

16.512, Rocket Propulsion
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Lecture 14: Non-Equilibrium Flows

Reacting Nozzle Flow

14.1 Introduction

As indicated in the introductory discussion of section 12.1, the actual expansion process in a rocket or ramjet nozzle is intermediate between the extremes of “frozen” and “equilibrium” flow, with the latter producing higher performance due to recovery of some of the chemical energy tied up in the decomposition of complex molecular species in the chamber - a kind of afterburning effect.

The two limits, “frozen” and “equilibrium” flow share an important property: both are isentropic flows (if we ignore friction or heat losses). This is because, in the frozen case no chemical change during expansion), there are no rate processes at all occurring, the molecules preserving their identity all the way, while in the equilibrium case, in which reactions do occur, their rate is so high (compared to the expansion rate) that conditions adjust continuously to maintain equilibrium at the local pressure and enthalpy level, with the result that the whole process can be regarded as reversible (and hence isentropic). For any more realistic intermediate conditions, in which reactions may proceed at rates comparable to that of the expansion, these finite rate reactions produce an irreversibility, and a consequent entropy increase.

In this Section we will discuss in detail an example of each, frozen and equilibrium expansion. We will use for this purpose the results of the equilibrium chamber calculations of Sec. 13.1, relative to the space Shuttle Main Engine.

14.2 Frozen Flow Calculation

The simple ideal gas model we have used throughout most of this course (constant molecular mass, constant specific heats) is an example of a frozen flow model, since it is implied by these assumptions that no chemical change takes place. Thus all of our “constant γ ” results belong in this category, and can be used as a first approximation for nozzle flow calculations (using for instance the value of γ and M computed for the combustor). However, even with no chemical changes, the specific heats of the various molecules do change with temperature, generally decreasing as temperature decreases in the range encountered in nozzles. This means that $\gamma = C_p/C_v = C_p/(C_p - R_g)$ is not a constant, since R_g , the gas constant, does not vary due to the constancy of the molecular mass.

For a more precise calculation, we make use of the constant-entropy condition for frozen flow. Suppose, for instance that the nozzle exit pressure is specified. This pressure, together with the chamber entropy are enough to determine all other thermodynamic variables of the frozen gas at the exit plane, in particular its enthalpy h_e per unit mass. Since the chamber enthalpy h_o is already known, we can find the exit velocity by the steady-state energy equation:

$$h_0 = h_e + \frac{1}{2} u_e^2$$

$$u_e = \sqrt{2(h_0 - h_e)} \quad (14.1)$$

The process by which h is found once P and S are given depends on the data available. Tables or graphs (Mollier charts) are the simplest method, but these are unlikely to exist for the particular composition of interest. More fundamentally, one can repeat the steps at the end of Sec. 13.1, when S was calculated after the gas composition was converged upon. In this case, the composition (i.e., x_{H_2} , x_H , x_{OH} , etc) is fixed throughout ("frozen"), and for each P , we will try various temperatures until S , the entropy, equals the chamber value.

In addition to the exit conditions, it is usually of interest to calculate the throat conditions, since it is the throat area that determines the mass flow rate. Two alternative procedures can be followed for this:

- Try a range of pressures about 1/2 the chamber pressure, calculate the corresponding $u = \sqrt{2(h_0 - h)}$ and density ρ , and look for a maximum of ρu . This occurs at the throat.
- For the same P range, calculate the local speed of sound, find where it is equal to the local velocity u . The local speed of sound is given in general by

$$a = \sqrt{\frac{\partial P}{(\partial \rho)_s}} \quad (14.2)$$

and for frozen flow this can be shown to have the familiar form

$$a = \sqrt{\gamma R_g T} \quad (14.3)$$

Conditional Throat : $A = \frac{1}{\rho u}$, $u = \sqrt{2(h_c - h)}$

$$\frac{dA}{A} = -\frac{d\rho}{\rho} - \frac{du}{u} = 0 \text{ at throat}$$

$$\frac{du}{u_t} = -\frac{1}{2} \frac{dh}{h_c - h_t} \xrightarrow{S = \text{const.}} = -\frac{1}{2} \frac{\frac{1}{\rho_t} d\rho}{h_c - h_t} = -\frac{d\rho}{\rho_t u_t^2}$$

So,
$$\frac{d\rho}{\rho_t} = -\frac{du}{u_t} = \frac{d\rho}{\rho_t u_t^2} \qquad \frac{dp}{d\rho} = u_t^2 \rightarrow \frac{u_t}{\sqrt{\left(\frac{\partial P}{\partial \rho}\right)_s}} = 1 \quad M_t = 1$$

(both, equil. and frozen)

Frozen and Equil. Speed of Sound

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_s \qquad c_p dT = \mathcal{I}ds + \frac{1}{\rho} d\rho = \frac{R_s T}{\rho} d\rho$$

and $\frac{P}{\rho} = R_g T$

Frozen: $R_g = \text{const} \qquad \frac{dp}{p} - \frac{d\rho}{\rho} = \frac{dT}{T}$

$$C_p \mathcal{I} \left(\frac{dP}{P} - \frac{d\rho}{\rho} \right) = \frac{R_g \mathcal{I}}{P} dP \qquad \underbrace{(-R_g + C_p)}_{C_v} \frac{dp}{p} = C_p \frac{d\rho}{\rho}$$

$$\left(\frac{dp}{d\rho}\right)_s = \frac{C_p P}{C_v \rho} = \gamma R_g T \quad \rightarrow \quad \left[a^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \gamma(T) R_g T \right]$$

\uparrow
 $\gamma(T)$

Equil. : $R_g = \frac{R}{M} \qquad \frac{dp}{p} - \frac{d\rho}{\rho} + \frac{dM}{M} = \frac{dT}{T}$

$$C_p \mathcal{I} \left(\frac{dp}{p} - \frac{d\rho}{\rho} + \frac{dM}{M} \right) = \frac{R_g \mathcal{I}}{p} dp$$

$$C_v \frac{dp}{p} = C_p \left(\frac{d\rho}{\rho} - \frac{dM}{M} \right)$$

$$\left(\frac{dp}{d\rho}\right)_s = \gamma(T) \frac{P}{\rho} \left(1 - \frac{\rho}{M} \frac{dM}{d\rho}\right)$$

In equil., during expansion $M \uparrow$ (recombination)

and $\rho \downarrow$ (expansion) $\rightarrow \frac{dM}{d\rho} < 0, \quad a^2 > \gamma \frac{P}{\rho}$

where the only novelty is that γ itself is variable, and must be taken to be the local γ .

A general calculation procedure can be as follows:

- (1) Given P_0, T_0, S_0 , all x_i 's, R
- (2) Specify an exit pressure P_e
- (3) Calculate $T_0 = T(P_0, S_0; x_i)$
- (4) Calculate $h_e, \rho_e, u_e = \sqrt{2(h_0 - h_e)}$
- (5) Calculate the specific impulse. For a rocket,

$$g I_{sp} = \frac{F}{\dot{m}} = \frac{\dot{m} u_e + (P_g - P_a) A_e}{\rho_e u_e A_e} = u_e + \frac{P_g - P_a}{\rho_e u_e} \quad (14.4)$$

where P_g is the external (ambient) pressure? All the above is independent of size. If a particular thrust F is desired (or an $\dot{m} = \frac{F}{g I_{sp}}$), we must also

find the required throat area A^* :

- (6) Locate P^* using one of the procedure (a) or (b) above.
- (7) Calculate $\rho^* u^* = (\rho u)_{MAX}$, i.e., from method (a) above.

$$(8) \quad A^* = \frac{\dot{m}}{(\rho u)_{MAX}} \quad ; \quad \frac{A_g}{A^*} = \frac{(\rho u)_{MAX}}{\rho_e u_e}$$

$$(9) \quad \text{Thrust coefficient} = c_F = \frac{F}{P_0 A^*}$$

14.3 Frozen Flow example (Shuttle Main Engine)

Using a simple computer program, and starting from the chamber conditions established in Sec 13.1, the procedures above lead to the results shown in Table 14.1. We have assumed matched exit conditions throughout ($P_g = P_e$)

P_e/P_0	0.001	0.0005	0.0002
P_e (atm)	0.21	0.105	0.042
T_e (K)	998	862	707
u_e (m/sec)	4227	4320	4421
I_{sp} (sec)	431	440	451
A_e/A^*	62.9	106.3	213.0
P^* (atm)	118.6	118.6	118.6
T^* (K)	3316	3316	3316

TABLE 14.1 Frozen flow performance of nozzle, from $P_0 = 210$ atm, $T_0 = 3640$ K, (LOX – LH₂, O/F = 6).

For reference, the Shuttle nozzle has an area ratio of $A_e/A^* = 76.5$, which would give a (matched) frozen specific impulse of about 435 sec, according to Table 14.1.

If we had simply used the “constant γ ” approximation, using (from Sec. 13.1) $\gamma = 1.191$ and $M = 13.48$ g/mole, the exit velocity would have been simply:

$$u_e = \sqrt{\frac{2\gamma}{\gamma-1} \frac{R}{M} T_0 \left[1 - \left(\frac{P_e}{P_0} \right)^{\frac{\gamma-1}{\gamma}} \right]}$$

For the case of $P_e / P_0 = 0.0005$, this would have given an exit velocity = 4316 m/sec, which is quite close to the 4320 m/sec shown in Table 14.1. Thus, in this case, constant γ is a good model, but this may not be true in even higher temperature cases, like in electrically heated gases (arc-jet rockets).

14.4 Equilibrium Flow Calculation

Here we must impose at each pressure below P_0 the same equilibrium conditions that were used in Sec. 13.1, with the difference that the entropy, not the enthalpy, is now prescribed. The mole fractions (x_{H_2} , x_H , x_{OH} , etc.) are now variable along the expansion, and so are therefore the molecular mass, the specific heat and γ . The calculational difficulty resides precisely in the need to perform these repeated equilibrium calculations, but, once again, computer programs are available to ease the burden.

Otherwise, the procedure is entirely analogous to that outlined in Sec. 14.2 (steps (1) through (9)). The one noteworthy difference is that the speed of sound, if

required, cannot be calculated as the local value of $\sqrt{\gamma R_g T}$, but must be found from the basic Eq. (14.2). Also, of course, the x_i values are understood to be unknown in principle, and are, in fact results of each local equilibrium calculation.

14.5 Equilibrium Flow Example (Shuttle Main Engine)

For the same chamber conditions as in Sec. 14.3 and once again assuming matched exit conditions throughout, the results of a calculation using a simple computer program are as shown in Table 14.2:

P_e/P_0	0.001	0.0005	0.0002
P_e (atm)	0.21	0.105	0.042
T_e (K)	1216	1058	877
$(X_{H_2})_e$	0.250	0.250	0.250
$(X_{H_2O})_e$	0.750	0.750	0.750
$(X_{O_2})_e$	0	0	0
$(X_O)_e$	0	0	0
$(X_{OH})_e$	0	0	0
$(X_H)_e$	0	0	0
U_g (m/sec)	4407	4511	4626
I_{sp} (sec)	449	460	472

A_e / A^*	69.7	118.5	239.4
P^* (atm)	120.7	120.7	120.7
T^* (K)	3422	3422	3422
$(X_{H_2})^*$	0.2502	0.2502	0.2502
$(X_{H_2O})^*$	0.6968	0.6968	0.6968
$(X_{O_2})^*$	0.0015	0.0015	0.0015
$(X_O)^*$	0.0010	0.0010	0.0010
$(X_{OH})^*$	0.0282	0.0282	0.0282
$(X_H)^*$	0.0222	0.0222	0.0222

TABLE 14.2 Equilibrium flow nozzle performance
LOX-LH, O/F = 6, $P_0 = 210$ atm, $T_0 = 3640$ K.

Once again, for the Shuttle, ($A_e/A^* = 76.5$), we would obtain $I_{sp} \approx 451$ sec in this case, compared with 435 sec for the frozen flow case. If we want to find the specific impulse in vacuum rather than at the matched pressure point, we would simply add

$\frac{P_g}{\rho_g u_g g}$ (see Eq. (14.4)) and we would obtain $(I_{SP})_{vac, equil} = 465$ sec. This is indeed

quite close to the actual performance of the Shuttle main engines, indicating that equilibrium does prevail during expansion. This is a result of the high pressure and large size of these engines, and would most likely not be the case in a smaller, lower pressure engine.

In addition to the higher exit velocity in the equilibrium case, other interesting differences between the results of Tables 14.1 and 14.2 are:

- (a) The exit temperatures are higher in the equilibrium case by about 200 K (a result of the afterburning).
- (b) The exit area ratios are larger in the equilibrium case (for a given pressure ratio). This is also due to the same "reheating" effect, which produces more volume increase.

Notice, finally, that the "constant γ " approximation would still give $u_g = 4316$ m/sec for the case of $P_e/P_0 = 0.0005$; this is now well below the 4511 m/sec shown in Table 14.2 for this case. Thus, constant γ may seriously underestimate performance in large, high pressure rockets.