EXAMPLE FLASH CALCULATION

Comments to this spreadsheet are given in red text below

Problem Statement: A subcooled liquid feed composed of n-pentane, n-hexane, n-heptane, benzene, and toluene at 298 K and 5 atm enters a flash chamber whose pressure is 2 atm. The flow rate of the feed is 1 mole/s. A heat exchanger present in the flash chamber provides 20 kJ of heat per mole of feed. Determine the composition of the vapor and liquid product streams, the vapor and liquid product flow rate, and the temperature in the flash chamber. Use the virial equation of state, the Pitzer and Curl correlation, and the Lewis fugacity rule for determining the vapor phase activity coefficients and regular solution theory for determining the liquid-phase activity coefficients. Assume ideal mixtures when determining the enthalpies of the liquid and vapor phases.

PART 1: INPUT DATA

Components:	n-C5	benzene	n-C6	n-C7	toluene
Antoine consts.					
A	15.833	15.9	15.83	15.873	16
B	2477.07	2788	2697.55	2911.32	3096.52
C	-39.94	-52.36	-48.78	-56.5	-53.67

These constants give the vapor pressure in mm Hg

Critical Constants					
Tc (K)	469.6	562.1	507.4	540.2	591
Vc (cm^3/mol)	304	259	370	432	316
Zc	0.262	0.271	0.264	0.263	0.264
Pc	33.3	44.6	29.3	27	40.6
omega	0.251	0.212	0.296	0.351	0.257
Liquid mol. vol. (cm^3/gmol)	115.26	88.26	130.77	146.49	106.23
Regular Solution Theory Solubility Parameters (cal/cm^3)^(1/2)	7.05	9.15	7.3	7.45	8.9

These Cpi values are approximate average values for the temperature range that applies to the problem. This avoids the use of temperature dependent heat capacities

Enthalpy Data (units: J, g-mole, K)

Note units for enthalpy parameters

Cpi liquid	150.47	180	180	220.99	200

heat vaporiz @ Tb	25256	30143.2	28273.6	31061.6	32513
Tb (Normal boiling pt.)	309.2	353	342	371	383

PART 2: PROBLEM SPECIFICATION

In this problem the feed parameters as well as the flash chamber pressure and the value of Q/F are specified.

Based on 1 mole of feed:

	z1	z2	z3	z4	z5
zi:	0.2	0.2	0.2	0.2	0.2
P:	2				

Flash chamber pressure

Feed is all liquid at 298 K, so by definition the enthalpy is zero. Note the feed pressure does not matter (since feed is all liquid).

Feed enthalpy/mole: 0

(Liq. enth. @ 298K = 0)

Enthalpy is defined to be zero for each component at 298 K in liquid sate

Heat input/mole feed 20000

This is Q/F (enthalpy input per mole of feed)

PART 3: INITIAL GUESS AND FINAL SOLUTION:

These are the changing cells in the solver. The values shown here are the final solution.

y1	y2	y3	y4	y5	T
0.378440903	0.192811904	0.220987144	0.116634164	0.091125884	368.7014896

x1	x2	x3	x4	x5	V/F
0.137029864	0.202536639	0.192593859	0.229419063	0.238420576	0.260842105

PART 4: UPPER AND LOWER LIMITS OF VARIABLES DURING SOLUTION SEARCH:

Upper limit of y&x	1
Lower limit of y&x	0
Upper limit of T	500
Lower limit of T	200

These can be used for inequality constraints to helo Solver find a solution

PART 5: GAS PHASE CALCULATIONS

These pressures are in atm (not mm Hg)

Note that R = 82.06 cm^3 atm / (mol K) in the relations given in this section

Pi_sat (atm)	5.286366803	1.573686447	2.148498203	0.918098945	0.629670849
B_i (cm^3/mol)	-720.7037032	-962.257141	-1099.753064	-1553.19729	-1313.682923
phi_i	0.953476078	0.938372358	0.929882187	0.902423305	0.916824815
phi_i_sat	0.881682074	0.951181989	0.924876469	0.953962104	0.973030402

phi_i is given by the Lewis fugacity rule here so it does not depend on composition

PART 6: LIQUID PHASE CALCULATIONS

Note that R = 2 cal/(mole K) when this parameter is needed in this section.

Regular soln theory

Volume fraction is given by x_i * v_i /(Σ x_i * v_i) where v_i is the molar volume of pure i.

xi * vi	15.79367686	17.87586083	25.1856655	33.60788026	25.32703003
Volume fractions	0.134083213	0.151760282	0.213818161	0.285320043	0.215018301
sol par_i * vol fr_i	0.945286651	1.38860658	1.560872578	2.125634322	1.913662875
Sol. par. of mixture	7.934063006				
gamma_i	1.12993505	1.19358603	1.073900071	1.047649431	1.143862295

PART 7: ENTHALPY

Need to incorporate "if" statement in formula so ΔH_v = 0 if T is greater than Tc for a component. Watson equation gives an imaginary result if you don't do this.

heat vaporiz (T) (Watson eqn.)	21176.93567	29262.20241	26443.86312	31221.27397	33344.85757

These are x_i * h_i .

	1457.785785	2577.535567	2451.001085	3584.517352	3371.337971
Liq. Tot. Enthalpy/mole	13442.17776				

This is Σ x_i * h_i (denoted at h_L below).

These are y_i * H_i .

	12040.24447	8095.876966	8656.095449	5463.796965	4327.12675
Gas Tot. Enthalpy/mole	38583.1406				

This is Σ y_i * H_i (denoted at H_v below).

Combined Products enth/mole 19999.99943

This is (V/F) * H_v + (1-V/F) h_L

PART 8: SELECTION OF THERMODYNAMIC MODELS

Assume ideal liquid (y/n)? n

Assume ideal gas (y/n)? n

Collect all the previous calculations for parameters here, but with an "if" statement so if the questions on lines 113-4 are answered with "y", unity appears in appropriate cell

PART 9: FINAL CALCULATIONS (SOLVE EQUATIONS IN RESIDUAL FORM)

	comp 1	comp 2	comp 3	comp 4	comp 5
phi_i	0.953476078	0.938372358	0.929882187	0.902423305	0.916824815
phi_i_sat	0.881682074	0.951181989	0.924876469	0.953962104	0.973030402
gamma_i	1.12993505	1.19358603	1.073900071	1.047649431	1.143862295

The residuals below use the parameters in the table immediately above, which will be unity if ideal conditions are assumed.

Equations to be solved (in residual form):

Note that f_i = gamma_i * x_i * phi_i_sat * P_i_sat / (ph_i * P)

Phase equilibrium residuals:

	y1 - f1	y2 - f2	y3 - f3	y4 - f4	y5 - f5	Σ y_i - 1
Residuals:	-1.25878E-07	-4.52083E-08	-4.93147E-08	-3.63089E-09	1.3264E-07	0

Material and Enthalpy Balances (in residual form):

	comp 1	comp 2	comp 3	comp 4	comp 5	Enthalpy Balance/1000
Residuals:	-2.75721E-08	-1.84381E-08	-2.31869E-08	-1.25574E-08	8.17546E-08	5.68731E-07

y_i *(V/F) + x_i * (1 - V/F) - z_i

(H_v *(V/F) + h_L* (1 - V/F) - Q/F - h_feed)/1000
Note that enthalpy balance residual is divided by 1000 to provide additional scaling to help Solver find the solution.

The above 12 residual are entered as contraints to be equal to zero in the Excel solver. The 12 residuals are set equal to zero by chaning the 12 changing cells shown earlier. .