Homework Review

Special Problem 9a
(Heat of Reaction at Different T’s)

See Excel Sheet

Level 3 Competency Exam

• See booklet
• Also on ChE web page
  – Undergraduate page

Business

• Winter and Spring TA positions available (apply online through ChE web page)
  – “Department” Menu → TA Application
  – Or email Serena (Department Secretary)
• Scholarships (applications due April 15)
  – Department (some are need-based)
  – Returned missionary (if in first-year back)
  – College (see advisement center)
• Answers to next two problems are now in the homework hints! (9.23 and 9.32)

Goals Today

1. Energy Balance with $\Delta H_r^0$ (single rxn)
2. Energy Balance with $\Delta H_f^0$ (multiple rxns)

The End is Near!!
1. Energy Balance with only One Reaction

Board Problem

A → bB

Path method, incomplete conversion

Caution on Enthalpy Tables

Find $\hat{H}_{H_2O,liq}$ at 25°C, 1 atm
1. Use steam tables (Table B.5)
   $(104.8 \text{ kJ/kg/1000 g}) \times (18 \text{ g/mol}) = 1.886 \text{ kJ/mol}$
   sat'd liquid (0.0317 bar)
2. Use $\Delta H_f$
   Table B.1 says $\Delta H_f = -285.84 \text{ kJ/mol}$ at 25°C and 1 atm
   What about VdP term since reference for steam tables is at 0.0317 bar?
   $V_dP = (0.0001\text{ m}^3/\text{kg})(1 \text{ atm} - 0.0317 \text{ bar}) (1.01325 \text{e5 N/m}^2/\text{atm})$
   $= (99.1 \text{ N-m/kg})(18 \text{ g/mol}) (J/\text{N-m})(\text{kJ}/1000\text{J})$
   $= 1.78 \times 10^{-3} \text{ kJ/mol}$ (not enough to make a difference)

Bottom line: Do not mix and match enthalpies from different tables!

Look at Table B.7

- How does $\hat{H}_{liq}$ water change with pressure at 50°C? (use steam tables)
  - 0.5 bar → 209.3 kJ/kg
  - 1.0 bar → 209.3 kJ/kg
  - 5.0 bar → 209.7 kJ/kg (0.19% above 0.5 bar value)
- Pretty small change!! (for a liquid)
- But relatively small change in pressure
- What about for steam?
  - At 350°C, $\Delta \hat{H}_{liq}$ vs $\Delta \hat{H}_{liq,liq} = 0.28\%$ decrease

2. Energy Balance with Multiple Reactions using $\Delta H_f$

- Most common approach
- Most reliable approach
  $\Delta H + \Delta E_k + \Delta E_p = Q - W_s$
  $\Delta H + \Delta E_k + \Delta E_p = Q - W_s$

Where is the $\Delta H_{rxn}$ term?

Idea: Construct a Table

<table>
<thead>
<tr>
<th>In</th>
<th>$n_i$</th>
<th>$T$</th>
<th>$T_{ref}$</th>
<th>$s_i$</th>
<th>$s_{ref}$</th>
<th>$n_i \Delta H_{i,f}$</th>
<th>$\int T\Delta C_p dT$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2</td>
<td>298</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>A 5 900</td>
<td>?</td>
</tr>
<tr>
<td>B</td>
<td>1</td>
<td>400</td>
<td>?</td>
<td>?</td>
<td>B     1 900</td>
<td>?</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5</td>
<td>700</td>
<td>?</td>
<td>?</td>
<td>C 0.05 900</td>
<td>?</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>-</td>
<td>?</td>
<td>?</td>
<td>D 1 900</td>
<td>?</td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>0</td>
<td>-</td>
<td>?</td>
<td>?</td>
<td>E 1.3 900</td>
<td>?</td>
<td></td>
</tr>
</tbody>
</table>

Example: Problem 9.20

4 NH$_3$ + 5 O$_2$ → 4 NO + 6 H$_2$O
2 NH$_3$ + 3/2 O$_2$ → N$_2$ + 3 H$_2$O

Step 1: Write the mole balance (already done)
Step 2: Write the energy balance
Energy Balance with $\Delta H^\circ$

$$\Delta H + \Delta E_l + \Delta E_p = Q - W_s$$

- $\Delta \dot{H} = \dot{H}_{\text{out}} - \dot{H}_{\text{in}} = \left(\sum n_i \dot{H}_i\right)_{\text{out}} - \left(\sum n_i \dot{H}_i\right)_{\text{in}}$
- $\dot{H}_i = \Delta H_{i,f}^\circ + \int_{T_{\text{ref}}}^T c_p \, dT$

Example: Problem 9.20

$$4 \text{NH}_3 + 5 \text{O}_2 \rightarrow 4 \text{NO} + 6 \text{H}_2\text{O}$$
$$2 \text{NH}_3 + 3/2 \text{O}_2 \rightarrow \text{N}_2 + 3 \text{H}_2\text{O}$$

<table>
<thead>
<tr>
<th>Species</th>
<th>$n_i$</th>
<th>$\dot{H}_i$</th>
<th>$\Delta H_{i,f}^\circ$</th>
<th>$c_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH$_3$</td>
<td>100</td>
<td>25</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>O$_2$</td>
<td>189</td>
<td>150</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>N$_2$</td>
<td>711</td>
<td>150</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>NO</td>
<td>0</td>
<td>-</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>H$_2$O (g)</td>
<td>0</td>
<td>-</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

Find $Q = \Delta H$

<table>
<thead>
<tr>
<th>Species</th>
<th>$n_i$</th>
<th>$\dot{H}_i$</th>
<th>$T$</th>
<th>$\Delta H_{i,f}^\circ$</th>
<th>$c_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH$_3$</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>O$_2$</td>
<td>69</td>
<td>700</td>
<td>?</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>N$_2$</td>
<td>716</td>
<td>700</td>
<td>?</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>NO</td>
<td>90</td>
<td>700</td>
<td>?</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>H$_2$O (g)</td>
<td>150</td>
<td>700</td>
<td>?</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

Excel Sheet