modeling and numerical methods. The iterative procedure of the Wang and Henke method can be too difficult for them to grasp at this stage of their educational development. This may also be the case for the detailed material balances on the three-stage column. An appropriate assignment in this course can be providing the students the flow rates and compositions of the various streams and asking them to calculate liquid bubble point temperatures and carry out enthalpy balances on the various stages. This assignment is presented in problem questions 1a and 1b. This assignment can be solved using either POLYMATH or a spreadsheet program such as Excel. Calculation of the bubble point temperatures involves solution of a single non-linear algebraic equation which can be accomplished using the Nonlinear Equation Solver of POLYMATH or the "Goal Seek" option of Excel, without the need to be familiar with the numerical methods.

In Figure 1A¹, the data and solutions of question 1a are presented as obtained with Excel. Most students in the advanced stages of a "Basic Principles and Calculations" course should arrive at the correct solution using Excel or POLYMATH without major difficulties. The report of the numerical results can be well organized and presented clearly by Excel, as shown in Figure 1A¹. The major weakness of the spreadsheet programs is the unsatisfactory documentation of the equations used for solution. Figure 2A¹ shows most of the equations that were used for calculating bubble point temperatures, enthalpies and enthalpy balances. The need to convert variable names to cell addresses makes this documentation very difficult to read and consequently difficult to debug. This essentially limits the practical use of spreadsheets for solution of simple mathematical models only, in chemical engineering applications.

In Figure 3A¹ the POLYMATH input for calculating bubble point temperature and liquid and vapor molar enthalpies for one equilibrium stage is shown. The POLYMATH input can be very conveniently used for documentation and debugging because the equations used essentially retain their mathematical form and the variable names may remain unchanged. This makes POLYMATH especially suitable for courses where the course objectives do not include learning of computer programming and/or numerical methods.

II. Separation Processes

The objectives of this course typically include learning various techniques for calculations involving staged processes and investigating behavior of such processes when changing operating conditions.

¹ All Figures and Tables with the A suffix are found in the Appendices.

Questions 2 and 4 can be useful in such a course. Question 2 involves carrying out a single Wang and Henke iteration using the data provided in Tables 2A² and 5A². Solution of this question includes carrying out all the steps of the Wang and Henke algorithm shown previously, except the repetition of the iterations until convergence. Question 2 can be solved with either POLMATH or Excel. Figure 4A² shows the POLYMATH input for material balance on the three stages of the column, for the first component. While this material balance yields a system of three simultaneous linear equations it is preferable to solve it using POLYMATH's non-linear equation solver program because it provides more detailed and clear documentation of the equations used. The complete solution of question 2, using POLYMATH, involves solution of two sets of material balance equations (as shown in Figure 4A²), five bubble point temperature and enthalpy calculations (as shown in Figure 3A²) for the three stages, condenser, and the feed stream, and enthalpy balance. Because of the limit on the number of equations in POLYMATH (maximum number of equations is 32 for one input file), the complete set of equations cannot be entered into one file. Consequently, the iterative solution of the distillation column (as requested in question 3) is too cumbersome and time consuming if POLYMATH is used. Excel is also inappropriate for this purpose. Question 4 involves parametric study of the distillation column behavior under different operating conditions. The most appropriate software for solving this question in a "Separation Processes" course where programming and numerical methods are not among the course objectives is a process simulation program such as Hysis or Aspen.

III. Process Modeling and Simulation

This is the course where students typically learn various techniques for simulating unit operations including distillation columns. The subject matter includes also learning numerical methods for solving steady state and unsteady state models. To enable the students to carry out modeling and simulation of complex unit operations, programming is essential. Question 3 involves iterative solution of the material and energy balance equations of the distillation column using the Wang and Henke method. Matlab, for example, can be used for solving this question. The script file "distil.m" shown in Appendix B is used to solve this question. The final results obtained by this program are shown in Table 4A² as "refined estimates". Note that the script file "distil.m" uses additional functions for calculating vapor liquid equilibrium k values, bubble point temperatures and vapor and liquid molar enthalpies. These functions are not shown in Appendix B.

For steady state simulation of a distillation column, Matlab enables similar results to a programming language like FORTRAN. Its main strengths are the

convenience in which complex matrix operations can be carried out as well as the subprograms and toolboxes that are provided for various purposes that can save a lot of programming. Because it enables students to solve complex modeling and simulation assignments, Matlab is an appropriate package for the "Process Modeling and Simulation" course. For demonstration of simple models POLYMATH and Excel can also be useful. Commercial process simulators should be used for simulation and parametric studies of complete processes or complex unit operations.

CONCLUSIONS

This work demonstrates that several mathematical packages should be used throughout the undergraduate curriculum in order to obtain the most benefits from the use of mathematical software packages in the undergraduate chemical engineering education. If there is a need to solve mathematical models in a particular course without consideration of the technical details of the solution (numerical methods and programming), mathematical software packages such as POLYMATH can be the most beneficial. If the course involves study of numerical methods and/or programming, then Matlab or packages with similar capabilities should be used. When course objectives include the simulation of complex unit operations or complete chemical processes, commercial simulation packages such as Hysis or Aspen should be utilized.

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² All Figures and Tables with the A suffix are found in the Appendices.

APPENDIX

	A	B	C	D	E	F	G	H	I	J	K
1	DATA			K-value constants				liquid and vapor enthalpy constants			
2	F (kgmol/hr)	100		A	B	C		al	av	bv	cv
3	z1	0.5	n-hexane	6.87776	1171.53	224.366		51.72	7678	31.83	0.04515
4	z2	0.5	n-octane	6.92374	1355.126	209.517		66.07	10444.7	41.836	0.0609
5	D (kgmol/hr)	36									
6	B (kgmol/hr)	64									
7	P (mm Hg)	760									
8	Q (kcal/hr)	5.80E+05									
9											
10		Estimated Values				Calculated values					
11		L(kgmol/hr)	V(kgmol/hr)	x1	x2	T (deg C)	k1	k2	f(T)	hl(cal/mol)	Hv(cal/mol)
12	Condenser	14	0	0.89725	0.10275	71.66984	1.0953526	0.16734717	7.29E-08	3812.439	10252.463
13	Stage 1	9	50	0.59349	0.40651	82.522401	1.51182	0.25276101	-7.7E-08	4749.446	10992.298
14	Feed	100	0	0.5	0.5	86.784325	1.7052531	0.29474998	1.54E-06	5111.163	11333.609
15	Stage 2	134	45	0.47128	0.52872	88.211151	1.7740903	0.31000707	2.14E-07	5231.55	11455.324
16	Stage 3	64	70	0.26853	0.73147	100.36232	2.4503205	0.46757344	5.05E-07	6244.202	12671.291
17											
18								Enthalpy Balance			
19								In	Out	Difference	
20							Stage 1	568863.743	592359.9	-23496.2	
21							Stage 2	1440851.69	1216517	224334.3	
22							Stage 3	1281027.75	1286619	-5591.55	

Figure 1A. Excel Solution Spreadsheet for Problem 1a

	F	G	H	I	J
10		Calculated values			
11	T (deg C)	k1	k2	f(T)	hl(cal/mol)
12	71.669840	=10^(\$D\$3-\$E\$3/(F12+\$F\$3))/B\$7	=10^(\$D\$4-\$E\$4/(F12+\$F\$4))/B\$7	=G12*D12+H12*E12-1	=\$H\$3*\$F12*D12+\$H\$4*\$F12*E12
13	82.522401	=10^(\$D\$3-\$E\$3/(F13+\$F\$3))/B\$7	=10^(\$D\$4-\$E\$4/(F13+\$F\$4))/B\$7	=G13*D13+H13*E13-1	=\$H\$3*\$F13*D13+\$H\$4*\$F13*E13
14	86.784325	=10^(\$D\$3-\$E\$3/(F14+\$F\$3))/B\$7	=10^(\$D\$4-\$E\$4/(F14+\$F\$4))/B\$7	=G14*D14+H14*E14-1	=\$H\$3*\$F14*D14+\$H\$4*\$F14*E14
15	88.211151	=10^(\$D\$3-\$E\$3/(F15+\$F\$3))/B\$7	=10^(\$D\$4-\$E\$4/(F15+\$F\$4))/B\$7	=G15*D15+H15*E15-1	=\$H\$3*\$F15*D15+\$H\$4*\$F15*E15
16	100.36232	=10^(\$D\$3-\$E\$3/(F16+\$F\$3))/B\$7	=10^(\$D\$4-\$E\$4/(F16+\$F\$4))/B\$7	=G16*D16+H16*E16-1	=\$H\$3*\$F16*D16+\$H\$4*\$F16*E16
17					
18		Enthalpy Balance			
19		In	Out	Difference	
20	Stage 1	=B12*J12+C15*K15	=B13*J13+C13*K13	=H20-I20	
21	Stage 2	=B13*J13+C16*K16+B14*J14	=B15*J15+C15*K15	=H21-I21	
22	Stage 3	=B15*J15+B\$8	=B16*J16+C16*K16		

Figure 2A. Partial Excel Solution Spreadsheet Calculations for Problem 1a

```

Figure 3. Tray bubble point and enthalpy calculations with POLYMATH
f(t)=k1*x1+k2*x2-1
x1=0.59349
x2=0.40651
h11=51.72*t
hv1=7678+t*(31.83+0.04515*t)
h12=66.07*t
hv2=10444.7+t*(41.836+0.0609*t)
P=760
k1=10^(6.87776-1171.53/(t+224.366))/P
k2=10^(6.92374-1355.126/(t+209.517))/P
h1=(h11*x1+h12*x2)
hv=(hv1*k1*x1+hv2*k2*x2)
t(min)=50, t(max)=150

```

Figure 3A. POLYMATH Problem File for Calculation of Bubble Point and Liquid and Vapor Molar Enthalpies

```

Figure 4. 1st component' material balance on the 3 equilibrium stages
f(x11)=-((V1-L0)*k11+L1)*x11+V2*k12*x12
f(x12)=L1*x11-(V2*k12+L2)*x12+V3*k13*x13+0.5*F
f(x13)=L2*x12-(V3*k13+B)*x13
V1=50
V2=45
V3=70
F=100
B=64
D=36
t1=80
t2=90
t3=100
P=760
L3=B
L0=V1-D
k11=10^(6.87776-1171.53/(t1+224.366))/P
L1=V2-D
k12=10^(6.87776-1171.53/(t2+224.366))/P
k13=10^(6.87776-1171.53/(t3+224.366))/P
L2=V3+F-D
x11(0)=0.5
x12(0)=0.4
x13(0)=0.3

```

Figure 4A. POLYMATH Problem File for Calculation of First Material Balance on the Three Equilibrium Stages

APPENDIX A

Table 1A. Pure Component Vapor Pressure and Enthalpy Equation Constants

	A	B	C	al	av	bv	cv
n-hexane	6.87776	-1171.53	224.366	51.72	7678	31.83	0.04515
n-octane	6.92374	-1355.126	209.517	66.07	10444.7	41.836	0.0609

Table 2A. Data for the Distillation Column Example

F (kgmol/hr)	100
z1	0.5
z2	0.5
D (kgmol/hr)	36
B (kgmol/hr)	64
P (mm Hg)	760
Q (kgcal/hr)	5.80E+05

Table 3A. Initial Estimates for Vapor and Liquid Flowrates and Liquid Compositions for the Various Stages

	L (kgmol/hr)	V (kgmol/hr)	x1	x2
Condenser	14	0	0.89725	0.10275
Stage 1	9	50	0.59349	0.40651
Feed	100	0	0.5	0.5
Stage 2	134	45	0.47128	0.52872
Stage 3	64	70	0.26853	0.73147

Table 4A. Refined Estimates for Vapor and Liquid Flowrates and Liquid Compositions for the Various Stages

	L(kgmol/hr)	V(kgmol/hr)	x1	x2
Condenser	43.53	0	0.93935	0.06065
Stage 1	37.501	79.531	0.71359	0.28641
Feed	100	0	0.5	0.5
Stage 2	132.72	73.502	0.45211	0.54789
Stage 3	64	68.717	0.25287	0.74713

Table 5A. Initial Estimates for Temperature and Vapor Flowrates for the Various Stages

	t (C)	V(kgmol/hr)
Stage 1	80	50
Stage 2	90	45
Stage 3	100	70

APPENDIX B

MATLAB SCRIPT FILE FOR SOLVING QUESTIONS 2 AND 3 FROM APPENDIX A.

```
%distil.m - a script file for binary distillation calculation for a three
% equilibrium stages distillation column. It solves questions 3 and 4 in the
% problem presented in Appendix A. All the data is included in the program
% total pressure and heat added to the reboiler, which should be supplied
% by the user.
% uses subprograms kvalue.m, bubble.m, entliq.m and entvap.m
format compact
F = 100.0;
z(1,1)=0.5;
z(2,1)=1-z(1,1);
PA=input('Input Pressure in the tower(atm)')
P=760*PA;
D = 36;
B = 64 ;
T0 = 100 ;
Q=input('Input Heat Added to the Reboiler (kcal/hr) ');
% CALCULATE FEED TEMPERATURE AND ENTHALPY
[TF,Yz]=bubble(z,T0,P)
HF=entliq(z,TF)
% SET INITIAL VALUES
T=[80 90 100]';
V=[50 45 70]';
TOLD=T;
VOLD=V;
for IT=1:20
% START WANG AND HENKE ITERATIONS
disp(['##### Iteration No: ' num2str(IT)]);
L0 = V(1) - D;
L(1,1) = V(2) - D;
L(2,1) = V(3) + F - D;
L(3,1)= 64;
disp('      Tray No.      L(I)      K(1,I)      K(2,I)');
for I=1:3
    K(:,I)=kvalue(T(I),P);
    Res=[I L(I) K(1,I) K(2,I)];
    disp(Res);
end
% BUILD AND SOLVE THE COEFFICIENT MATRIX
for I=1:2
    A(1,1)=-((V(1)-L0)*K(I,1)+L(1));
    A(2,2)= -(V(2)*K(I,2)+L(2));
    A(3,3) = -(V(3)*K(I,3)+B);
    A(2,1) = L(1);
    A(3,2) = L(2);
    A(1,2) = V(2)*K(I,2);
    A(2,3) = V(3)*K(I,3);
    A(1,3) =0;
    A(3,1)=0;
    BB =[0.0 -F*z(I) 0.0]';
    X(:,I)=inv(A)*BB;
end
% NORMAILZE LIQUID MOLE FRACTIONS
for J = 1:3
    XN(J,1) = X(J,1)/(X(J,1)+X(J,2));
    XN(J,2) = X(J,2)/(X(J,1)+X(J,2));
end
end
```

```

% CALCULATE BUBBLE POINT TEMPERATURES
for J=1:3
    T0=T(J);
    [T(J,1),YN(:,J)]=bubble(XN(J,:),T0,P);
end
T0 = T(1);
KC=kvalue(T(1),P);
XC(1)=XN(1,1)*KC(1);
XC(2)=XN(1,2)*KC(2);
[TC,YC]=bubble(XC',T0,P);
H0=entliq(XC',TC);
% CALCULATE ENTHALPIES
for J=1:3
    HL(J,1)=entliq(XN(J,:),T(J));
    HV(J,1)=entvap(YN(:,J),T(J));
end
% CALCULATE NEW VAPOR FLOWRATES

V(3,1) = (L(2)*HL(2)-B*HL(3)+Q)/HV(3);
V(2,1) = (V(3)*HV(3)+F*HF+L(1)*HL(1)-L(2)*HL(2))/HV(2);
V(1,1) = (V(2)*HV(2)+L0*H0-L(1)*HL(1))/HV(1);

% CALCULATE ERROR SUMS
VSUM = 0;
TSUM = 0;
for J = 1:3
    VSUM = VSUM + (VOLD(J)-V(J))^2;
    TSUM = TSUM + (TOLD(J)-T(J))^2;
end
format short e
disp(' *** Condenser');
disp('      Temp.      X1          X2          Enthalpy');
Resc=[TC XC(1) XC(2) H0];
disp(Resc);
disp('*** Feed');
disp('      Temp.      Enthalpy');
Resf=[TF HF];
disp(Resf);
disp(' *** Column Trays')
disp('      Temp.      X1          X2          Enth. Liq.   Ent. Vap.
Vap. flow rate');
RES=[T X(:,1) X(:,2) HL HV V(:,1)];
disp(RES);
VOLD=V;
TOLD=T;
pause
if ((VSUM+TSUM)<1e-5)
    return
end
end

```