A VBA Solution to "SEMI-BATCH STEAM DISTILLATION OF A BINARY ORGANIC MIXTURE"

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Introduction

It is the purpose of this paper to:

1. Present a VBA/spreadsheet solution to solve a steam distillation problem [1].
2. Compare a "controlled integration" solution[1] which uses POLYMATH[TM] and a MATLAB® solution to the VBA/spreadsheet solution.
3. Implement a "controlled integration" VBA/spreadsheet solution and compare it to the authors[1] solution

The problem is first reviewed together with the solution given by the authors[1,2,3].
The VBA solution and its spreadsheet implementation are then presented. The VBA solution is compared with the POLYMATH™[4] /MATLAB®[5] solutions.

Finally a spreadsheet solution using "controlled integration" is presented which differs from that of the authors[1].

Problem Statement and Solution [1]

"Initially M = 0.0.015 kmol of organics (Fig 1) with composition x_1 = 0.725 is charged into the still.
The initial temperature in the still is T_o = 25 C. Starting at time t=0, steam at a temperature T_{steam} = 99.2° C is bubbled continuously through the organic phase at a rate of M_S = 3.85E-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 surroundings is UA = 1.05 J/s-K.
The ambient pressure is P = 9.839E+04 Pa."

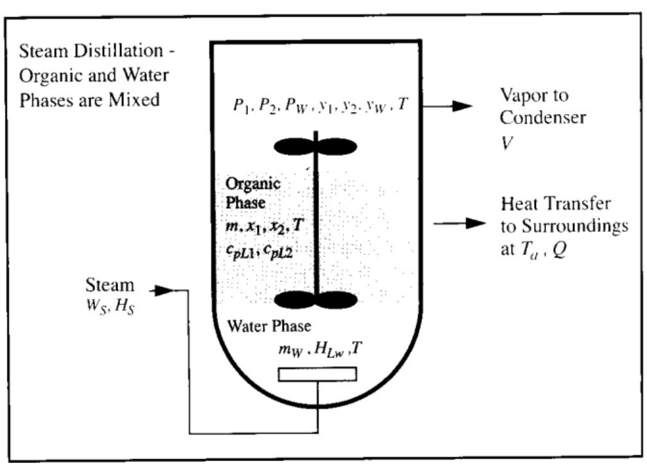

Figure I Schematic Plot of steam distillation (From Reference 1 with permission)

The differential equations representing this steam distillation are given in Reference 1. Figure II are the results [1] presented by the authors for the heating and distillation cycles. Figure III is additional results.

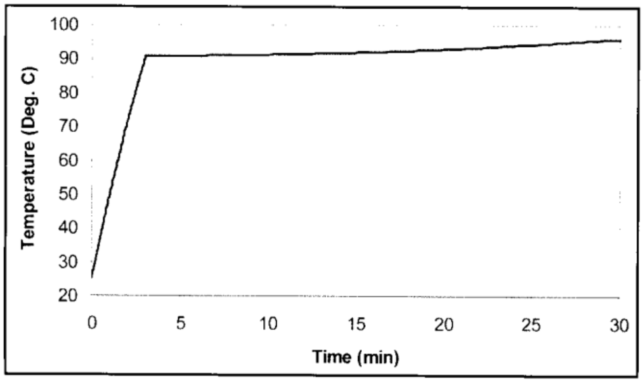

Figure 2. *Temperature change during semi-batch steam distillation (POLYMATH results).*

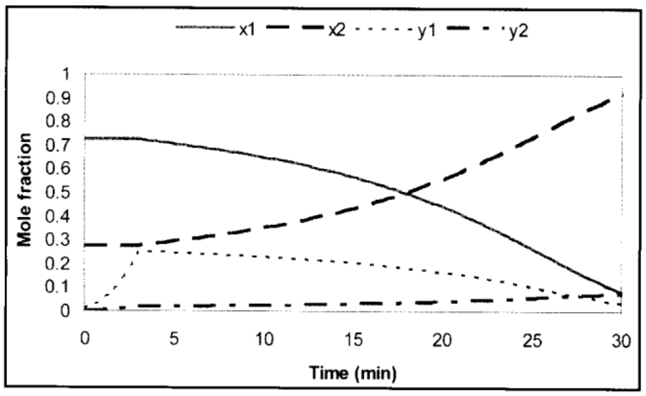

Figure 3. *Change of organic phase composition during semi-batch steam distillation (POLYMATH results).*

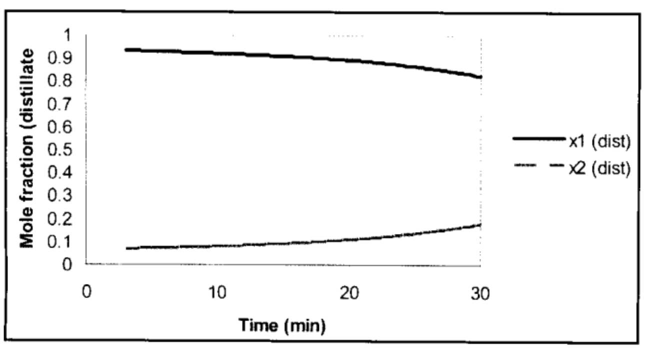

Figure 4. *Change of organic phase distillate composition during semi-batch steam distillation (POLYMATH results).*

Figure II Results of the integrations from Reference 1 (with permission)

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

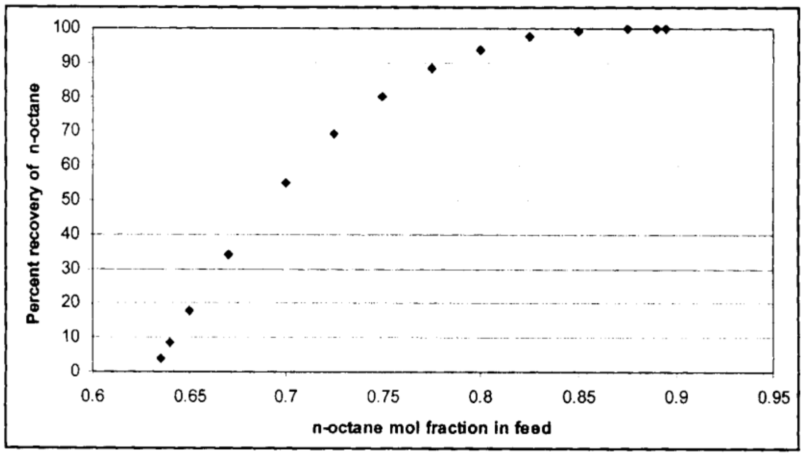

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Figure III Additional Results from Reference 1 (with permission)

VBA Functions

The VBA function procedures used by the current author are listed in the Appendix. The functions are:

1. Integ - This is the function invoked from the spreadsheet with Ctrl+ Shft+Enter with input of time, Temperature and Mass of Water (Heating) or time, Mass Water (MW), Mx1 and Mx2 (Distillation). Output is to the cells which are highlighted.
2. Rk4a – This is a classical fourth-order Runge-Kutta integration procedure.
3. dydx - This provides the right hand sides for the integration procedures for heating and distillation.
4. DMM – A bubble point procedure called during distillation. The bubble point is calculated each time the integration routine evaluates the right hand side of the differential equations. The bubble point temperature is used to evaluate the physical property equations.

   The bubble point is calculated using Newton's method:
   Find TK which makes f(TK) = 0

   f(TK) = 1 – y1-y2-yw.
   f'(TK) = -d y1 /d TK - dy2 /d TK - dyw /d TK

   Each derivative in turn is determined analytically then evaluated numerically. Then

   TKnew = TK - f(TK)/f'(TK)

   The above is repeated until f(TK) is less than 1.E-6 (see Figure A5)

5. Interp – a general interpolation procedure.
   Generally quadratic interpolation is used.
6. Coth and Tanh – VBA does not provide these functions.
   Note: In VBA ln (natural log) is log.

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Heating Cycle

Table I is a spreadsheet implementation of the heating cycle. Two differential equations (for T and MW) are solved (Reference 1). The initial conditions are set at time zero (line 7) utilizing values from the parameter vector (at L6) and the physical properties of n-octane and n-decane.

On the line following the time 0 line, the cells A8 to C8 are high lighted. The command = integ($A7,$B7:$C7,$L$6) is entered with Ctrl+Shift+Enter which invokes the integ procedure (Figure A1). The remaining entries on the line 8 are calculated from the values returned from the integ procedure (time, MW and T) and by copying parts of line 7. The entries at subsequent times (h = 20 sec) are calculated by copying the line above.

The function dydx (Figure A3) is called by the integration routine rk4a (4^{th} Order Runge- Kutta – Figure A2) which is called in turn by function integ. Each step repeats the above until fT (value of 1 – y1-y2-yw) crosses 0. The time to reach the bubble point (fT = 0) is determined by interpolation (Figure A6) of fT vs. Time.

When the time to the bubble point is determined, that time is used to find (by interpolation) the corresponding values of y1, y2, MW and yw.

Table II compares the VBA solution to that of Reference 3 at the bubble point. Both solutions agree with each other very well. This assures that the equations used to evaluate the physical properties in the spreadsheet solution and those given in Reference 1 are consistent.

Heatinc x10 = 0.725

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Time Sec	T (Deg C)	Mass Water in Still (kmol)	TK	Y1	Y2	YW	fT	(Min)	Prm	
									2	Number Dependent Varables
0	25	0	298.15	0.01379	0.000506	0.03222	0.95348	0	20	Step Size (seconds)
20	33.53362	0.00077	306.68362	0.02192	0.000897	0.05274	0.92444	0.33333	3.85E-05	Steam Flow Raste (kmol/s)
40	41.6893	0.00154	314.8393	0.0332	0.001497	0.0821	0.88321	0.66667	372.35	Steam Temperature (K)
60	49.49358	0.00231	322.64358	0.04822	0.002372	0.12242	0.82699	1	1.05	Heat Tranfer coef (J/(s-K)
80	56.97038	0.00308	330.12038	0.06758	0.003595	0.17591	0.75292	1.33333	25	Ambient Temperature deg C
100	64.14143	0.00385	337.29143	0.09183	0.005243	0.24479	0.65813	1.66667	273.15	Enthalpy Reference Deg C
120	71.02648	0.00462	344.17648	0.1215	0.007395	0.33124	0.53987	2	0.725	Mole Fraction n-octane
140	77.6436	0.00539	350.7936	0.15702	0.010132	0.43733	0.39552	2.33333	0.275	Mole Fraction n-decane
160	84.0093	0.00616	357.1593	0.19879	0.013532	0.56504	0.22264	2.66667	98390	Pa
180	90.13873	0.00693	363.28873	0.24713	0.017667	0.71615	0.01906	3	0.015	Initial Amount of Organics kmol
200	96.04581	0.0077	369.19581	0.30231	0.022607	0.89227	-0.21718	3.33333		
220	101.7433	0.00847	374.89335	0.36452	0.028417	1.09483	-0.48777	3.66667		

Interpolations

Time (Sec) When fT = 0 (fT vs Time)
181.7

MW at 181.70(Time vs Mass Water)
0.006995

(Deg C) at 181.701 (Time vs Temp)
90.65

YW at 181.70 (Time vs YW)
0.730097

Y1 at 1: (Time vs Y1)
0.252

Value of Q At Bubblepoint
68.92768

Y2 at 1: (Time vs Y2)
0.018

Table I Spreadsheet for Heating

Comparison of Solutions At The Bubble point

Variable	Initial Values	POLYMATH**	VBA*
MW	0	0.006996	0.0069954
Q	0	68.93874	68.927
T	25	90.65594	90.65
t	0	181.72	181.7012
y1	0.0137865	0.251608	0.25153
y2	0.0005059	0.01806	0.01805
yw	0.0322226	0.730306	0.730096

* Using Interpolation at the bubble point

**Reference 3

Table II Comparison of Solutions– Heating Cycle

Distillation Cycle

During the distillation cycle three differential equations are integrated - for MW, Mx1 and Mx2. Table III is the corresponding spreadsheet. The starting values for t, MW, Mx1 and Mx2 are taken from the ending values of the heating cycle and are entered on line 6. The temperature (Deg TK) is calculated by calling DMM with arguments of Mx1 and Mx2. The temperature. Deg C = TK - 273.15.

The remaining values on line 6: x1, x2, y1, y2, x1(dist), x2(dist) , yw are calculated from the value of TK, the values of Mx1 and Mx2, the physical properties of n-octane and n-decane, and the values in the parameter vector. The next time increment (line 7) is calculated from the values in line 6. Enter the command =Integ($A6,$B6:$D6,$T$4), highlight the output area $A7 to $D7 and enter Ctrl+Shift+Enter. T4 is the parameter vector which contains the step size h.

Once the output is obtained the rest of the line is obtained by copying the line above.
The copy command is then used to obtain as many time steps as desired.

The integ function (Figure A1) calls the Runge-Kutta function which carries out the integration.

The integrator (function rk4a) calls the function dydx (Figure A4) a number of times. In turn the dydx function calls the bubble point function (DMM – Figure A5) that determines the temperature at which the physical property routines are evaluated. The step size (h) on the spreadsheet is chosen so that it will end at a time of 2000 sec. (for purposes of comparison[1]). The parameter vector (prm) contains a starting value for the DMM bubble point procedure as well as other values used by the dydx function procedure.

Table IV compares the Reference 1 solution to the VBA spreadsheet solution at 2000 sec.

Comparison: Distillation -2000 seconds

Variable	Initial Value	Final VBA	Final Reference 3
x1	0.725	0.002332	0.01995
x2	0.275	0.9977	0.98005
y1	0.2516431	0.000995	0.008464
y2	0.0180626	0.08433	0.082287
x1(dist}	0	0.7628	0.791748
x2(dist)	0	0.2372	0.208252
Mx1	0.010875	1.74E-06	2.59E-05
Mx2	0.04125	7.44E-04	0.001271
T *	90.66	96.726	96.56247
MW	0.0069955	0.0170323	0.022794
Q	68.943	75.312	75.1406
eps		4E-07	1.77E-06

* Temperature determined from Bubble Point of DMM (VBA)

Table IV Comparison of VBA Solution and Reference 3

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>>> These are Dertermind from Mx1 and Mx2>>>>>>>>>>>>>>>

Time Sec	Mass Water in Still (kmol)	Mass n-Octane Still (kmol)	Mass n-decane Still (kmol)	T Deg C	TK Deg K	x1	x2	y1	y2	x1 (dist	x2 (dist	yw	eps	Percent Recovered	Q	Time (min)
181.7	0.006995	0.010875	0.00413	90.657	363.81	0.725	0.275	0.2516	0.0181	0	0	0.73	5E-07	0	68.9395	3.03
215.37	0.00727368	0.010526	0.0041	90.697	363.85	0.72	0.28	0.2501	0.0184	0.932	0.068	0.731	1E-08	3.212162	68.9818	3.59
249.05	0.00755097	0.010179	0.00407	90.739	363.89	0.714	0.286	0.2486	0.0188	0.931	0.069	0.733	5E-07	6.404205	69.0258	4.15
282.72	0.00782681	0.009834	0.00405	90.783	363.93	0.708	0.292	0.2469	0.0193	0.93	0.07	0.734	-2E-07	9.575284	69.0717	4.71
316.39	0.00810114	0.009491	0.00402	90.828	363.98	0.702	0.298	0.2452	0.0197	0.93	0.07	0.735	-4E-07	12.72449	69.1195	5.27
350.06	0.00837389	0.009151	0.00399	90.876	364.03	0.696	0.304	0.2435	0.0201	0.929	0.071	0.736	5E-07	15.85086	69.1694	5.83
383.73	0.00864499	0.008814	0.00396	90.925	364.08	0.69	0.31	0.2416	0.0206	0.928	0.072	0.738	2E-07	18.9534	69.2214	6.4
417.41	0.00891437	0.008479	0.00394	90.977	364.13	0.683	0.317	0.2397	0.0211	0.927	0.073	0.739	2E-08	22.031	69.2757	6.96
451.08	0.00918195	0.008147	0.00391	91.031	364.18	0.676	0.324	0.2377	0.0216	0.925	0.075	0.741	-5E-07	25.08252	69.3325	7.52
484.75	0.00944764	0.007818	0.00387	91.088	364.24	0.669	0.331	0.2355	0.0222	0.924	0.076	0.742	-5E-07	28.10673	69.392	8.08
518.42	0.00971136	0.007493	0.00384	91.147	364.3	0.661	0.339	0.2333	0.0227	0.923	0.077	0.744	4E-07	31.10231	69.4541	8.64
552.1	0.00997301	0.00717	0.00381	91.209	364.36	0.653	0.347	0.231	0.0233	0.922	0.078	0.746	4E-07	34.06786	69.5193	9.2
585.77	0.01023248	0.006851	0.00378	91.274	364.42	0.645	0.355	0.2285	0.024	0.921	0.079	0.748	-2E-07	37.00191	69.5876	9.76
619.44	0.01048967	0.006536	0.00375	91.342	364.49	0.636	0.364	0.2259	0.0246	0.92	0.08	0.749	4E-08	39.90285	69.6592	10.3
653.11	0.01074446	0.006224	0.00371	91.414	364.56	0.627	0.373	0.2232	0.0253	0.918	0.082	0.751	2E-08	42.76897	69.7345	10.9
686.78	0.01099673	0.005916	0.00367	91.489	364.64	0.617	0.383	0.2203	0.0261	0.917	0.083	0.754	2E-07	45.59846	69.8135	11.4
720.46	0.01124634	0.005613	0.00364	91.568	364.72	0.607	0.393	0.2173	0.0268	0.915	0.085	0.756	-6E-07	48.38935	69.8967	12
754.13	0.01149316	0.005314	0.0036	91.652	364.8	0.596	0.404	0.2141	0.0277	0.914	0.086	0.758	4E-07	51.13958	69.9841	12.6
787.8	0.01173702	0.005019	0.00356	91.739	364.89	0.585	0.415	0.2107	0.0285	0.912	0.088	0.761	-2E-07	53.84689	70.0762	13.1
821.47	0.01197777	0.00473	0.00352	91.832	364.98	0.573	0.427	0.2072	0.0295	0.911	0.089	0.763	-6E-07	56.5089	70.1733	13.7
855.14	0.01221524	0.004445	0.00348	91.929	365.08	0.561	0.439	0.2034	0.0304	0.909	0.091	0.766	-6E-07	59.12304	70.2756	14.3
888.82	0.01244923	0.004167	0.00344	92.032	365.18	0.548	0.452	0.1994	0.0315	0.907	0.093	0.769	-9E-07	61.68659	70.3835	14.8
922.49	0.01267955	0.003894	0.00339	92.14	365.29	0.534	0.466	0.1952	0.0326	0.905	0.095	0.772	-3E-07	64.1966	70.4974	15.4
956.16	0.01290599	0.003627	0.00335	92.255	365.4	0.52	0.48	0.1907	0.0337	0.903	0.097	0.776	-7E-07	66.64997	70.6176	15.9
989.83	0.01312832	0.003367	0.0033	92.376	365.53	0.505	0.495	0.186	0.035	0.901	0.099	0.779	-5E-07	69.04336	70.7444	16.5
1023.5	0.01334631	0.003113	0.00325	92.503	365.65	0.489	0.511	0.1809	0.0363	0.899	0.101	0.783	-4E-07	71.37325	70.8784	17.1
1057.2	0.0135597	0.002867	0.0032	92.638	365.79	0.473	0.527	0.1756	0.0377	0.896	0.104	0.787	-5E-07	73.63588	71.0197	17.6
1090.9	0.01376822	0.002629	0.00315	92.78	365.93	0.455	0.545	0.17	0.0391	0.894	0.106	0.791	-3E-07	75.82733	71.1687	18.2
1124.5	0.0139716	0.002399	0.00309	92.929	366.08	0.437	0.563	0.164	0.0407	0.891	0.109	0.795	2E-08	77.94344	71.3257	18.7
1158.2	0.01416956	0.002177	0.00303	93.087	366.24	0.418	0.582	0.1576	0.0424	0.889	0.111	0.8	5E-07	79.97992	71.491	19.3
1191.9	0.01436179	0.001965	0.00297	93.252	366.4	0.398	0.602	0.1509	0.0441	0.886	0.114	0.805	2E-07	81.93231	71.6647	19.9
1225.5	0.01454799	0.001762	0.00291	93.426	366.58	0.377	0.623	0.1439	0.046	0.883	0.117	0.81	-5E-07	83.79609	71.8468	20.4
1259.2	0.01472786	0.00157	0.00285	93.607	366.76	0.355	0.645	0.1364	0.0479	0.879	0.121	0.816	2E-07	85.56669	72.037	21
1292.9	0.0149011	0.001388	0.00278	93.795	366.95	0.333	0.667	0.1287	0.05	0.876	0.124	0.821	-3E-07	87.23964	72.2352	21.5
1326.6	0.01506742	0.001217	0.00271	93.991	367.14	0.31	0.69	0.1205	0.0521	0.872	0.128	0.827	5E-07	88.81064	72.4407	22.1
1360.2	0.01522658	0.001058	0.00264	94.193	367.34	0.286	0.714	0.1121	0.0544	0.868	0.132	0.834	-4E-08	90.2757	72.6525	22.7
1393.9	0.01537834	0.00091	0.00256	94.399	367.55	0.262	0.738	0.1034	0.0567	0.864	0.136	0.84	1E-07	91.63136	72.8694	23.2
1427.6	0.01552252	0.000775	0.00248	94.609	367.76	0.238	0.762	0.0945	0.0591	0.86	0.14	0.846	-1E-07	92.87484	73.0899	23.8
1461.2	0.01565901	0.000652	0.0024	94.821	367.97	0.214	0.786	0.0855	0.0615	0.856	0.144	0.853	1E-07	94.00429	73.3117	24.4
1494.9	0.01578778	0.000542	0.00232	95.031	368.18	0.19	0.81	0.0764	0.0639	0.851	0.149	0.86	-2E-07	95.01897	73.5327	24.9
1528.6	0.01590887	0.000444	0.00223	95.238	368.39	0.166	0.834	0.0674	0.0663	0.846	0.154	0.866	2E-07	95.91948	73.7499	25.5
1562.3	0.01602243	0.000358	0.00214	95.439	368.59	0.144	0.856	0.0587	0.0687	0.841	0.159	0.873	-6E-07	96.70795	73.9606	26
1595.9	0.01612872	0.000284	0.00204	95.63	368.78	0.122	0.878	0.0503	0.0709	0.836	0.164	0.879	3E-07	97.3881	74.1617	26.6
1629.6	0.01622812	0.000221	0.00194	95.81	368.96	0.102	0.898	0.0423	0.0731	0.83	0.17	0.885	3E-07	97.96527	74.3502	27.2
1663.3	0.01632109	0.000169	0.00184	95.975	369.13	0.084	0.916	0.035	0.0751	0.824	0.176	0.89	5E-07	98.44636	74.5238	27.7
1697	0.01640818	0.000126	0.00174	96.124	369.27	0.068	0.932	0.0283	0.0769	0.818	0.182	0.895	5E-07	98.83958	74.6802	28.3
1730.6	0.01649003	9.2E-05	0.00163	96.255	369.41	0.053	0.947	0.0224	0.0785	0.812	0.188	0.899	5E-07	99.15417	74.818	28.8
1764.3	0.01656728	6.52E-05	0.00153	96.368	369.52	0.041	0.959	0.0173	0.0799	0.806	0.194	0.903	2E-07	99.40002	74.9368	29.4
1798	0.01664063	4.49E-05	0.00142	96.463	369.61	0.031	0.969	0.013	0.0811	0.8	0.2	0.906	2E-07	99.58726	75.0364	30
1831.6	0.01671074	2.98E-05	0.00131	96.541	369.69	0.022	0.978	0.0095	0.082	0.794	0.206	0.909	4E-08	99.72582	75.1178	30.5
1865.3	0.01677822	1.9E-05	0.0012	96.602	369.75	0.016	0.984	0.0067	0.0828	0.788	0.212	0.911	-3E-07	99.82509	75.1824	31.1
1899	0.01684366	1.16E-05	0.00108	96.65	369.8	0.011	0.989	0.0045	0.0834	0.781	0.219	0.912	-2E-07	99.89361	75.232	31.6
1932.7	0.01690756	6.64E-06	0.00097	96.685	369.83	0.007	0.993	0.0029	0.0838	0.775	0.225	0.913	-2E-07	99.9389	75.2688	32.2
1966.3	0.01697033	3.56E-06	0.00086	96.709	369.86	0.004	0.996	0.0018	0.0841	0.769	0.231	0.914	-3E-07	99.96731	75.2948	32.8
2000	0.01703232	1.74E-06	0.00074	96.726	369.88	0.002	0.998	0.001	0.0843	0.763	0.237	0.915	4E-07	99.98401	75.3123	33.3

prm			
1	N	3	Number Dep Varables
2	h	33.6722	Step Size in seconds
3	MS	3.85E-05	Steam Flow (kmol/s)
4	TSK	372.35	Steam Temp(K)
5	U	1.05	Heat Tran coef (J/(s-K)
6	Ta	25	Ambient Temp deg C
7	T0	273.15	Enthalpy Ref Deg C
8	x01	0.725	Mole Fraction n-octane
9	x02	0.275	Mole Fraction n-decane
10	P	98390	Pa
11	M0	0.015	Init Amt Organ (kmol)
12	TC	90.66	Guess For Bub Pt
13	Iter	25	Max Iterations DMM

Interpolation To Find
Percent Recovered
When x1(dist) = 0.90
(x10 = 0.725)
x1(dist) vs Pecent
Recovered

70.05617407

Time for recovery

16.73935206

Table III Spreadsheet of the Distillation Cycle

Note: TK is determined at each step by the function DMM.

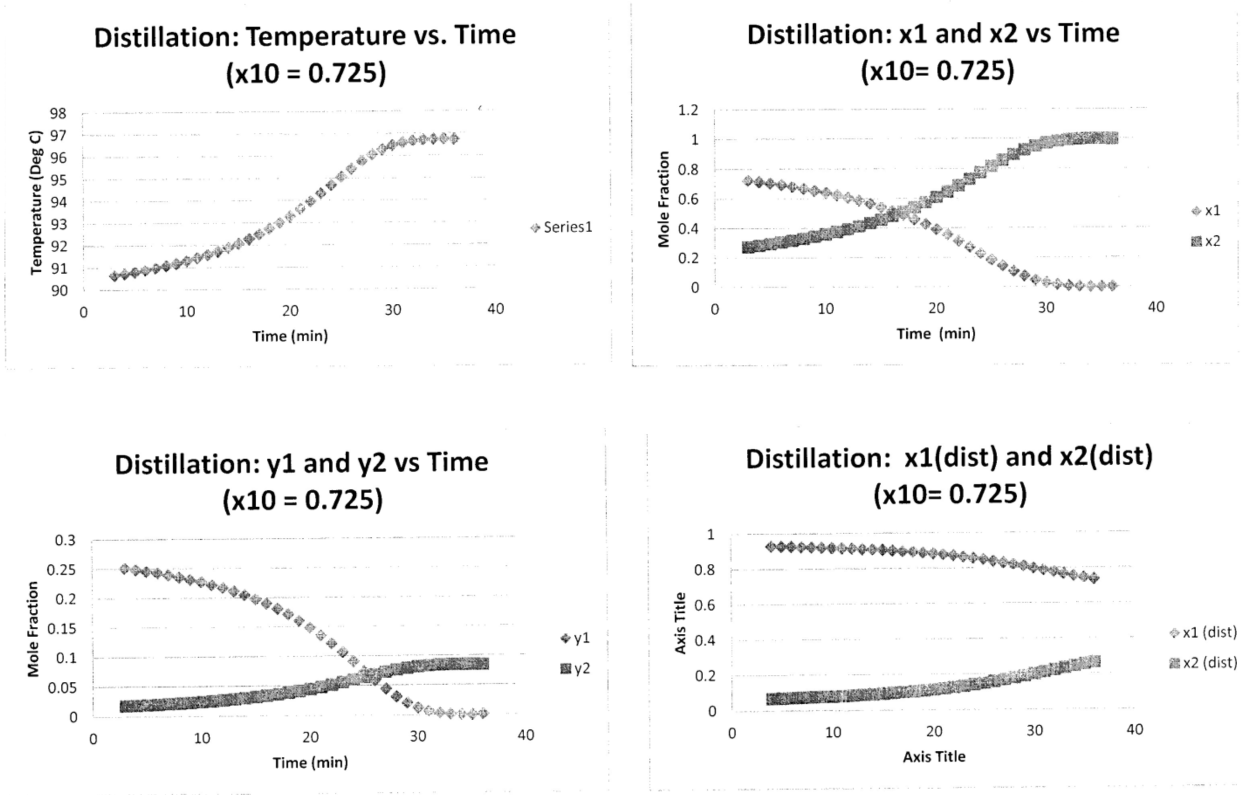

Figure IV Plots from the VBA Solution for Distillation

Figure IV are plots of several of the dependent variables vs. time from the spreadsheet solution. They are distinctly different from the authors'[1] plots shown in Figure II.

The spreadsheet (Table III) keeps track of the percent octane recovered in a column so designated. Interpolation (Figure A6) is used to determine the percent of n-octane recovered when x1(dist) =0.90 (plot of x1(dist) vs. percent recovered). Similarly an interpolation of x1(dist) vs. time determines the recovery time (at x1(dist) =0.90). Parametric cases (different feed concentrations) are evaluated by changing the entries in the parameter list (prm). ("Set Formulas, Calculation Options, Manual. To evaluate the spreadsheet enter Calculate Now"). Simply changing the values of the feed in the prm vector and recalculating the spreadsheet allows the parametric study.

Table V indicates how the %Recovery (and Recovery Time) varies as a function of the feed fraction of n-octane. A plot of the authors'[1] results are shown in Figure II (Additional Results).

Comparison: %Recovery of n-octane - VBA Solution and
Reference 3 when x1(dist) = 0.90

n-Octane Mole Fraction in Feed	Reference 3 t (min) to Recovery	Reference 3 % Recovery	VBA Spreadsheet t (min) to Recovery	VBA Spreadsheet % Recovery
0.635	3.82	3.71	3.68	3.82
0.64	4.75	8.61	4.56	8.89
0.65	6.52	17.8	6.27	18.47
0.67	9.85	34.21	9.46	35.54
0.7	14.41	55.03	13.69	56.43
0.725	17.87	69.42	16.74	70.06
0.75	20.74	80.23	19.35	80.65
0.775	23.14	88.29	21.55	88.57
0.8	25.1	93.98	23.34	94.11
0.825	26.62	97.56	24.74	97.61
0.85	27.75	99.39	25.79	99.37
0.875	28.58	99.96	26.57	99.95
0.89	29	100	26.96	99,99
0.895	29.13	100	27.09	100

Table V % Recovery as a function of fraction n-Octane in Feed

A Spreadsheet Solution Using "Controlled Integration[6] "

The author's spreadsheet solution was modified by adding a fourth differential equation $dT/dt = Kc * eps$ in place of the DMM routine. The dydx routine was replaced by the one in Figure A8 to allow integration with "controlled integration". Thus, the bubble point temperature is determined by this differential equation rather than by the DMM function. Figure VI is plot of the still temperature vs. time and Figure VII is a plot of x1 and x2 vs. time resulting from "controlled integration".

The shapes of T vs. time and x1, x2 vs. time compares well with this author's VBA solution (Figure IV) rather than with the shape presented in Figure II by the authors[1]. It was found that, a small value of Kc (2 rather than 1000) and a step size of 33.67 sec (to end up at 2000 sec) was needed to achieve stability. The numerical output at 2000 sec compared very well with that obtained by the VBA solution (Table VI).

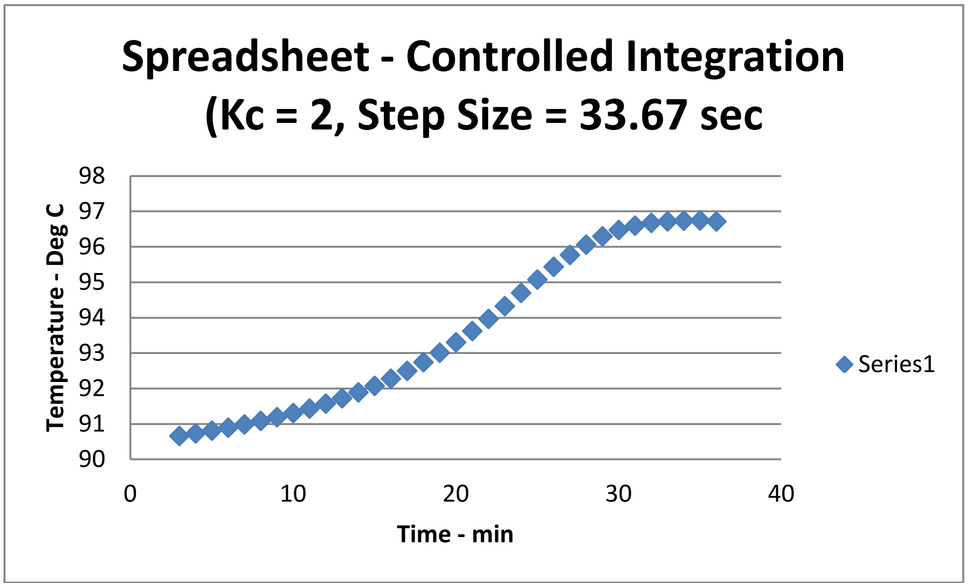

Figure VI Temperature vs. Time Using "controlled integration"

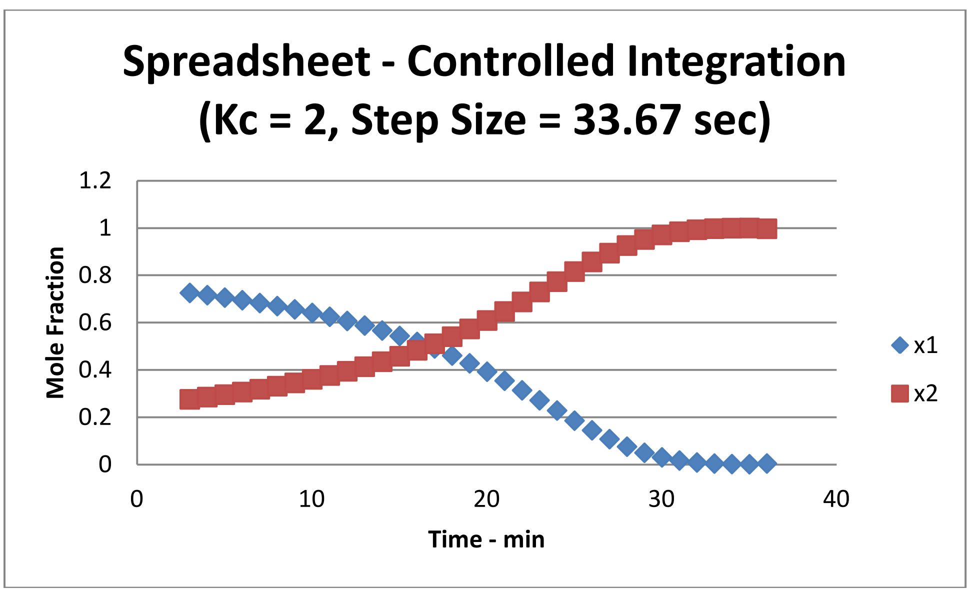

Figure VII x1 and x2 vs. Time Using "controlled Integration"

Comparison VBA vs. "Controlled Integration"
Spreadsheet Solutions
At 2000 Sec X10 = 0.725 h = 33.6722

Variable	VBA	"Controlled Integration" Kc = 2
MW	0.01703	0.01703
Mx1	2.00E-06	2.00E-06
Mx2	0.00074	0.00074
Deg C	96.728	96.719
x1	0.002	0.002
x2	0.998	0.998
y1	0.001	0.001
y2	0.0843	0.0843
x1(dist)	0.763	0.763
x2(dist)	0.237	0.237
yw	0.915	0.914
eps	4.00E-07	0.0002
%Recovered	99.98401	99.98411
Q	75.3123	75.3054

Table VI VBA solution vs. “Controlled Integration” solution on a Spreadsheet

Conclusions

The VBA solution and the POLYMATH[TM] solution listed in Reference 3 match almost exactly for the heating cycle (Table II) which integrates T and Mx1. However, in the distillation cycle the POLYMATH [TM] and VBA results (Table IV) differ both in the results after 2000 sec and in the shape of the dependent variable values with time (Figures II and IV). The POLYMATH[TM] solution uses “controlled integration” [1] with Kc = 1000. This requires [1] a “stiff “integrator (available in POLYMATH{TM} [7]) and an additional differential equation, dT/dt = Kc * eps where eps is the bubble point error. The differences between the “stiff” integrator which integrates four equations (MW, Mx1, Mx2 and T) and the classical Runge-Kutta integrator used in the VBA solution which integrates three equations (MW, Mx1 and Mx2) may cause the differing results.

Table V (% Recovery of n-octane when x1(dist)= 0.90) shows that the differences between the VBA solution and the MATLAB® solution are not large. These differences may result from interpolation errors in the VBA solution and/or equation solving errors in MATLAB® .

This author was successful in generating a "controlled integration" solution for the distillation cycle with a value of Kc = 2. The solution matched the VBA distillation solution almost exactly. The integration was carried out with a Runge-Kutta routine and the average value of eps was 0.0053. This suggests that the need for a large value of Kc (with the need for a "stiff" integrator) was not needed. It is unknown if this results can be generalized. Setting Kc = 1000 caused the Runge-Kutta integrator to "blow up".

Acknowledgement

The author would like to thank *Chemical Engineering Education* and the authors of Reference 1 for permission to copy the Tables and Figures of their paper.

References

1. Shacham, M. , M. B. Cutlip, and M. Elly, " SEMI-BATCH STEAM DISTILLATION OF A BINARY ORGANIC MIXTURE", *Chemical Engineering Education*, **46**(3), 173 (2012)
2. Shacham, M. , M. B. Cutlip, and M. Elly, " SEMI-BATCH STEAM DISTILLATION OF A BINARY ORGANIC MIXTURE" , *CACHE News*, *Summer 2012*
3. Shacham, M. , M. B. Cutlip, and M. Elly, " SEMI-BATCH STEAM DISTILLATION OF A BINARY ORGANIC MIXTURE – a Demonstration of Advance :problem Solving Techniques and Tools", ftp://ftp.bgu.ac.il/Shacham/SteamDist/
4. POLYMATH is a product of Polymath Software <http://www.polymath.software.com>
5. MATLAB is a product of Mathworks, Inc., <http://www.mathworks.com>
6. Shacham, M., N. Brauner and M. Pozin, "Application of Feedback Control Principles for Solving Differential Algebraic Systems of Equations In Process Control Education", *Computers Chemical Engineering* Vol . 20, Suppl., pp 1329-1334, 1996
7 POLYMATH Integration Algorithms ,<,http://www.polymath-software.com

APPENDIX

Listing of VBA Functions

```
Option Explicit

Private Function Integ(x, y, prm)
'
'This function is invoked from the spreadsheet
'It sets up the call to the classical 4th order Runge-Kutta Integration Routine
'
Dim N, IR, NN, I As Integer
Dim h, xx As Single

N = prm(1)

NN = N + 1

ReDim yy(1 To N) As Single
ReDim ddd(1 To NN)

h = prm(2)
xx = x

For I = 1 To N
  yy(I) = y(I)
Next

IR = rk4a(N, h, xx, yy, prm)

xx = xx + h

ddd(1) = xx

For I = 2 To NN
  ddd(I) = yy(I - 1)
Next I

Integ = ddd


End Function
```

Figure A1   Function Integ

```
Private Function rk4a(N, h, x, y, prm)
'
'Modified from Pedro L. Claveria abril/2002
'based in EMR Technology Group Library
'
'
'N = number of equations
'h  = step size for integration
'x = independent variable
'y = vector of dependent variables
'prm = vector of parameters

 ReDim ccc(N), fff(N)
 ReDim k1(N), k2(N), k3(N), k4(N)
 ReDim Y2(N), Y3(N), y4(N)

 Dim muda1, muda2, muda3, muda4 As Single
 Dim I As Integer

 'Calculation of k1
 muda1 = dydx(x, y, prm, fff)
 For I = 1 To N: k1(I) = fff(I): Next
 'Calculation of k2
 For I = 1 To N: Y2(I) = y(I) + 0.5 * h * k1(I): Next
 muda2 = dydx(x + h / 2, Y2, prm, fff)
 For I = 1 To N: k2(I) = fff(I): Next
 'Calculation of k3
 For I = 1 To N: Y3(I) = y(I) + 0.5 * h * k2(I): Next
 muda3 = dydx(x + h / 2, Y3, prm, fff)
 For I = 1 To N: k3(I) = fff(I): Next
 'Calculation of k4
 For I = 1 To N: y4(I) = y(I) + h * k3(I): Next
 muda4 = dydx(x + h, y4, prm, fff)
 For I = 1 To N: k4(I) = fff(I): Next

 'New values of the dependent variables
 For I = 1 To N
    ccc(I) = y(I) + (h / 6) * (k1(I) + 2 * k2(I) + 2 * k3(I) + k4(I))
 Next I

 For I = 1 To N
    y(I) = ccc(I)
 Next I

 rk4a = 0
 End Function
```

Figure A2 Function rk4a – Classical Fourth Order Runge-Kutta

```
Private Function dydx(x, y, prm, fff)
'
' The right hand side for the heating cycle equations
'
Dim T, MW, MS, TK, TSK, HS, U, Ta, Q, T0, x1, x2, M As Single
Dim HL_H2O, LCP_C8H18, LCP_C10H22, LCP_H2O, CpL
Dim Test1, Test2
'
' The Two Dependent variables  T and MW
'
T = y(1)
MW = y(2)

' Work on fff(1)

MS = prm(3)
TK = T + 273.15
TSK = prm(4)

Test1 = coth(2610.5 / TSK)
Test2 = tanh(1169 / TSK)

HS = 33363# * TSK + 26790# * 2610.5 * ((Test1) ^ 2) _
    + 8896# * 1169# * (Test2) - 44710000#

U = prm(5)
Ta = prm(6)
Q = U * (T - Ta)
T0 = prm(7)

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 _
    + 0.000009371 * (TK ^ 5 - T0 ^ 5) / 5

LCP_C8H18 = (0 - 186.63 * TK + 0.95891 * TK ^ 2 + 224830#)

LCP_C10H22 = (0 - 197.91 * TK + 1.0737 * TK ^ 2 + 278620#)

LCP_H2O = (276370# - 2090.1 * TK + 8.125 * TK ^ 2 - 0.014116 * TK ^ 3 + 0.0000093701 * TK ^ 4)

x1 = prm(8)
x2 = prm(9)
M = prm(11)
CpL = MW * LCP_H2O + M * (x1 * LCP_C8H18 + x2 * LCP_C10H22)
'
```

Figure A3 Function dydx – Right Hand Side of Runge-Kutta for Heating Cycle

```
' Set up the Differential Equatiosn for Heating
'
fff(1) = (MS * (HS - HL_H2O) - Q) / CpL
fff(2) = MS

dydx = 0
End Function
```

Figure A3 Function dydx – Right Hand Side of Runge-Kutta for Heating Cycle (Continued)

```
Private Function dydx(x, y, prm, fff)
' This calculates the right hand side of the differential equations
' For Distillation

Dim TK, MW, MX1, MX2 As Single
Dim MS, M, M0, Q, HV As Single
Dim X1, X2, P, T0, V1, V2, VW, Y1, Y2, YW As Single
Dim TSK, HS, T, Ta, U, V As Single
Dim HL_C8H18, HL_C10H22, HL_H2O As Single
Dim HIG_C8H18, HIG_C10H22, HIG_H2O As Single
Dim TEST1, TEST2
'
' Obtain the three dependent variables
'
MW = y(1)
MX1 = y(2)
MX2 = y(3)
'
'Determine the bubble point in the still based on Mx1 and Mx2
' Note the bubble point does not depend on MW
'
TK = DMM(MX1, MX2, prm)
' T is the temperature C
T = TK - 273.15
'
' Make the parameters available
'
MS = prm(3)
M0 = prm(11)
P = prm(10)
T0 = prm(7)
TSK = prm(4)
U = prm(5)
Ta = prm(6)

M = MX1 + MX2
X1 = MX1 / M
X2 = MX2 / M
'
' Prepare vapor pressures
'
V1 = 96.084 - 7900.2 / TK - 11.003 * Log(TK) + 0.0000071802 * TK ^ 2
V2 = 112.73 - 9749.6 / TK - 13.245 * Log(TK) + 0.0000071266 * TK ^ 2
VW = 73.649 - 7258.2 / TK - 7.3037 * Log(TK) + 0.0000041653 * TK ^ 2
```

Figure A4 Function dydx: Right Hand Side of Differential Equations for Distillation

```
Y1 = (X1 / P) * Exp(V1)
Y2 = (X2 / P) * Exp(V2)
YW = (1 / P) * Exp(VW)


TEST1 = coth(2610.5 / TSK)
TEST2 = tanh(1169 / TSK)

HS = (33363# * TSK + 26790# * 2610.5 * ((TEST1) ^ 2) _
    + 8896# * 1169# * (TEST2) - 44710000#)


HL_C8H18 = (224830 * (TK - T0) - 186.63 * (TK ^ 2 - T0 ^ 2) / 2 + 0.95891 * (TK ^ 3 - T0 ^ 3) / 3)
HL_C10H22 = (278620 * (TK - T0) - 197.91 * (TK ^ 2 - T0 ^ 2) / 2 + 1.0737 * (TK ^ 3 - T0 ^ 3) / 3)
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 + 0.0000093701 * (TK ^ 5 - T0 ^ 5) / 5)


Q = U * (T - Ta)


HIG_C8H18 = (135540 * TK + 443100 * 1635.6 * (coth(1635.6 / TK)) - 305400 * 746.4 * (tanh(746.4 / TK))
- 492800000#)
HIG_C10H22 = (167200 * TK + 535300 * 1614.1 * (coth(1614.1 / TK)) - 378200 * 742 * (tanh(742 / TK)) -
579100000#)
HIG_H2O = (33363# * TK + 26790# * 2610.5 * (coth(2610.5 / TK)) ^ 2 + 8896# * 1169# * (tanh(1169 /
TK)) - 44710000#)

HV = YW * HIG_H2O + Y1 * HIG_C8H18 + Y2 * HIG_C10H22

V = (MS * (HS - HL_H2O) + Q) / (HV - (HL_H2O * YW + (Y1 * HL_C8H18 + Y2 * HL_C10H22)))

' Set Right Side of Differential equations

fff(1) = MS - V * YW
fff(2) = -V * Y1
fff(3) = -V * Y2

dydx = 0
End Function
```

Figure A4 Function dydx: Right Hand Side of Differential Equations for Distillation (Continued)

```
Private Function DMM(MX1, MX2, prm)
' Given MX1 and Mx2  find the Temp (TK) that satisfies 1-y1-y2-y3 = 0 (bubble pt)

' Prepare for Newton Method

Dim X1, X2, P As Single
Dim TC, TK, TKnew As Single
Dim Y1, Y2, YW, FOX As Single

Dim FOXP, DY1, DY2, DYW As Single
Dim DERY1, DERY2, DERYW  As Single
Dim V1, V2, VW, NCOUNT, ITER As Single

X1 = MX1 / (MX1 + MX2)
X2 = MX2 / (MX1 + MX2)

P = prm(10)

TC = prm(12)
TK = TC + 273.15

NCOUNT = 0
ITER = prm(13)

Q1:

'  Start of Loop

 NCOUNT = NCOUNT + 1
 If NCOUNT > ITER Then MsgBox " MORE ITERATIONS THAN PRM(13) in DMM"
 If NCOUNT > ITER Then Exit Function


' Evaluate Bubble Point at TK

V1 = 96.084 - 7900.2 / TK - 11.003 * Log(TK) + 0.0000071802 * TK ^ 2
V2 = 112.73 - 9749.6 / TK - 13.245 * Log(TK) + 0.0000071266 * TK ^ 2
VW = 73.649 - 7258.2 / TK - 7.3037 * Log(TK) + 0.0000041653 * TK ^ 2

Y1 = (X1 / P) * Exp(V1)
Y2 = (X2 / P) * Exp(V2)
YW = (1 / P) * Exp(VW)

'Evaluate FOX (f(x))

FOX = 1# - Y1 - Y2 - YW
```

```
If Abs(FOX) >= 0.000001 Then GoTo Q2:

DMM = TK

Exit Function

Q2:

' Evaluate FOXP  (f'(x))

DERY1 = Exp(V1) * ((7900.2 / (TK ^ 2) - 11.003 / TK + 2 * 0.0000071802 * TK))
DERY2 = Exp(V2) * ((9749.6 / (TK ^ 2) - 13.245 / TK + 2 * 0.0000071266 * TK))
DERYW = Exp(VW) * ((7258.2 / (TK ^ 2) - 7.3037 / TK + 2 * 0.0000041653 * TK))


DY1 = (X1 / P) * DERY1
DY2 = (X2 / P) * DERY2
DYW = (1 / P) * DERYW

FOXP = -(DY1 + DY2 + DYW)

' Newton's method

TKnew = TK - FOX / FOXP

TK = TKnew

GoTo Q1:

End Function
```

```
Private Function Interp(N, x, fx, arg, NN)

'  N is the order of interpolation  -1 for Linear, 2 for second order
'  x is the x array of numbers to be used -
'         the name for the range is used in the call
' fx is the array corresponding values of f(x) -
'         the the first element of the range may be used
'arg is the x argument
' The return is the value of f(arg)
' NN = 1  Ascend  NN = -1  Decend for the x array

Dim xarg, X1, X2, x3, fx1, fx2, fx3 As Single
Dim Term1, Term2, Term3
Dim NC, Num, NX As Integer

NX = NN
xarg = arg

'Nc is the total array length
 NC = Application.Count(x)

'Num is the index of the element in the range less than or equal to arg

Num = Application.Match(arg, x, NX)

Setn:

If (N = 2 And NC < 3) Then
     Interp = 0
     Exit Function
 End If


 If (N = 1 And NC < 2) Then
     Interp = 0
     Exit Function
 End If

 xarg = arg

 X1 = x(Num)
 fx1 = fx(Num)
```

Figure A6   Function Interp- General Interpolation Routine

```
X2 = x(Num + 1)
fx2 = fx(Num + 1)

If (N = 2 And NC >= Num + 2) Then GoTo Second:




If (N = 2 And NC < Num + 2) Then GoTo Third:

Term1 = (xarg - X2) / (X1 - X2)
Term2 = (xarg - X1) / (X2 - X1)

Interp = Term1 * fx1 + Term2 * fx2

Exit Function
Second:

x3 = x(Num + 2)
fx3 = fx(Num + 2)
GoTo Continue:

Third:

X1 = x(NC - 2)
fx1 = fx(NC - 2)

X2 = x(NC - 1)
fx2 = fx(NC - 1)

x3 = x(NC)
fx3 = fx(NC)

Continue:
Term1 = (xarg - X2) * (xarg - x3) / ((X1 - X2) * (X1 - x3))
Term2 = (xarg - X1) * (xarg - x3) / ((X2 - X1) * (X2 - x3))
Term3 = (xarg - X1) * (xarg - X2) / ((x3 - X1) * (x3 - X2))

Interp = Term1 * fx1 + Term2 * fx2 + Term3 * fx3

End Function
```

Figure A6 Function Interp- General Interpolation Routine (Continued)

```
Private Function coth(x)

coth = (Exp(x) + Exp(-x)) / (Exp(x) - Exp(-x))

End Function

Private Function tanh(x)

tanh = (Exp(x) - Exp(-x)) / (Exp(x) + Exp(-x))

End Function
```

Figure A7 Function coth and tanh

```
 Private Function dydx(x, y, prm, fff)
' For Distillation

Dim TK, MW, MX1, MX2 As Single
Dim MS, M, M0, Q, HV As Single
Dim X1, X2, P, T0, V1, V2, VW, Y1, Y2, YW As Single
Dim TSK, HS, T, Ta, U, V As Single
Dim HL_C8H18, HL_C10H22, HL_H2O As Single
Dim HIG_C8H18, HIG_C10H22, HIG_H2O As Single
Dim TEST1, TEST2
Dim Kc, EPS As Single

'
' The Four Dependent Variables for Controlled Distillation
'
MW = y(1)
MX1 = y(2)
MX2 = y(3)
T = y(4)

TK = T + 273.15

MS = prm(3)
M0 = prm(11)
P = prm(10)
T0 = prm(7)
TSK = prm(4)
U = prm(5)
Ta = prm(6)

M = MX1 + MX2
X1 = MX1 / M
X2 = MX2 / M


V1 = 96.084 - 7900.2 / TK - 11.003 * Log(TK) + 0.0000071802 * TK ^ 2
V2 = 112.73 - 9749.6 / TK - 13.245 * Log(TK) + 0.0000071266 * TK ^ 2
VW = 73.649 - 7258.2 / TK - 7.3037 * Log(TK) + 0.0000041653 * TK ^ 2

Y1 = (X1 / P) * Exp(V1)
Y2 = (X2 / P) * Exp(V2)
YW = (1 / P) * Exp(VW)

Kc = prm(14)
EPS = 1 - Y1 - Y2 - YW
```

Figure A8 Function dydx - The Right Hand Side of Equations for “Controlled Distillation”

```
TEST1 = coth(2610.5 / TSK)
TEST2 = tanh(1169 / TSK)

HS = (33363# * TSK + 26790# * 2610.5 * ((TEST1) ^ 2) _
     + 8896# * 1169# * (TEST2) - 44710000#)


HL_C8H18 = (224830 * (TK - T0) - 186.63 * (TK ^ 2 - T0 ^ 2) / 2 + 0.95891 * (TK ^ 3 - T0 ^ 3) / 3)
HL_C10H22 = (278620 * (TK - T0) - 197.91 * (TK ^ 2 - T0 ^ 2) / 2 + 1.0737 * (TK ^ 3 - T0 ^ 3) / 3)
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 + 0.0000093701 * (TK ^ 5 - T0 ^ 5) / 5)


Q = U * (T - Ta)


HIG_C8H18 = (135540 * TK + 443100 * 1635.6 * (coth(1635.6 / TK)) - 305400 * 746.4 * (tanh(746.4 / TK))
- 492800000#)
HIG_C10H22 = (167200 * TK + 535300 * 1614.1 * (coth(1614.1 / TK)) - 378200 * 742 * (tanh(742 / TK)) -
579100000#)
HIG_H2O = (33363# * TK + 26790# * 2610.5 * (coth(2610.5 / TK)) ^ 2 + 8896# * 1169# * (tanh(1169 /
TK)) - 44710000#)

HV = YW * HIG_H2O + Y1 * HIG_C8H18 + Y2 * HIG_C10H22

V = (MS * (HS - HL_H2O) + Q) / (HV - (HL_H2O * YW + (Y1 * HL_C8H18 + Y2 * HL_C10H22)))

fff(1) = MS - V * YW
fff(2) = -V * Y1
fff(3) = -V * Y2
fff(4) = Kc * EPS
dydx = 0
End Function
```

Figure A8 Function dydx - The Right Hand Side of Equations for “Controlled Distillation” (Continued)