SECTION 16: USING ENTHALPY IN PROBLEM-SOLVING

$\Delta H$ is used the same way that $\Delta E$ is used, and all of the problem-solving methods from pages 24-27 apply to $\Delta H$ as well. However, whenever we relate $\Delta H$ to heat and (useful) work, we must be sure that we are using constant-pressure conditions. If the pressure is not constant, we must use $\Delta E = q + w$ to interrelate energy, heat and work.

The first example shows how we can get a value for $\Delta H$ if we know $\Delta E$.

**Sample Problem 21:** “What is $\Delta H$ for the reaction below at 25ºC, given that $\Delta E$ for this reaction is $-3346$ kJ?”

$$4 \text{ Al}(s) + 3 \text{ O}_2(g) \rightarrow 2 \text{ Al}_2\text{O}_3(s)$$

**Answer:** We can use $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$ to calculate $\Delta H$. However, you must be careful in using this equation: there are two common errors we see.

- **Energy units:** these must match! $\Delta E$ and $\Delta H$ are usually given in kJ, but R is not. You actually are faced with several choices for $R$: 8.314 J/mol·K, or 0.08206 L·atm/mol·K, or 62.36 L·torr/mol·K. You can reconcile the energy units by choosing the first value of $R$ (in joules) and then converting $RT\Delta n_{\text{gases}}$ from joules to kilojoules.

- **Moles of gases:** be sure that you consider only gases! It’s easy to forget this and to add up the moles of everything.

In this example, the balanced equation implies that we start with 4 moles of aluminum and 3 moles of oxygen, and we produce 2 moles of aluminum oxide. Oxygen is the only gas, so we go from 3 moles of gases to zero: $\Delta n_{\text{gases}} = 0$ mol $- 3$ mol $= -3$ mol. Now we’re ready to do the computation.

$$\Delta H = \Delta E + RT\Delta n_{\text{gases}}$$

$$= -3346$ kJ $+ (8.314$ J/mol·K$)(298$ K$)(-3$ mol$)$

$$= -3346$ kJ $+ (-7433$ J$)$

$$(\text{Be sure to make your energy units agree!})$$

$$= -3346$ kJ $+ (-7.4$ kJ$)$

$$= -3353$ kJ

Next, let us look at the relationship between $\Delta H$ and the number of moles of reactant.

**Sample Problem 22:** “What will $\Delta H$ be if I allow 225 moles of Al to react with 175 moles of $O_2$ at 25ºC?”

**Answer:** In the previous example, we found that $\Delta H = -3353$ kJ for the reaction:

$$4 \text{ Al}(s) + 3 \text{ O}_2(g) \rightarrow 2 \text{ Al}_2\text{O}_3(s)$$

However, the answer to this question is not $-3353$ kJ, because this $\Delta H$ value specifically applies to the reaction of 4 moles of aluminum with 3 moles of oxygen (check the balanced equation).

To find $\Delta H$ for a different number of moles of reactant, we must first determine the limiting reactant. In this problem, the limiting reactant is Al, since 225 moles of Al reacts with
only 168.75 moles of O₂ (using the 4:3 mole ratio from the balanced equation). As we saw when we examined ΔE, we must then use the limiting reactant in our direct proportion:

\[
\frac{\Delta H}{225 \text{ mol Al}} = \frac{-3353 \text{ kJ}}{4 \text{ mol Al}}
\]

\[\Delta H = -1.89 \times 10^5 \text{ kJ}\]

(If you’re curious, this is enough energy to lift a 2000 pound car about 13 miles into the air.)

The enthalpy of a reaction can be divided up between heat and useful work. Here is an example of this:

**Sample Problem 23:** “225 moles of Al reacts with excess oxygen in a battery. The battery is connected to a motor, which does 150000 kJ of useful work. How much heat is given off?”

**Answer:** We have already determined that \(\Delta H = -1.89 \times 10^5 \text{ kJ}\) for the reaction of 225 moles of aluminum with excess oxygen. This means that the total of the heat given off and the useful work done by the reaction will equal 189000 kilojoules. (All three of these quantities will be negative numbers.) In this example, \(w_{\text{useful}} = -150000 \text{ kJ}\), so...

\[
\Delta H = q + w_{\text{useful}}
\]

\[-189000 \text{ kJ} = q + (-150000 \text{ kJ})
\]

\[q = -39000 \text{ kJ}\]

The battery will give off 39000 kilojoules of heat. Note that we made the assumption that the battery was operating at constant pressure: this is a safe assumption unless the problem specifically states otherwise.

Here is a pair of examples that explore the difference between open (constant-pressure) and closed (constant-volume) systems.

**Sample Problem 24:** “For the reaction below, \(\Delta H = -1532 \text{ kJ}\):

\[
4 \text{ NH}_3(g) + 3 \text{ O}_2(g) \rightarrow 2 \text{ N}_2(g) + 6 \text{ H}_2\text{O}(l)
\]

How much heat will be given off when 0.124 moles of ammonia reacts with oxygen in an open container at 25°C?”

**Answer:** We need to make an initial assumption that no useful work is done. This is always a safe assumption if you are not told explicitly that “X joules of useful work is done” or something similar. Reactions do not do useful work unless you carry them out in some sort of machine (a combustion engine, a battery that is connected to a motor, etc.).

In an open container, the pressure will be constant, so the heat of the reaction will equal \(\Delta H\). As in the previous example, we must set up a direct proportion to correct the number of moles, since we are given \(\Delta H\) for 4 moles of NH₃ (look at the balanced equation), but we are asked for the heat when we use 0.124 moles of NH₃.
\[
\frac{\Delta H}{0.124 \text{ mol NH}_3} = -1532 \text{ kJ} \quad \frac{4 \text{ mol NH}_3}{\Delta H}
\]

\[
\Delta H = -47.5 \text{ kJ}
\]

The reaction is carried out at constant pressure, so \( q = \Delta H = -47.5 \text{ kJ} \). We can say that 47.5 kJ of heat will be given off.

**Sample Problem 25:** “For the reaction below, \( \Delta H = -1532 \text{ kJ} \):

\[
4 \text{ NH}_3(g) + 3 \text{ O}_2(g) \rightarrow 2 \text{ N}_2(g) + 6 \text{ H}_2\text{O}(l)
\]

How much heat will be given off when 0.124 moles of ammonia reacts with oxygen in a sealed, rigid container at 25ºC?”

**Answer:** This problem looks very similar to the previous one, but now we have a constant volume (rather than constant pressure). Under constant-volume conditions, no “useless work” is done, since the gases cannot expand or contract. We assume (as we did in the previous example) that no useful work is done. Therefore, \( w = 0 \) and \( q = \Delta E \), which in turn means that we will need to convert \( \Delta H \) (the useful energy, which was given to us) to \( \Delta E \) (the total energy available from the reaction). This would seem to be straightforward, since we have a formula that does exactly what we want: \( \Delta H = \Delta E + RT\Delta n_{\text{gases}} \).

Unfortunately, life is not so simple. The \( \Delta H \) value we were given (and the \( \Delta E \) value we can calculate from it) are the energy we get when 4 moles of ammonia reacts with oxygen: the balanced equation says “4 NH\(_3\)”’. However, the problem asks us for the heat when 0.124 moles of ammonia reacts with oxygen. Neither the \( \Delta H \) value we were given nor the \( \Delta n_{\text{gases}} \) value we would get from the balanced equation will apply to this situation. However, we can still solve the problem if we are very careful about our system. Here are the two possible strategies we could use:

**Strategy #1:**
1) Convert \( \Delta H \) (for 4 moles of NH\(_3\)) to \( \Delta E \) (for 4 moles of NH\(_3\)), using the fact that \( \Delta H = \Delta E + RT\Delta n_{\text{gases}} \). In this case, \( \Delta n_{\text{gases}} \) can be obtained directly from the balanced equation: \( 2 - 7 = -5 \) moles (remember that the water is a liquid).
2) Use a direct proportion to calculate \( \Delta E \) for 0.124 moles of ammonia.

**Strategy #2:**
1) Use a direct proportion to calculate \( \Delta H \) for 0.124 moles of ammonia (starting with the \( \Delta H \) for 4 moles of ammonia).
2) Use stoichiometry to calculate the correct value of \( \Delta n_{\text{gases}} \) when we only use 0.124 moles of ammonia.
3) Use \( \Delta H = \Delta E + RT\Delta n_{\text{gases}} \) to calculate \( \Delta E \) for 0.124 moles of ammonia.

Strategy #1 is easier to use (since it involves only two calculations), so that’s the method we’ll use here.
Step 1: converting $\Delta H$ to $\Delta E$, based on 4 moles of ammonia…

$$\Delta H = \Delta E + RT\Delta n_{\text{gases}}$$

$$-1532 \text{ kJ} = \Delta E + (8.314 \text{ J/mol} \cdot \text{K})(298 \text{ K})(-5 \text{ mol})$$

$$-1532 \text{ kJ} = \Delta E - 12388 \text{ J}$$

(Be sure to reconcile the energy units!)

$$-1532 \text{ kJ} = \Delta E - 12.4 \text{ kJ}$$

$$\Delta E = -1519.6 \text{ kJ}$$

(This value is only good to the ones place, but we need not round it off yet, since this is not our final answer.)

Step 2: calculating $\Delta E$ for 0.124 moles of ammonia…

$$\frac{\Delta E}{0.124 \text{ mol NH}_3} = \frac{-1519.6 \text{ kJ}}{4 \text{ mol NH}_3}$$

$$\Delta E = -47.1 \text{ kJ}$$

As explained above, $\Delta E = q$ under these conditions (constant volume), so $q = -47.1 \text{ kJ}$. Since the question asked “how much heat will be given off…”, you should say “47.1 kJ of heat will be given off.” You do not need the negative sign, since you said that the heat was given off. (However, if the question asked “what is q?”), you would need to include the sign.

It is useful to look at two sets of numbers in this example: the values of $\Delta H$, $\Delta E$ and $\Delta n$ for the reaction of 4 moles of ammonia and 0.124 moles of ammonia.

<table>
<thead>
<tr>
<th></th>
<th>4 moles of NH₃</th>
<th>0.124 moles of NH₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta H$</td>
<td>-1532 kJ</td>
<td>-1520 kJ</td>
</tr>
<tr>
<td>$\Delta E$</td>
<td>-1520 kJ</td>
<td>-47.5 kJ</td>
</tr>
<tr>
<td>$\Delta n_{\text{gases}}$</td>
<td>-5 mol</td>
<td>-0.155 mol</td>
</tr>
</tbody>
</table>

Each set of values is internally consistent: in each column, $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$ (try it yourself!). Also, in every case you can get from the “4 moles” column to the “0.124 moles” column by setting up a direct proportion. For $\Delta n_{\text{gases}}$, the proportion would look like this:

$$\frac{\Delta n_{\text{gases}}}{0.124 \text{ mol NH}_3} = \frac{-5 \text{ mol gases}}{4 \text{ mol NH}_3}$$

$$\Delta n_{\text{gases}} = -0.155 \text{ mol}$$
You can use this technique yourself to calculate the $\Delta n_{\text{gases}}$ value for any problem (if you want to use strategy #2 above), but it usually isn’t worth the trouble. You can also calculate $\Delta n_{\text{gases}}$ using stoichiometry: you know how many moles of NH$_3$ are used up (0.124 moles) and you have the balanced equation….

**Sample Problem 26:** “When 5.000 grams of iron reacts with oxygen to produce solid Fe$_2$O$_3$ in an open container, 36.97 kJ of heat is given off. How much heat would be given off if 5.000 grams of iron were to react with oxygen in a closed, rigid container? The temperature is 25ºC in both cases.”

**Answer:** Let us spend a moment piecing together the information we are given.

1) The first reaction is carried out in an open container, which means that the pressure is constant. Under these conditions, the heat given off will equal $\Delta H$, so in the first reaction, $\Delta H = -36.97$ kJ.

2) The second reaction is carried out in a closed, rigid container, which means that the volume is constant. Under these conditions, the heat given off will equal $\Delta E$.

3) The reaction involves Fe combining with O$_2$ to form Fe$_2$O$_3$. Iron (Fe) is a solid at 25ºC, and oxygen is a diatomic gas (O$_2$). The balanced equation for this reaction is therefore:

$$4 \text{ Fe(s)} + 3 \text{ O}_2(\text{g}) \rightarrow 2 \text{ Fe}_2\text{O}_3(\text{s})$$

4) In both reactions, we are starting with 5.000 grams of Fe: converting this to moles gives 0.089526 mol Fe.

A reasonable strategy would be to convert $\Delta H$ (which we are given) to $\Delta E$ using the relationship $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$. However, we must be very careful to get the correct $\Delta n_{\text{gases}}$. When 4 moles of Fe react, $\Delta n_{\text{gases}} = -3$ mol (from the balanced equation). What about when we use 0.089526 moles of Fe? We can set up a direct proportion:

$$\frac{\Delta n_{\text{gases}}}{0.089526 \text{ mol Fe}} = \frac{-3 \text{ mol gases}}{4 \text{ mol Fe}}$$

$$\Delta n_{\text{gases}} = -0.067144 \text{ mol}$$

(You can also do this using normal stoichiometry. The choice is yours.)

Now, let us apply our magic formula:

$$\Delta H = \Delta E + RT\Delta n_{\text{gases}}$$

$$-36.97 \text{ kJ} = \Delta E + (8.314 \text{ J/mol} \cdot \text{K})(298 \text{ K})(-0.067144 \text{ mol})$$

$$-36.97 \text{ kJ} = \Delta E - 166 \text{ J}$$

$$-36.97 \text{ kJ} = \Delta E - 0.166 \text{ kJ}$$

$$\Delta E = -36.81 \text{ kJ}$$

Since $\Delta E = q$, **36.81 kJ of heat will be given off.**
Once again, to illustrate the importance of keeping track of the amount of chemical, here is a table illustrating the values of $\Delta H$, $\Delta E$ and $\Delta n_{\text{gases}}$ for the reaction of 4 moles of Fe versus 0.089526 moles of Fe. All of the values in the middle column are calculated from the values in the right-hand column by setting up a direct proportion.

<table>
<thead>
<tr>
<th></th>
<th>4 moles of Fe</th>
<th>0.089526 moles of Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta H$</td>
<td>$-1652 \text{ kJ}$</td>
<td>$-36.97 \text{ kJ}$</td>
</tr>
<tr>
<td>$\Delta E$</td>
<td>$-1645 \text{ kJ}$</td>
<td>$-36.81 \text{ kJ}$</td>
</tr>
<tr>
<td>$\Delta n_{\text{gases}}$</td>
<td>$-3 \text{ mol}$</td>
<td>$-0.06714 \text{ mol}$</td>
</tr>
</tbody>
</table>

Once again, each set of values is internally consistent: $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$ is satisfied. Whenever you interconvert $\Delta H$ and $\Delta E$, ask yourself: “how many moles of reactants does my value of $\Delta H$ or $\Delta E$ apply to? and does my value of $\Delta n_{\text{gases}}$ agree with this?”