Questions for Class 6  
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 \(V_\infty\) 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 model using the following rate constants:

<table>
<thead>
<tr>
<th></th>
<th>(A_1) (sec(^{-1}))</th>
<th>(A_2) (sec(^{-1}))</th>
<th>(E_1) (kcal/mol)</th>
<th>(E_2) (kcal/mol)</th>
<th>(\alpha_1)</th>
<th>(\alpha_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kobayashi 2-step</td>
<td>2.0e5</td>
<td>1.3e7</td>
<td>25</td>
<td>40</td>
<td>0.3</td>
<td>1.0</td>
</tr>
<tr>
<td>Ubhayakar 2-step</td>
<td>3.7e5</td>
<td>1.46e13</td>
<td>17.6</td>
<td>60</td>
<td>0.39</td>
<td>0.80</td>
</tr>
</tbody>
</table>

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.

5. Please discuss what the blowing factor is in relation to coal devolatilization.

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