

## 16.50 Lecture 10

### Subjects: Models for rocket engines; Flow of reacting gases

#### Models for Rocket Engines

In Lecture 6 we described in general terms a set of models we might use to describe the various features of rocket engines, making the point that no one model incorporates all the features. The models we have discussed thus far are:

##### Model 1;

$$\frac{c^2}{2} = c_p T_c$$

which simply equates the kinetic energy of the exhaust to the thermal energy in the chamber, ignoring all questions of efficiency and gas dynamics.

Model 2; which describes the nozzle flow for  $c_p$  and  $\gamma$  constant, enabling an approximate description of the effects of the pressure expansion ratio and of the gas properties. This resulted in the definitions of the Thrust Coefficient  $c_F$ , and Characteristic Velocity  $c^*$ , which are applicable for more general situations than this model represents. The model in turn gave us approximate formulae for estimating  $c_F$  and  $c^*$  for particular nozzle geometries and propellants.

Model 3, which describes the behavior of the flow in terms of the actual geometry of the nozzle, but within the simplification of ideal gas behavior.

Model 4, which dealt with Solid Propellant Internal Ballistics. This models the gas formation process for solid rockets, combined with the most important fluid mechanical phenomena governing the burning rate and stability.

In all of these models, the properties of the gases in the combustion chamber were taken as given. It should be clear by now that this is a key issue in understanding rocket engines. So we need a model that connects the properties of the gases in the chamber to the propellant characteristics, i.e. a model that describes the combustion process. This set of processes we term Combustion Thermochemistry. We will treat it as Model 5.

#### Model 5 - Combustion Thermochemistry

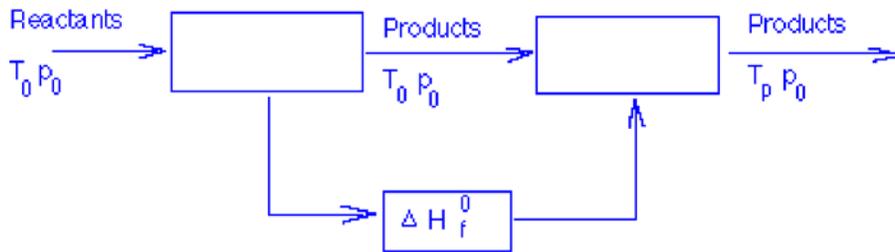
In this model we want to represent what happens in the combustor, to convert liquid propellants (one or two) to hot gases at  $T_c$  and  $p_c$ . Qualitatively, what happens is that the difference between the chemical energies of the reactants (the chemicals injected into the combustion chamber) and that of the reaction products (the hot gases we seek to describe) shows up as thermal energy of the latter. To describe this quantitatively it is helpful to show it as a sequence of two steady flow processes. The first is the formation by chemical reactions of the products from the reactants at standard temperature and pressure. Of course such a process cannot happen in an isolated reactor, but we can think of it as a process in

which the reactions occur at standard temperature and pressure while heat is added or removed in the amount necessary to keep the temperature constant, and the volume is expanded or contracted as needed to maintain the pressure constant as well. The heat added in such an ideal process is defined as the Standard Heat of Formation  $\Delta H_f^0$  of the products if the reactants are the elements in their standard states.

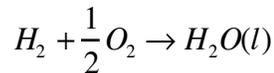
The second step involves using the heat added in the first step to change the temperature of the products. The temperature change is then given by the Steady Flow Energy Equation as

$$h(T_p, p_0) - h(T_0, p_0) = -\Delta H_f^0$$

where the products are indicated by the subscript p and the reactants by the subscript 0, but note that the pressure is the same in both states.



Every chemical substance has a Standard Heat of Formation defined in this way. For example for water,



$$\Delta H_{f, H_2O(l)}^0 = -68.3174 \text{ kcal / mole}$$

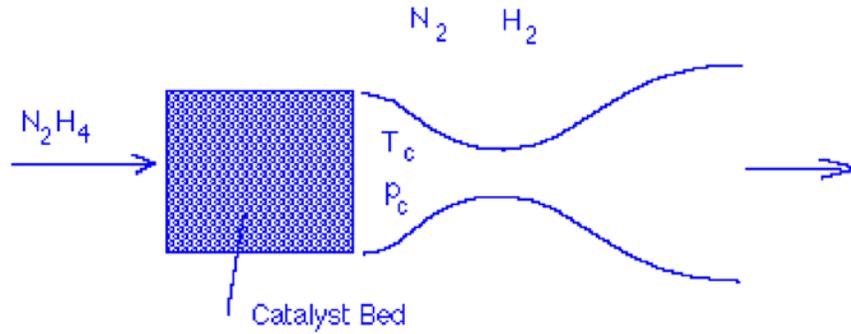
The rather cumbersome notation is necessary to indicate that the reaction product in this case is liquid water. The heat of formation of gaseous water would differ from this by the heat of vaporization.

Note that the heat of formation of water is negative, so that heat is released in its formation. The convention that heat added is positive is purely arbitrary.

From the definition of the heat of formation, it is zero for the elements in their standard states.

In general one should remember that substances that are stable at normal temperature and pressure have negative heats of formation, those that are unstable (explosives) have positive heats of formation.

As a simple example of the application of these ideas to rocket engines, consider a monopropellant rocket engine using Hydrazine,  $N_2H_4$ :

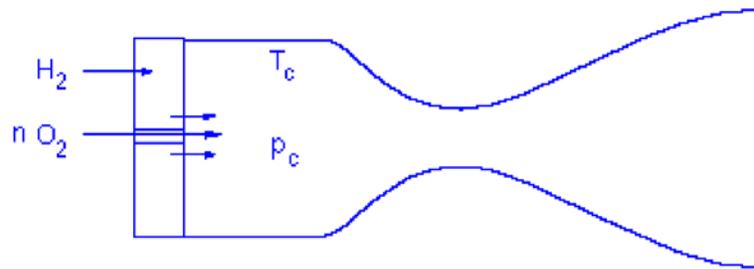


This substance has physical properties much like those of water, but has a positive Standard Heat of Formation of 50.6 kJ/ mole. If we assume for now that it decomposes to produce N<sub>2</sub> and H<sub>2</sub>, and the enthalpy of each can be approximated by c<sub>p</sub>T, then the chamber temperature is given by

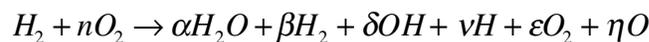
$$[c_{pN_2} + 2c_{pH_2}](T_c - T_0) = \Delta H_{f,N_2H_4}^0$$

where the specific heats are per mole if the heat of formation is as well. In this argument we have assumed that the products of combustion are nitrogen and hydrogen. In general there might be some ammonia and perhaps other compounds in the decomposition products of hydrazine. We will see how to deal with this in the following discussion. For a first-cut estimate, say both N<sub>2</sub> and H<sub>2</sub> behave as ideal diatomic molecules with  $\gamma=1.4$ , so that, for each of them,  $c_p = \gamma/(\gamma-1)\mathcal{R} = 1.4/0.4 * 8.314 = 29.1$  J/mole/K. We then obtain  $T_c - T_0 = 580$ K, and if  $T_0 = 298$ K,  $T_c = 878$ K.

Now let us extend the argument to the somewhat more complex situation of a H<sub>2</sub> - O<sub>2</sub> liquid bipropellant rocket



To avoid some complexity, we assume that the hydrogen and oxygen are gases, at 298.16°K. They react to form products according to



Here n is set by the mix of propellants injected, but the coefficients on the right side are to be determined. We regard p<sub>c</sub> as given for this discussion. Actually it is set by the nozzle throat area for specified mass flows of hydrogen and oxygen, which in turn are determined by the pressure differential across their injector orifices, and the total orifice areas. So we have to find T<sub>c</sub> and the values of  $\alpha, \beta, \delta, \nu, \epsilon, \eta$  for given n.

To find  $\alpha, \beta, \delta, \nu, \varepsilon, \eta$  (6 unknowns), we first note that the total moles of hydrogen and oxygen atoms must be equal on the right and left. In general we must have Conservation of Atomic Species

$$H: 2\alpha + 2\beta + \delta + \nu = 2 \quad (1)$$

$$O: \alpha + \delta + 2\varepsilon + \eta = 2n \quad (2)$$

If the reaction products are in Chemical Equilibrium (as we shall assume) the other four relations needed to find the six unknowns are provided by the Law of Mass Action, which provides a set of relationships between the pressure of each of the compounds which is not an element and the pressures of its elementary constituents. These expressions take the form of Equilibrium Constants defined through the stoichiometric relationship for formation of each of the compounds:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad K_{p_{H_2O}}(T_c) = \frac{P_{H_2O}}{P_{H_2}(P_{O_2})^{\frac{1}{2}}} \quad (3)$$

$$H_2 \rightarrow 2H \quad K_{p_H}(T_c) = \frac{P_H^2}{P_{H_2}} \quad (4)$$

$$H_2 + O_2 \rightarrow 2OH \quad K_{p_{OH}}(T_c) = \frac{P_{OH}^2}{P_{H_2}P_{O_2}} \quad (5)$$

$$O_2 \rightarrow 2O \quad K_{p_O}(T_c) = \frac{P_O^2}{P_{O_2}} \quad (6)$$

The actual choice of reactions to be “equilibrated” is arbitrary, as long as the chosen set can be used to generate by linear combinations any of the included species out of the “major” expected product species. In our case we mainly expect to see  $H_2O$  and, since the mixture is purposely fuel-rich ( $n < 1/2$ ), excess hydrogen in the form of  $H_2$ . It is a good practice to select reactions in which only one of the “minor” species appears, so as to facilitate iteration starting with the majors only. In the set above, this is true of all but reaction (5), in which two “minors” ( $O_2, OH$ ) appear. We can replace (5) by the result of eliminating  $O_2$  between (3) and (5), namely

$$H_2 + 2OH \rightarrow 2H_2O \quad \frac{K_{p_{H_2O}}^2}{K_{p_{OH}}} = \frac{P_{H_2O}^2}{P_{H_2}P_{OH}} \quad (5')$$

As indicated by the functional expression, the K's are dependent only on the temperature. This can be shown fairly readily by general thermodynamic arguments. Because of the wide latitude in selecting the set of reactions to equilibrate, Standard thermodynamic tables do not list all possible  $K_p(T)$ , but they do list the basic quantities from which they can be calculated, namely, the “Standard Chemical Potentials”,  $\mu_i^0(T)$  (molar Gibbs Free Energies at 1 atm.

partial pressure), or the Standard Entropies,  $s_i^0(T)$ , also at 1 atm. pressure. For example, the equilibrium constant for reaction (3) above is calculated as

$$K_{p_{H_2O}} = \exp\left[-\frac{\mu_{H_2O}^0 - \mu_{H_2}^0 - \frac{1}{2}\mu_{O_2}^0}{RT}\right]$$

where each of the chemical potentials is read from the tables for the given T. If the standard molar entropies are listed instead, we can calculate first each of the standard chemical potentials as  $\mu_i^0(T) = h_i(T) - T s_i^0(T)$ , where  $h_i$  is the molar enthalpy.

Returning to Eqs. (3)-(6), each of the p's can be written in terms of  $\alpha, \beta$ , etc, if  $p_c$  is set.

Thus if  $\sigma \equiv \alpha + \beta + \delta + \nu + \varepsilon + \eta$  then by Dalton's Law of Partial Pressures,

$$p_{H_2O} = \frac{\alpha}{\sigma} p_c \quad p_{H_2} = \frac{\beta}{\sigma} p_c \dots p_{OH} = \frac{\delta}{\sigma} p_c \quad p_H = \frac{\nu}{\sigma} p_c \quad p_{O_2} = \frac{\varepsilon}{\sigma} p_c \quad p_O = \frac{\eta}{\sigma} p_c$$

We will continue this discussion in the next lecture.

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