16.50 Lecture 12

Subject: Nozzle flow of reacting gases

In the last two lectures we discussed the phenomena that occur in the combustor, and how to estimate the properties of the gas in the (near) stagnation state there. Suppose now that we have determined the composition of the gases in the rocket chamber, and we wish to compute the flow through the nozzle, <u>taking account of chemical reactions</u>.

There are three things that we must account for, that were not included in the simple model based on ideal gas behavior. The first is that the composition of the gas is not necessarily constant in the flow, so that all the properties that are composition dependent must be treated as variables along the flow direction. These include the specific heats, the gas constant R and the ratio of specific heats γ. Second, the sum of the thermal enthalpy and the kinetic energy is no longer constant because there can be exchange of chemical energy and thermal energy. But if the enthalpy is defined as in the previous two lectures, i.e., including in it the chemical enthalpy of formation, then the sum of it and the kinetic energy is indeed conserved. Finally, because of this energy exchange between chemical and kinetic, there can be a change in the entropy of the flow. Fortunately we can neglect this entropy change in some important special cases, as will be explained.

To take these effects into account quantitatively we may proceed as follows:

The chamber condition is specified by T_c, p_c and the mole (y_i), or mass (x_i), fractions of the various chemical constituents. As explained in the last two lectures we can compute all the thermodynamics properties of the gas per unit mass at chamber conditions:

$$H_c = \sum x_i H_i \quad ; \quad H_i = (\Delta h_i(T_c) + H^{\circ}_{f\,i})/M_i$$

$$S_c = \sum x_i S_i \qquad S_i = \int_{T_r}^{T} c_{pi} \frac{dT}{T} - R_i \ln \frac{p_i}{p_r} \qquad \text{(S}_i, \text{ c}_{pi} \text{ per unit mass)}$$

where it will be recalled that x_i is the mass fraction of species i and therefore
$$\sum x_i = 1$$
Notice also that each enthalpy H_i is now <u>per unit mass</u>, and so is H_c.

To deal with the flow we note first that energy conservation for the gas flow gives

$$H_c = H(T,p) + \frac{u^2}{2} \tag{1}$$

which replaces the ideal gas energy equation
$$(c_p T_c = c_p T + \frac{u^2}{2})$$

We must have some statement about the variation of the entropy, since in general the transfer of energy from chemical to thermal takes place at a finite rate and there is therefore an entropy increase.

But there are two limiting cases for which the entropy change is very small

      a)   chemical equilibrium
      b)   frozen flow

The case of Chemical Equilibrium will be approached if the reactions occur fast enough to keep up with the temperature and pressure changes caused by the expansion (flow time $\gg$ reaction time), so the chemical energy is transferred through an infinitesimal ΔT, and

$$S = \sum x_i(p,T)S_i(p,T) = S_c \qquad (2e)$$

and the x_i are determined by Equilibrium at the local T & p. Re-calculating all these mass fractions is clearly a tedious task, but conceptually not very different from what was done for the chamber conditions, with the major difference that Entropy per unit mass, rather than Enthalpy per unit mass is now constrained.

In the case of Frozen Flow the reactions occur so slowly that the x_i are fixed at their chamber values (flow time $\ll$ reaction time). In this case there is no chemical energy release and again

$$S = \sum x_i(p_c,T_c)S_i(p,T) = S_c \qquad (2f)$$

These are two limiting cases, which provide upper and lower limits for the velocity u, at a given p, since the case of Equilibrium Flow gives the maximum thermal energy availability for conversion to kinetic energy, while the Frozen Flow case gives the minimum.

In these calculations, the entropy per unit mass S_i of one species at (p,T) is related to that per mol, $S_i(p,T) = \tilde{S}_i(p,T)/M_i$, and this can be calculated from tabulated "standard molar entropies", which are at p=1atm, as

$$\tilde{S}_i(p,T) = \tilde{S}_i^{\,0}(T) - \Re\ln(p_i(atm)); \qquad p_i = py_i \qquad (2g)$$

It is important to note that the conservation laws for both energy and entropy are per unit mass. Thus it is the total energy and the entropy of a fixed mass of gas that is conserved. At times it will be convenient to write the relations in terms of moles of the constituents (using y_i rather than x_i) but a fixed mass of gas may contain different numbers of moles at different points in the flow, so if we use the y_i we must be careful to keep track of the changes in the number of moles.

To go from mole fractions to mass fractions or vice-versa,

$$x_i = \frac{y_i M_i}{\sum y_i M_i}; \qquad y_i = \frac{x_i / M_i}{\sum x_i / M_i}$$

For example for a mixture of $H_2 + H_2O$

$$y_{H_2} = \frac{1}{2}, \quad y_{H_2O} = \frac{1}{2}$$

$$x_{H_2} = \frac{\frac{1}{2}(2)}{\frac{1}{2}(2) + \frac{1}{2}(18)} = \frac{1}{10}$$

$$x_{H_2O} = \frac{\frac{1}{2}(18)}{\frac{1}{2}(2) + \frac{1}{2}(18)} = \frac{9}{10}$$

The above are all the relationships we need, so let us see how we proceed, for given chamber conditions, p_c and T_c.

a) Compute $\quad x_i (p_c, T_c)$
$\qquad\qquad\qquad H_c$
$\qquad\qquad\qquad S_c$

b) Select a value of $p < p_c$. <u>We can treat p as the independent variable</u>, finding all the other properties as functions of it. If we wish to find the conditions at the nozzle exit then the pressure is the exit pressure, $p = p_e.$

c) From the Entropy equation (2e or 2f), find T

(This replaces $\dfrac{T}{T_c} = (\dfrac{p}{p_c})^{\frac{r-1}{\gamma}}$ of the Ideal Gas model)

1) For Frozen Flow, since $x_i (p, T) = x_i (p_c, T_c)$ are known, Eqs. (2f) and (2g) contain only T as an unknown, and can be solved iteratively at each p (this replaces the enthalpy conservation iteration we did in the chamber).

2) For Equilibrium Flow, we still have $s = s_c$, but now we don't know the x_i, so we have to solve for them at each p, as noted above.
   - A. <u>Assume a T</u>
   - B. Compute the y_i (and x_i) from $K_{p_i}(T)$
   - C. Compute $S(T,p)$ and <u>Iterate on T</u> until it equals $S_c(T_c, p_c)$.

d) In either Fozen or Equilibrium cases, having T and $x_i(T,p)$ compute $H(T,p)$, then the velocity is given by

$$\frac{u^2}{2} = H_c - H(T,p)$$

These procedures enable you to describe the flow in the nozzle with p as the independent variable. Having u, p, T we can find ρ and hence ρu and the variation of the nozzle area with p. In particular, to find the throat area we can compute ρu for a set of values of p near $(1/2)p_c$ and by plotting them determine the p that maximizes ρu. This is the throat pressure, and the maximum value of ρu defines $c^* = p_c / (\rho u)_t$

Normally, of course, such calculations are handled by standardized computer programs. They all follow the logic outline above although the numerical procedures may become quite complex because of considerations of stability etc. You don't need to know all the details, but it is important that you understand the logic they follow. As we say, Garbage In-Garbage Out. Be sure you know what the computer is doing.

A very widely used suite of codes for thermochemical problems in aerospace is the CEA set, available at http://cearun.grc.nasa.gov.

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