- 1. Read the paper by <u>Fletcher et al., 23rd Combustion Institute (1990)</u> and comment on the main conclusions that would apply to network models.
- 2. Please review the main features of the network models. Discuss why you might want to use a network model instead of a simpler model (1-step, 2-step, etc.).
- 3. How does a flash calculation (used in CPD and FLASHCHAIN) differ from just using the vapor pressure as a cutoff value (like in FG-DVC)?
- 4. Compare the maximum MW vaporized at 1 atm at 550 K for the three models, assuming that everything with vapor pressure > ambient pressure vaporizes.
- 5. Please discuss the coal-dependent input parameters used by the three models, and how they pertain to macromolecular structure.
- 6. Using the flash program provided, or one of your own choosing, calculate

(1) the average molecular weight of tar vapor and of tar liquid

(2) the molecular weight distribution (fraction of tar vapor at each molecular weight) for ambient pressures of 1.e-3 atm, 1 atm, and 100 atm and a temperature of 800 K. Use the Fletcher-Grant-Pugmire vapor pressure correlation. Assume the following feed distribution:

	Mol. Wt.	Moles of feed
Light gas	30.	2.603E-03
Tar precursor	292.	3.674E-04
(feed metaplast)	595.	8.835E-05
	898.	3.431E-05
	1201.	1.667E-05
	1504.	9.226E-06
	1807.	5.566E-06
	2111.	3.570E-06
	2414.	2.396E-06
	2717.	1.666E-06
	3020.	1.191E-06
	3323.	8.717E-07
	3626.	6.502E-07
	3929.	4.929E-07
	4233.	3.789E-07
	4536.	2.948E-07
	4839.	2.317E-07
	5142.	1.839E-07
	5445.	1.471E-07
	5748.	1.185E-07
	6051.	9.618E-08

A copy of this fortran program and a python program can be obtained from the ChE 733 web page followed by /flash (<u>http://www.et.byu.edu/~tom/classes/733/flash</u>)

- I recommend using the <u>FORCE</u> fortran compiler. Please click <u>here</u> for some background on how this flash program works.
- 7. Please run the base case for the cpd model at 3 different pressures (1, 20, and 50 atm) and plot the tar and total volatiles yields as a function of temperature for each pressure. You will need the fortran and input files. Zip files for the CPD Heat model in Matlab and Fortran are located <a href="http://www.et.byu.edu/~tom/classes/733/cpd/">http://www.et.byu.edu/~tom/classes/733/cpd/</a>.