**Questions for Class 8**
**Chemical Engineering 733**

1. One step devolatilization models are of the form:

$$\frac{dV}{dt} = k(V_\infty - V)$$

where V is the fractional yield of volatiles (mass of volatiles per mass of daf coal), and $V_\infty$ is the hypothetical ultimate yield. Assuming a $V_\infty$ of 0.5, please integrate this expression at $10^4$ K/s from 300 K to 1400 K for the following two rates:

(a) Badzioch & Hawksley (1970): $k = 3.12 \times 10^5 \exp[-8961/T]$

(b) Solomon, et al. (1976): $k = 4.3 \times 10^{14} \exp[-27{,}544/T]$

where T is in Kelvin and k is in seconds$^{-1}$. Plot V versus T. What is the time and corresponding temperature when the yield reaches V = 0.4? You will probably have to integrate this numerically.

2. Repeat problem 1 for the 2-step competing model using the following rate constants:

| | $A_1$ $sec^{-1}$ | $A_2$ $sec^{-1}$ | $E_1$ (kcal/mol) | $E_2$ (kcal/mol) | $\alpha_1$ | $\alpha_2$ |
|---|---|---|---|---|---|---|
| Kobayashi 2-step | 2.0e5 | 1.3e7 | 25 | 40 | 0.3 | 1.0 |
| Ubhayakar 2-step | 3.7e5 | 1.46e13 | 17.6 | 60 | 0.39 | 0.80 |

3. Why was the distributed activation energy model (DAEM) developed (i.e., what was the underlying idea)? Please find the typos in Equation 3.7 in Smoot and Smith. Repeat Problem 1 for the DAEM model using the following coefficients:

$V_\infty = 0.5$
$k_0 = 1.67e13$ $sec^{-1}$
$E_0 = 50.65$ kcal/mol
$\sigma = 7.01$ kcal/mol

4. Please compare the capabilities of the 3 simple models (1-step, 2-step, and DAEM) with respect to calculation of total volatiles yields as a function of time, temperature, heating rate, pressure, and coal type. You may want to look at the paper by Richards et al., *Fuel*, **185**, 171-180 (2016).
5. Please discuss what the blowing factor is in relation to coal devolatilization. You may want to look at the paper by Fletcher, *Combustion Science and Technology* **63**, 89 (1989).

6. If the coal ignites heterogeneously before devolatilization, why will the heterogeneous reaction quickly quit and then restart at a later time?