Conservation of energy and combustion

Consider H<sub>2</sub> reacting with O<sub>2</sub> in a steady-state reaction chamber, resulting in heat transfer out of the system. All inlets and exits are maintained at standard temperature and pressure,  $T_0$  and  $P_0$ . The reaction produces 1 kmol/s of H<sub>2</sub>O using stoichiometric flow rates of H<sub>2</sub> and O<sub>2</sub>:



## $H_2$ + $\frac{1}{2}$ $O_2$ → $H_2O$

Write conservation of energy for the process. Will you use a mass-based specific enthalpy or a mole-based specific enthalpy? Why?

We have different chemical species entering and leaving the chamber. This poses a problem concerning a reference state for specific enthalpy. And so, let us choose  $T_0$  and  $P_0$  to be the reference state where all species have zero enthalpy. But wait, what just happened to conservation of energy? We know from experience that reacting hydrogen with oxygen produces large rates of heat transfer. The problem is that our standard thermodynamic conservation of energy equation only tracks internal energy, kinetic energy, and gravitational potential energy. In systems involving chemical reactions, chemical energy (stored in chemical bonds) is also involved. We can fix this by adding specific chemical energy (energy per unit mass or mole) to the mass flow terms:

Though it is called an enthalpy, it actually represents the chemical energy stored in a chemical species. Think of it as a *chemical* enthalpy if you like. We'll call the normal, everyday enthalpy a *thermodynamic* enthalpy. If we add the two together to get a total, thermochemical enthalpy, we have

Remember how we said we wanted specific enthalpy to be zero for any chemical species at  $T_0$  and  $P_0$ ? We really want the *thermodynamic* enthalpy part to be zero. If we're at some T and P other than  $T_0$  and  $P_0$  we can make this work by subtracting the value for h at  $T_0$  and  $P_0$  from the value of h:

If we now use the total thermochemical enthalpy in our conservation of energy equation it will work in cases involving chemical reactions too!

But there is still a problem. We need information on any chemical reaction we can dream up, which is a big pain in the behonkus. As a way around this, we give a special name to chemical enthalpy of compounds formed at  $T_0$  and  $P_0$  with stoichiometric amounts of re-

actant	 	And
that is		

$$\Delta h_f^0 =$$

Lastly, we can catalog pretty much any chemical reaction happening with any reactants forming any products at any temperature/pressure by pretending like it happens as follows.





And so for any one species, reactant or product

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h =
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