Homework Hints

• See online hint for Problem 9-56

Review of Enthalpy

<table>
<thead>
<tr>
<th>Term</th>
<th>Units</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>J</td>
<td>Total enthalpy ($H = U + PV$)</td>
</tr>
<tr>
<td>$\dot{H}$</td>
<td>J/s</td>
<td>Enthalpy per time</td>
</tr>
<tr>
<td>$\tilde{H}$</td>
<td>J/mol or kJ/kg</td>
<td>Specific enthalpy (i.e., enthalpy per unit mass or mole)</td>
</tr>
<tr>
<td>$\Delta H^\circ$</td>
<td>kJ/mol</td>
<td>Standard heat of formation ($^\circ$ means at 1 atm, 25°C)</td>
</tr>
<tr>
<td>$\Delta H_r$</td>
<td>kJ/mol</td>
<td>Heat of reaction</td>
</tr>
<tr>
<td>$\Delta H_{comb}$</td>
<td>kJ/mol</td>
<td>Heat of combustion (in book, this corresponds to the high heating value with liquid H2O as a product) ($^\circ$ means reactants and products at 1 atm, 25°C)</td>
</tr>
<tr>
<td>$\Delta H_{vap}$</td>
<td>kJ/mol</td>
<td>Heat of vaporization (liquid $\rightarrow$ vapor) (Value in Table B.1 at boiling temperature, 1 atm)</td>
</tr>
<tr>
<td>$\Delta H_m$</td>
<td>kJ/mol</td>
<td>Heat of melting (Value in Table B.1 at melting temperature, 1 atm)</td>
</tr>
</tbody>
</table>

Class 33

Adiabatic Flame Temperatures

Adiabatic Flame Temperature

• Very useful in industry
  – Maximum $T$ possible
  – Determines material used to confine the flame
• All energy from exothermic reaction goes into heating up products
• Iterative process because $C_p = f(T)$
• Numbers can be reasonable, but not with the $C_p$’s in the text

A. Path Method

[Diagram showing the path method]

If reactants are at 25°C, then

$$Q = 0 = n_{fuel} \Delta H_r + \sum_{products} n_i \int_{25^\circ C}^{T_{ad}} C_{p,i} \, dT$$

Good for simple reactions
B. In-Out Table to Calculate $T_{ad}$

1. Guess $T_{ad}$
2. Make H table on in and out streams based on $T_{ad}$
3. Compute $Q = (\sum n_i H_i)_{out} - (\sum n_i H_i)_{in}$
4. If $Q \neq 0$, go to step 1

- There are nice algorithms to make a series of guesses
- These are included in the solver in Excel and Mathcad

Example 1

- Fuel = methane at 25°C (basis: 1 mole of CH₄, stoichiometric air)
- $T_{in} = 25^\circ C$

CH₄ + 2 O₂ $\Rightarrow$ CO₂ + 2 H₂O

- What is $T_{adiabatic}$ in stoichiometric air?
- What is $T_{adiabatic}$ in stoichiometric O₂?

See Excel Sheet

Then set $n_{N₂} = 0$ and redo solver.

Heat Capacity Correlations Can Go Crazy at High Temperatures!

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Cp (kJ/mol-C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.05</td>
</tr>
<tr>
<td>2000</td>
<td>0.1</td>
</tr>
<tr>
<td>4000</td>
<td>0.15</td>
</tr>
<tr>
<td>6000</td>
<td>0.2</td>
</tr>
<tr>
<td>8000</td>
<td></td>
</tr>
</tbody>
</table>

Cp Comparison

- CO/CO₂ Felder
- CO₂ JANAF
- CO-JANAF
- CO₂-DIPPR
- CO-DIPPR

With More Complex Chemistry

<table>
<thead>
<tr>
<th>CH4-Air Stoichimetric</th>
<th>CH4-O₂ Stoichimetric</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar 0.84%</td>
<td>CO 15.52%</td>
</tr>
<tr>
<td>CO 0.85%</td>
<td>CO₂ 11.38%</td>
</tr>
<tr>
<td>CO₂ 8.60%</td>
<td>H 4.86%</td>
</tr>
<tr>
<td>H 0.06%</td>
<td>HO₂ 0.01%</td>
</tr>
<tr>
<td>H₂ 0.34%</td>
<td>CO 3.76%</td>
</tr>
<tr>
<td>H₂O 18.32%</td>
<td>H₂ 7.15%</td>
</tr>
<tr>
<td>NO 0.10%</td>
<td>H₂O 39.23%</td>
</tr>
<tr>
<td>O₂ 70.10%</td>
<td>O 9.93%</td>
</tr>
<tr>
<td>O 0.02%</td>
<td>O₂ 8.18%</td>
</tr>
<tr>
<td>OH 0.30%</td>
<td></td>
</tr>
<tr>
<td>D 0.43%</td>
<td></td>
</tr>
</tbody>
</table>

T_ad = 2212 K

T_ad = 3048 K

Spreadsheet with high T Cp’s

http://www.et.byu.edu/~tom/classes/273/273.html
**Example 2**

- Fuel = 40 mol% CO, 60 mol% H₂ (basis: 100 moles of fuel)
- \( T_{in} = 25^\circ C \)

\[
\begin{align*}
\text{CO} + \frac{1}{2}\text{O}_2 & \rightarrow \text{CO}_2 \\
\text{H}_2 + \frac{1}{2}\text{O}_2 & \rightarrow \text{H}_2\text{O}
\end{align*}
\]

- What is \( T_{adiabatic} \) in stoichiometric air?
- What is \( T_{adiabatic} \) in stoichiometric \( \text{O}_2 \)?

See Excel Sheet

Then set \( n_{N_2} = 0 \) and redo solver.

**Mistake Students Made on Exam**

- Fuel = 40 mol% CO, 60 mol% H₂ (basis: 100 moles of fuel)
- \( \text{CO} + \text{H}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \)
- Rationalize: 1 mole of \( \text{O}_2 \) needed
- Problems with this idea:
  - There are actually 2 moles fuel in this equation (1 CO and 1 H₂)
  - There are not equal amounts of CO and H₂ (although this would not have caused the error)

**40% CO, 60% H₂ Example**

- In Air
  - \( T = 2649 \text{ K} \) using Felder \( C_p \)’s
  - \( T = 2584 \text{ K} \) using JANAF \( C_p \)’s
  - \( T = 2371 \text{ K} \) using chemical equilibrium code
    - 6.10 mol% \( \text{H}_2 \)
    - 0.99 mol% \( \text{O}_2 \)
    - 0.11 mol% \( \text{H} \)
    - 0.07 mol% \( \text{O} \)
    - 0.61 mol% \( \text{OH} \)
    - 2.06 mol% \( \text{CO} \)
    - 0.37 mol% \( \text{NO} \)

- In \( \text{O}_2 \)
  - \( T = 5047 \text{ K} \) using Felder \( C_p \)’s
  - \( T = 5038 \text{ K} \) using JANAF \( C_p \)’s
  - \( T = 3009 \text{ K} \) using chemical equilibrium code
    - 5.84 mol% \( \text{H}_2 \)
    - 8.79 mol% \( \text{O}_2 \)
    - 3.91 mol% \( \text{H} \)
    - 3.44 mol% \( \text{O} \)
    - 8.37 mol% \( \text{OH} \)
    - 17.41 mol% \( \text{CO} \)
    - Trace \( \text{HO}_2 \)

**Spreadsheet**

**Message:**

- If temperatures get too hot, other species (like radical species) become stable, lowering the flame temperature!
- In particular, CO is as stable as \( \text{CO}_2 \) at high temperatures (above 2700 K)
Special Problem 9c

Help on Special Problem 9c

\[ \text{CH}_4 + 2 \text{ O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O} \quad (\xi_1) \]
\[ \text{CH}_4 + 1.5 \text{ O}_2 \rightarrow \text{CO} + 2 \text{H}_2\text{O} \quad (\xi_2) \]

But \( \left( \frac{n_{\text{fuel}}}{n_{\text{fuel}}^{\text{stoch}}} \right)_{\text{stoch}} = \frac{2}{1} = 2 \)
(based only on first reaction!)
Therefore, \( \frac{n_{\text{fuel}}}{n_{\text{fuel}}^{\text{stoch}}} = 2 \)
Assuming \( n_{\text{CH}_4,0} = 1 \), then \( n_{\text{O}_2,0} = 2^*SR \)
Assuming all \( \text{O}_2 \) and \( \text{CH}_4 \) react,
\[ n_{\text{O}_2} = 0 = n_{\text{O}_2,0} - 2\xi_1 - 1.5\xi_2 \]
\[ n_{\text{CH}_4} = 0 = n_{\text{CH}_4,0} - \xi_1 - \xi_2 \]
\[ \xi_2 = \frac{2 - n_{\text{O}_2,0}}{1.5} \quad \text{(prove this)} \]
\[ \xi_1 = 1 - \xi_2 \quad \text{(prove this)} \]

Questions?

- Enthalpy
- Heat Capacities
- Heat of Formation
- Heat of Vaporization, Heat of Melting
- Heat of Combustion
- Energy Balances
- Adiabatic Flame Temperature