Lecture Notes No. 3
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FUNDAMENTAL CONCEPTS OF REAL GASDYNAMICS

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FUNDAMENTAL CONCEPTS OF GASDYNAMICS

1. THERMODYNAMICS OF GASES

We generally deal with fluids which fall into one of the five following categories: 1) constant density, incompressible fluids, 2) liquids whose density is spatially dependent, e.g. sea water, 3) barotropic gases, where the density, $\rho = \rho(p)$ only, 4) polytropic gases, where ρ is a function of two thermodynamic state variables, such as $\rho = \rho(p, s)$ or $\rho = \rho(p, T)$and 5) gases whose density depends upon two thermodynamic state variables and quantities related to the history of the flow, *e.g.*, chemical or thermodynamic non-equilibrium. Here, we will be primarily concerned with barotropic and polytropic gases.

In order to develop state relationships for barotropic and polytropic gases, we will present a brief review of the thermodynamics of gases. Our main objective is to develop an equation of state for a variety of flow conditions. Throughout our discussions we will be assuming the gas to be in thermodynamic equilibrium, and if reacting, in chemical equilibrium. In the following development, we will be considering single species gases and mixtures of gases, perfect and real gases and reacting flows in chemical equilibrium. In §1.1–1.8, we will deal primarily with single species gases. In §1.9 we will deal with mixtures of gases in general and with mixtures in chemical equilibrium in §1.10.

1.1 First and Second Laws

The *state* of a system in (local) thermodynamic equilibrium may be defined by any two *intensive* variables, such as the temperature T, the pressure, p, the specific volume $v \equiv 1/\rho$, internal energy per unit mass, e, entropy per unit mass s, *etc.* *Extensive* variables, such as the volume V, internal energy E, entropy S will also depend upon the mass M of the system.

The first law of thermodynamics may be stated that in going from state 1 to state 2, the change in internal energy per unit mass must equal the sum of the heat added per unit mass to the work done per unit mass on the system as

$$e_2 - e_1 = \int_1^2 dq + \int_1^2 dw \,. \tag{1.1}$$

The heat added to the system, $\int dq$, and the work done on the system, $\int dw$ depend upon the specific path of integration. The first law, (1.1) applies to any path. It is convenient to write this for an infinitesimal change as

$$de = dq + dw \,. \tag{1.2}$$

The second law of thermodynamics introduces the entropy, which satisfies the following inequality:

$$s_2 - s_1 \geq \int_1^2 \frac{dq}{T} \,. \tag{1.3}$$

For a *reversible* process, the equality portion of (1.3) applies, so that

$$(dq)_{rev} = Tds\,. \tag{1.4}$$

It may also be stated that if the work done on the system is done through a reversible process, then

$$(dw)_{rev} = -pdv\,. \tag{1.5}$$

Now let us consider going between the same states 1 and 2 as in (1.1), but this time by reversible processes. Then, from (1.4) and (1.5)

$$e_2 - e_1 = \int_1^2 Tds - \int_1^2 pdv\,. \tag{1.6}$$

Comparing (1.6) to (1.1), we must have

$$\int_1^2 dq + \int_1^2 dw = \int_1^2 Tds - \int_1^2 pdv\,,$$

where dq and dw correspond to heat added and work done through an arbitrary process, reversible or irreversible. This does not imply that $dq = Tds$ or $dw = -pdv$, but it does mean that $dq + dw$ must equal $Tds - pdv$. This is a consequence of e being a variable of state. Hence in general we may state that

$$de = Tds - pdv\,. \tag{1.7}$$

This relationship is valid for both reversible and irreversible processes. It is sometimes called the fundamental equation or a combined first and second law. In these notes, we will refer to it as the first law of thermodynamics.

Another form of the first law can be obtained by introducing the enthalpy, $h \equiv e + pv$, whereby we obtain

$$dh = Tds + vdp\,. \tag{1.8}$$

Introducing the Gibbs free energy per unit mass,

$$g \equiv h - Ts\,, \tag{1.9}$$

and the Helmholz free energy per unit mass

$$f \equiv e - Ts\,, \tag{1.10}$$

leads to

$$dg = -sdT + vdp \tag{1.11}$$

and

$$df = -sdT - pdv\,. \tag{1.12}$$

1.2 Derivative Relationships

Equations (1.7), (1.8), (1.11) and (1.12) may be used to obtain Maxwell's relations. For example, if we consider $e = e(s, v)$, then $de = (\partial e/\partial s)_v ds + (\partial e/\partial v)_s dv$ and by comparing to (1.7) we obtain

$$\left(\frac{\partial e}{\partial s}\right)_v = T\,, \qquad \left(\frac{\partial e}{\partial v}\right)_s = -p\,. \tag{1.13}$$

Similarly, by considering $h = h(s, p)$ we obtain from (1.8)

$$\left(\frac{\partial h}{\partial s}\right)_p = T\,, \qquad \left(\frac{\partial h}{\partial p}\right)_s = v\,. \tag{1.14}$$

Using $g = g(T, p)$ and (1.11) gives

$$\left(\frac{\partial g}{\partial T}\right)_p = -s\,, \qquad \left(\frac{\partial g}{\partial p}\right)_T = v\,, \tag{1.15}$$

and $f = f(T, v)$ and (1.12) results in

$$\left(\frac{\partial f}{\partial T}\right)_v = -s\,, \qquad \left(\frac{\partial f}{\partial v}\right)_T = -p\,. \tag{1.16}$$

Another set of useful relations, called the *reciprocity relations* may be developed starting from $e = e(v, T)$ and $s = s(v, T)$ and (1.7) whereby

$$\left(\frac{\partial e}{\partial v}\right)_T dv + \left(\frac{\partial e}{\partial T}\right)_v dT = T\left[\left(\frac{\partial s}{\partial v}\right)_T dv + \left(\frac{\partial s}{\partial T}\right)_v dT\right] - p dv\,.$$

Since dv and dT must be independent of each other,

$$\begin{aligned}\left(\frac{\partial e}{\partial v}\right)_T &= T\left(\frac{\partial s}{\partial v}\right)_T - p\,,\\ \left(\frac{\partial e}{\partial T}\right)_v &= T\left(\frac{\partial s}{\partial T}\right)_v\,.\end{aligned} \tag{1.17}$$

Now, we can eliminate the entropy by cross-differentiating the above expressions. Differentiating the first of (1.17) with respect to T and the second with respect to v yields

$$\begin{aligned}\frac{\partial^2 e}{\partial v \partial T} &= T\frac{\partial^2 s}{\partial v \partial T} + \left(\frac{\partial s}{\partial v}\right)_T - \left(\frac{\partial p}{\partial T}\right)_v\,,\\ \frac{\partial^2 e}{\partial T \partial v} &= T\frac{\partial^2 s}{\partial T \partial v}\,.\end{aligned}$$

Assuming continuity of second derivatives, we can interchange the order of differentiation, and subtracting, yields

$$\left(\frac{\partial s}{\partial v}\right)_T = \left(\frac{\partial p}{\partial T}\right)_v .$$

Now substituting this result into the first of (1.17) gives

$$\left(\frac{\partial e}{\partial v}\right)_T = -p + T\left(\frac{\partial p}{\partial T}\right)_v . \tag{1.18}$$

This is called the reciprocity relationship and it will be utilized in our discussion on the equation of state.

Another form of the reciprocity relationship involving the enthalpy may be developed from $h = h(p,T)$ and $s = s(p,T)$ and (1.7) which results in

$$\begin{aligned} \left(\frac{\partial h}{\partial p}\right)_T &= T\left(\frac{\partial s}{\partial p}\right)_T + v\,, \\ \left(\frac{\partial h}{\partial T}\right)_p &= T\left(\frac{\partial s}{\partial T}\right)_p . \end{aligned} \tag{1.19}$$

Again, eliminating s by cross differentiation gives the reciprocity relation in terms of the enthalpy as:

$$\left(\frac{\partial h}{\partial p}\right)_T = v - T\left(\frac{\partial v}{\partial T}\right)_p . \tag{1.20}$$

1.3 Thermal Equation of State

Under a wide range of conditions, most gases behave in a manner described as a *perfect* or *ideal* gas. From the physics of gases, analyses based upon the kinetic theory of gases and statistical mechanics, (*c.f.*, Vincenti and Kruger (1965), §II.3 and §IV.9), may be used to develop an equation of state in the form

$$pV = NkT\,, \tag{1.21}$$

where N is the number of molecules and Boltzman's constant k is equal to 1.38054×10^{-23} $J/^\circ K/molecule$. The assumptions made include the concept of a weakly interacting gas where intermolecular forces are neglected. We can write the result in terms of the number of moles of the gas, $\mathcal{N}$ by the relationship $N = \mathcal{N}\hat{N}$ where Avogadro's number $\hat{N} = 6.02252 \times 10^{23}$ $molecules/mole$. We obtain

$$pV = \mathcal{N}\hat{R}T\,, \tag{1.22}$$

where the universal gas constant $\hat{R} = \hat{N}k = 8314.3\ J/(kg\text{–}mol\ {}^\circ K)$. This result is consistent with the early experiments of Boyle, Charles and Gay-Lussac.

We can write the state equation in terms of the mass M by introducing the molecular mass (mass per mole) $\hat{M} = M/\mathcal{N}$ and the species gas constant $R = \hat{R}/\hat{M}$ so that

$$pV = MRT\,. \tag{1.23}$$

Finally, dividing by M we obtain the familiar perfect gas law

$$pv = RT\,, \tag{1.24}$$

or

$$p = \rho RT\,. \tag{1.25}$$

This result is called the *thermal equation of state* and gases obeying this law are called thermally perfect. (The term *perfect gas* is sometimes used to mean a gas which is both thermally perfect and has constant specific heats. So to avoid ambiguity we will use the term thermally perfect when we mean a gas where $p = \rho RT$.)

The condition where a gas may not be thermally perfect include very high pressures near the gas *triple point.* Here, a Van der Waal's equation of state is used, *c.f.*, Liepmann and Roshko (1957), pp. 9, where

$$p = \rho RT\left(\frac{1}{1-\beta\rho} - \frac{\alpha\rho}{RT}\right)\,, \tag{1.26}$$

and $\beta = RT_c/8p_c$, $\alpha = 27\beta RT_c/8$, with T_c and p_c being the critical temperature and critical pressure, respectively. Values of p_c and t_c for some common gaseous species are presented in Table 1.1. It is seen that the real gas effect is important at very high pressures and low temperatures. For example, diatomic nitrogen gas, N_2 has critical properties of $p_c = 33.5\ atm$ and $T_c = 126\ K$. At a moderate temperature of 315 K, the Van der Waal's equation of state will deviate from the thermally perfect equation of state by 1% when the pressure is higher than 67 *atm.* At a lower temperature of 210 K, a 1% variation occurs at pressures higher than 4.9 *atm.*

Table 1.1 Critical Pressures and Temperatures

	O_2	N_2	NO	H_2	He	A	CO_2
p_c (atm)	49.7	33.5	65.0	12.8	2.26	48.0	73.0
T_c (°K)	154.3	126.0	179.1	33.2	5.2	151.1	304.2

In Fig. 1.1 we present a plot of $z = p/\rho RT$ versus $\log_{10} p$ for nitrogen N_2 at temperatures of 200, 300 and 400 degrees Kelvin. The dotted curve represents the $T = 200K$ case and the dot-dashed curve is the $T = 400K$ case. Thus we see that

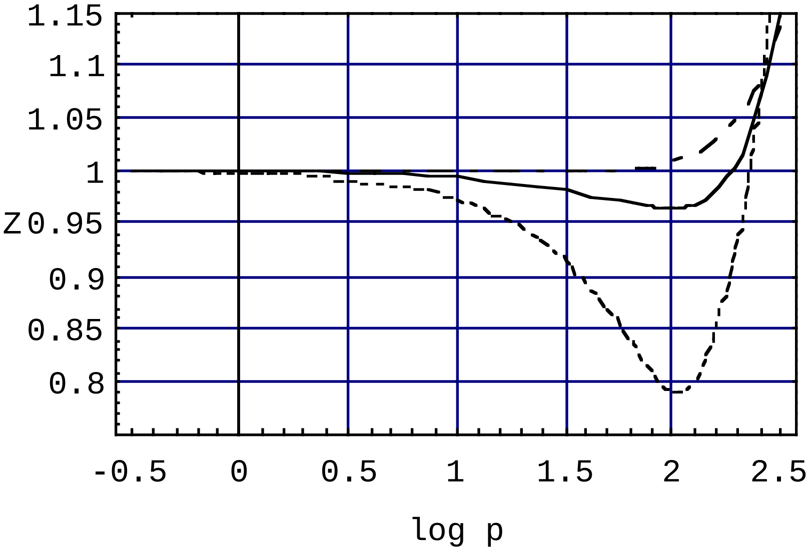

Figure 1.1. Thermal imperfection for N_2 *at* $T = 200K,\ T = 300K,\ T = 400K, \quad Z = p/\rho RT$.

major thermal equation of state imperfections occur at a combination of very high pressures and low temperatures for these gases.

On the other extreme, at very high temperatures and low pressures, the gas may dissociate and ionize and will no longer behave as a thermally perfect gas. However, even if reactions take place, the individual species will behave as a thermally perfect gas, but the mixture will not. For example, considering pure N_2 at temperatures above $4500K$, significant amounts of dissociated N will begin to be present. The perfect gas law will still hold for each species, $p_{N_2} = \rho_{N_2} R_{N_2} T$ and $p_N = \rho_N R_N T$. For the mixture of N and N_2, we have $p = p_N + p_{N_2} = \rho \tilde{R} T$ where ρ is the mass density of the mixture and $\tilde{R}$ is the mixture gas "constant". But, as will be shown later in this chapter, $\tilde{R}$ will depend upon the species mass fractions, which in turn depend upon the pressure and temperature, and hence will not be constant. Thus the mixture will not behave as a thermally perfect gas.

As a consequence of the assumption of a thermally perfect gas, it can be shown that the internal energy and the enthalpy will be functions of a single state variable, the temperature. We can show this by starting with the general specification of the internal energy as $e = e(v, T)$. Then from the thermal equation of state (1.25), we can take the derivative $(\partial p/\partial T)_v = R/v$. Then using the reciprocity relationship, (1.18), we find

$$\left(\frac{\partial e}{\partial v}\right)_T = -p + T\frac{R}{v} = 0\,. \tag{1.27}$$

Therefore, for a thermally perfect gas $e = e(T)$.

Similarly, considering $h = h(p, T)$, the thermal equation of state (1.25) will give $(\partial v/\partial T)_p = R/p$ and reciprocity (1.20) gives

$$\left(\frac{\partial h}{\partial p}\right)_T = v - T\frac{R}{p} = 0\,, \tag{1.28}$$

so that, for a thermally perfect gas $h = h(T)$.

1.4 Specific Heats

The specific heat is the amount of heat added per unit mass per unit temperature. For a gas, the process must be specified, either constant volume or constant pressure. From the First Law, (1.7), if the work done in a constant volume process is zero, then

$$c_v \equiv \left(\frac{dq}{dT}\right)_v = \left(\frac{\partial e}{\partial T}\right)_v\,, \tag{1.29}$$

and similarly for a constant pressure process, using (1.8), we obtain

$$c_p \equiv \left(\frac{dq}{dT}\right)_p = \left(\frac{\partial h}{\partial T}\right)_p\,, \tag{1.30}$$

For a thermally perfect gas, since $e = e(T)$ and $h = h(T)$, then $c_v = de/dT = c_v(T)$ and $c_p = dh/dT = c_p(T)$. Also for a thermally perfect gas $h = e + RT$ so that differentiating with respect to T gives

$$c_p(T) = c_v(T) + R\,, \tag{1.31}$$

noting that R is constant.

1.5 Internal Energy and Enthalpy

For a thermally perfect gas, $de = c_v(T)dT$ and $dh = c_p(T)dT$. If c_v and c_p are known functions of T, then e and h may be determined by quadrature as

$$\begin{aligned} e &= \int_{T_r}^{T} c_v\,dT + e_r\,, \\ h &= \int_{T_r}^{T} c_p\,dT + h_r\,, \end{aligned} \tag{1.32}$$

where the subscript r denotes an arbitrary reference state and $e_r = e(T_r)$ and $h_r = h(T_r)$. Often T_r is taken to be absolute zero, and since we are dealing with a thermally perfect gas where $h = e + RT$, then at $T = 0$, h_r will equal e_r. The value of this quantity cannot be obtained experimentally and can be obtained theoretically only for very simple molecules. However, in using e and h, only changes Δe and Δh will appear, so that the absolute value will not be needed. This issue becomes important in dealing with mixtures of gases and will be discussed in §1.9. It is common practice to take e_r and h_r equal to h_f^0, the heat of formation of the species at absolute zero. We will utilize the convention that the heat of formation of all atoms is zero. Note that some texts use the heat of formation of molecules to be zero. We will write

$$\begin{aligned} e &= \int_0^T c_v\, dT + h_f^0\,, \\ h &= \int_0^T c_p\, dT + h_f^0\,, \end{aligned} \tag{1.33}$$

Other choices for heat of formation include the standard heat of formation, referring to species at the standard temperature of 298.16 K and standard pressure of 1 *atm*. For a discussion of these issues see Anderson (1990) , pp. 550–551.

When c_p and c_v are constant we have a *calorically perfect gas* and upon neglecting h_f^0, we obtain

$$e = c_v T\,, \qquad h = c_p T\,, \tag{1.34}$$

The evaluation of c_p and c_v in general can be obtained from the physics of gases using quantum statistical mechanics, *c.f.*, Vincenti and Kruger (1965), §IV. The results for a *weakly interacting* gas are summarized here. The internal energy is composed of two parts, $e = e_{tr} + e_{int}$, where e_{tr} is the contribution to the internal energy due to molecular translation, which is found to be

$$e_{tr} = \frac{3}{2} RT\,, \tag{1.35}$$

and e_{int} is the contributions due to the internal structure of the molecules. The quantity e_{int} consists of contributions due to molecular rotation, molecular vibration and electron excitation. Strictly speaking, the effects of molecular rotation and vibration are coupled, it is common to approximate these effects separately. For a monatomic gas there would be no rotation or vibration effects. If we assume that the contributions to e_{int} act independently, then $e_{int} = e_{rot} + e_{vib} + e_{el}$. For a diatomic molecule, the rotational energy mode may be considered to be fully excited at very low temperatures so that

$$e_{rot} = RT\,. \tag{1.36}$$

The vibrational energy of a diatomic molecule may be approximately modeled as a quantum harmonic oscillator whereby

$$e_{vib} = \frac{R\Theta_v}{\exp(\Theta_v/T) - 1}\,, \tag{1.37}$$

Table 1.2 Vibration and Electronic Excitation Parameters

	vibration	electronic excitation			
Species	θ_v (°K)	g_0	g_1	Θ_1 (°K)	Θ_2 (°K)
O_2	2270	3	2	11,390	$\mathcal{O}$(19,000)
N_2	3390	1		$\mathcal{O}$(100,000)	
NO	2740	2	2	174	$\mathcal{O}$(65,000)
O		5	4	270	$\mathcal{O}$(23,000)
N		4		$\mathcal{O}$(19,000)	

with Θ_v a characteristic temperature for molecular vibration. Some typical values for θ_v from Vincenti and Kruger (1965) are given in Table 1.2, below.

The internal energy contribution due to electron excitation depends upon the quantum energy levels of the electrons, for which the electronic partition function takes the form

$$Q_{el} = g_0 + g_1 e^{-\Theta_1/T} + g_2 e^{-\Theta_2/T} + \dots\,, \tag{1.38}$$

where $g_0, g_1, g_2 \dots$ are the degeneracy factors for the lowest electronic energy levels and $\Theta_1, \Theta_2, \dots$ are the corresponding characteristic temperatures for electronic excitation. For a more complete discussion of these terms, see Vincenti and Kruger, (1965), pp. 130–132. A tabulation of a few of these constants for some of the constituents of air appear in Table 1.2. The *order of magnitude* terms in the table indicate the level of the first characteristic temperature term usually neglected. The corresponding internal energy is given by

$$e_{el} = R\left[\frac{g_1\Theta_1 e^{-\Theta_1/T} + g_2\Theta_2 e^{-\Theta_2/T} + \dots}{g_0 + g_1 e^{-\Theta_1/T} + g_2 e^{-\Theta_2/T} + \dots}\right]. \tag{1.39}$$

Often this contribution turns out to be negligible. For example, for N_2 and O_2, electron excitation effects will not become significant until a temperature of at least $10,000\ K$. For other gases, such as O and NO these effects can be important at low temperatures, 200–300 K, but not at high temperatures. Thus we can roughly see that these effects will not be important for air, since at low temperatures it is composed of N_2 and O_2 and at higher temperatures it will be composed of N, O and NO.

Thus, for a monatomic gas, neglecting electronic excitation gives

$$e = \frac{3}{2}RT\,, \tag{1.40}$$

so that $c_v = (3/2)R$. Thus this gas will be both thermally and calorically perfect and $c_p = c_v + R = (5/2)R$ and $\gamma = c_p/c_v = 5/3$.

For a diatomic gas, neglecting electronic excitation, gives

$$e = \frac{5}{2}RT + \frac{R\Theta_v}{\exp(\Theta_v/T) - 1}\,, \tag{1.41}$$

and

$$c_v = \frac{5}{2}R + R\left[\frac{\Theta_v/2T}{\sinh(\Theta_v/2T)}\right]^2\,. \tag{1.42}$$

This gas will be thermally perfect. If $T << \Theta_v$, then we can neglect e_{vib} and the gas will be calorically perfect with $c_v = (5/2)R$, $c_p = (7/2)R$ and $\gamma = 7/5$. The internal energy of gas mixtures will be discussed in §1.9.

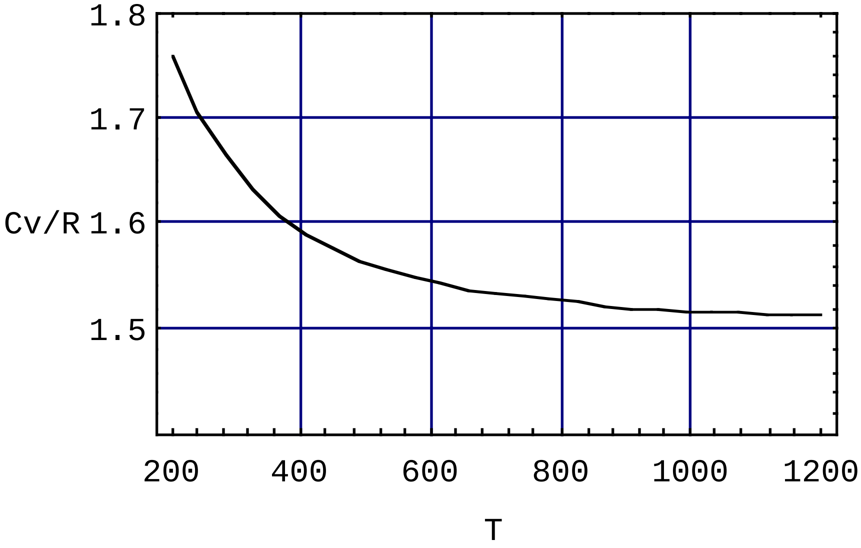

Figure 1.2. Specific heat distribution for pure monatomic oxygen.

Some example distributions of c_v/R versus T are shown in Figs. 1.2 – 1.4. Fig 1.2 is for monatomic oxygen. The specific heat is dominated at low temperatures by the electronic excitation. At temperatures above 1000 K, c_v returns to the translational value 3/2. In Fig. 1.3 is the distribution of c_v/R for pure diatomic oxygen O_2. (Note that we are evaluating c_v only for O_2 and are not evaluating it for a dissociating mixture of O and O_2. This will be discussed in §1.10.) The plot shows a dominance of vibrational effects at the low range of temperatures and the electronic excitation effects at the high range. In Fig. 1.4, we show the same c_v distribution for O_2, with the abscissa expanded to show low temperature effects. The variation of c_v with relatively low temperatures is seen due to the low characteristic vibration temperature for O_2.

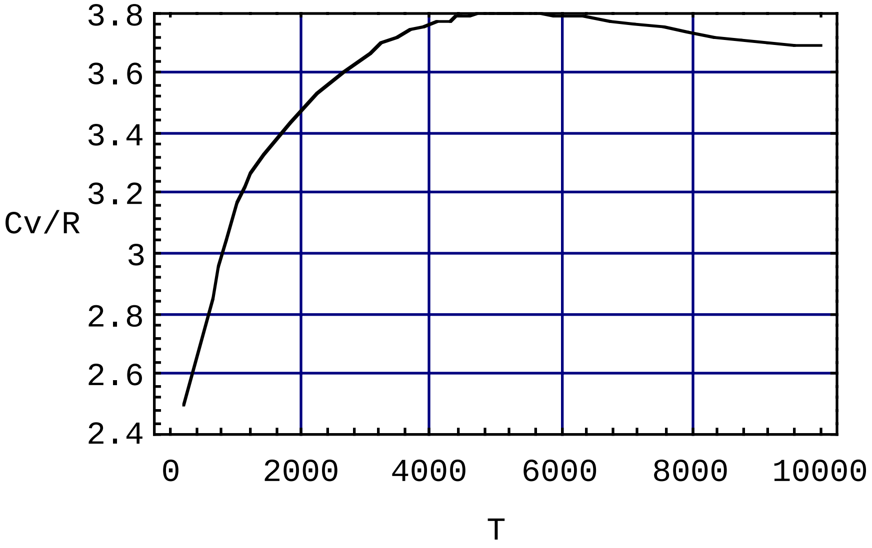

Figure 1.3. Specific heat distribution for pure diatomic oxygen O_2.

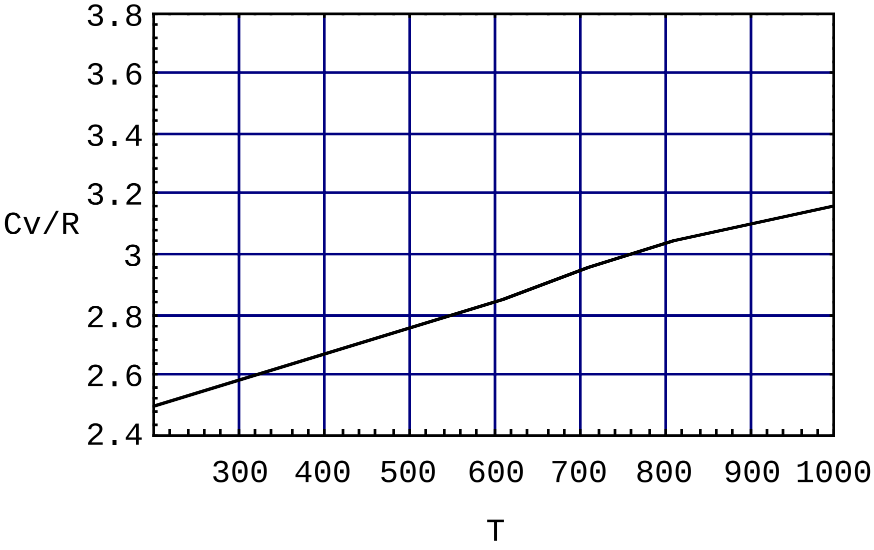

Figure 1.4. Specific heat distribution for pure diatomic oxygen O_2 at low temperatures.

1.6 Entropy and Free Energies

We may obtain a formula for the entropy for a thermally perfect gas starting from the first law (1.8), and substituting $dh = c_p dT$ along with the equation of state (1.24), to obtain

$$ds = c_p \frac{dT}{T} - R \frac{dp}{p} \, .$$

Integrating from the reference state, subscript r,

$$s = \int_{T_r}^{T} \frac{c_p}{T}\, dT - R \log \frac{p}{p_r} + s_r\,. \tag{1.43}$$

Under conditions of both a thermally and calorically perfect gas, we can obtain

$$\frac{s - s_r}{c_v} = \log \left[\left(\frac{T}{T_r} \right)^{\gamma} \left(\frac{p}{p_r} \right)^{1-\gamma} \right]. \tag{1.44}$$

Eliminating T in terms of p and ρ from the equation of state (1.25), upon rearranging terms,

$$\frac{p}{p_r} = \left(\frac{\rho}{\rho_r} \right)^{\gamma} \exp\left(\frac{s - s_r}{c_v} \right). \tag{1.45}$$

This important result may be viewed as a polytropic equation of state in the form $p = p(\rho, s)$.

For a flow where the entropy is unchanged, $s = s_r$, we have the familiar isentropic relationship

$$\frac{p}{p_r} = \left(\frac{\rho}{\rho_r} \right)^{\gamma}. \tag{1.46}$$

We see that the gas will be barotropic under these conditions.

We can also obtain an integrated form of the Gibb's free energy for a thermally perfect gas using the definition $g = h - Ts$ along with the expression for h, (1.32) and the expression for s, (1.43),

$$g = \omega(T) + RT \log p\,, \tag{1.47}$$

where

$$\omega(T) = \int_{T_r}^{T} c_p\, dT + h_r - T \left[\int_{T_r}^{T} \frac{c_p}{T}\, dT + R \log(p_r) + s_r \right]. \tag{1.48}$$

This result will be useful in developing the Law of Mass Action for a reacting gas in §1.9.

1.7 Sound Speeds

The speed of sound is defined as

$$a^2 \equiv \left(\frac{\partial p}{\partial \rho} \right)_s. \tag{1.49}$$

For a thermally and calorically perfect gas, we may take this derivative directly from the state relationship of the form $p = p(\rho, s)$ given in (1.45) to obtain

$$a^2 = \gamma \frac{p}{\rho} = \gamma R T\,. \tag{1.50}$$

Other forms of the sound speed relationship, which are useful when we do not have perfect gases may be developed from alternate specifications of the state equation. If we know, for example, $p = p(\rho, e)$, then we may derive the sound speed involving the known derivatives $(\partial p/\partial \rho)_e$ and $(\partial p/\partial e)_\rho$ by expanding $(\partial p/\partial \rho)_s = (\partial p/\partial \rho)_e + (\partial p/\partial e)_\rho (\partial e/\partial \rho)_s$. From (1.13), $(\partial e/\partial v)_s = -p$ and using $v = 1/\rho$ we obtain

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho . \tag{1.51}$$

This form is sometimes utilized in the numerical solutions of the governing equations for real gases in conservation-law form.

Another form of the sound-speed relationship may be developed for equations of state of the form $p = p(v, T)$, such as Van der Waal's gases, (1.26). Then if we consider $T = T(v, s)$ we see that $(\partial p/\partial v)_s = (\partial p/\partial v)_T + (\partial p/\partial T)_v (\partial T/\partial v)_s$. We can evaluate the temperature derivative by using $e = e(v, T)$ so that $de = (\partial e/\partial v)_T dv + (\partial e/\partial T)_v dT$ and with the first law (1.7) and consideration of $T(v, s)$ we find $(\partial e/\partial T)_v (\partial T/\partial v)_s = -(\partial e/\partial v)_T - p$. Then replacing $(\partial e/\partial v)_T$ with the reciprocity relationship (1.18) and using the definition of c_v, (1.29), we finally obtain

$$a^2 = -v^2\left(\frac{\partial p}{\partial v}\right)_s = -v^2\left[\left(\frac{\partial p}{\partial v}\right)_T - \frac{T}{c_v}\left(\frac{\partial p}{\partial T}\right)_v^2\right] , \tag{1.52}$$

or in terms of density derivatives

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_T + \frac{T}{\rho^2 c_v}\left(\frac{\partial p}{\partial T}\right)_\rho^2 . \tag{1.53}$$

Expressions (1.52) and (1.53) may be simplified further by eliminating one of the two partial derivatives. From the first law (1.7) with $e = e(v, T)$, we have $(\partial e/\partial T)_v = T(\partial s/\partial T)_v$. Then considering $s = s(T, p)$ and $p = p(T, v)$ we have $(\partial s/\partial T)_v = (\partial s/\partial T)_p + (\partial s/\partial p)_T (\partial p/\partial T)_v$ so that $(\partial e/\partial T)_v = T[(\partial s/\partial T)_p + (\partial s/\partial p)_T (\partial p/\partial T)_v]$. Substituting the definition of c_v in (1.29), c_p in (1.30) along with the second of (1.19) into the above expression gives $c_v = c_p + T(\partial s/\partial p)_T (\partial p/\partial T)_v$. Next we use the first of (1.19) and (1.20) to get $(\partial s/\partial p)_T = -(\partial v/\partial T)_p$. Then we implicitly differentiate $v = v(T, p)$ and $p = p(v, T)$ to obtain $(\partial v/\partial p)_T (\partial p/\partial v)_T = 1$ and $(\partial v/\partial T)_p + (\partial v/\partial p)_T (\partial p/\partial T)_v = 0$ from which $(\partial v/\partial T)_p = -(\partial p/\partial T)_v/(\partial p/\partial v)_T$. (The differentiation of implicit functions is clearly described in Hildebrand (1976), §7.2). Putting this together we finally obtain

$$a^2 = -v^2\frac{c_p}{c_v}\left(\frac{\partial p}{\partial v}\right)_T = \frac{c_p}{c_v}\left(\frac{\partial p}{\partial \rho}\right)_T . \tag{1.54}$$

This formula is valid for thermally and calorically imperfect gases as well as perfect gases. For the case of a gas which is thermally perfect but calorically imperfect, (1.54) reduces to $a^2 = [c_p(T)/c_v(T)]RT$. As an example, consider pure diatomic oxygen O_2, which due to molecular vibrational effects and electronic excitation, will be calorically imperfect at high temperatures. A plot of a/a_0 is presented in Fig 1.5, where $a_0^2 = 1.4RT$. The sound speed is initially reduced due to vibrational effects and then at very high temperatures begins to increase due to electronic excitation. Note that in this example we have ignored the effects of chemical dissociation, which would be significant at high temperatures. These effects will be considered later in this chapter.

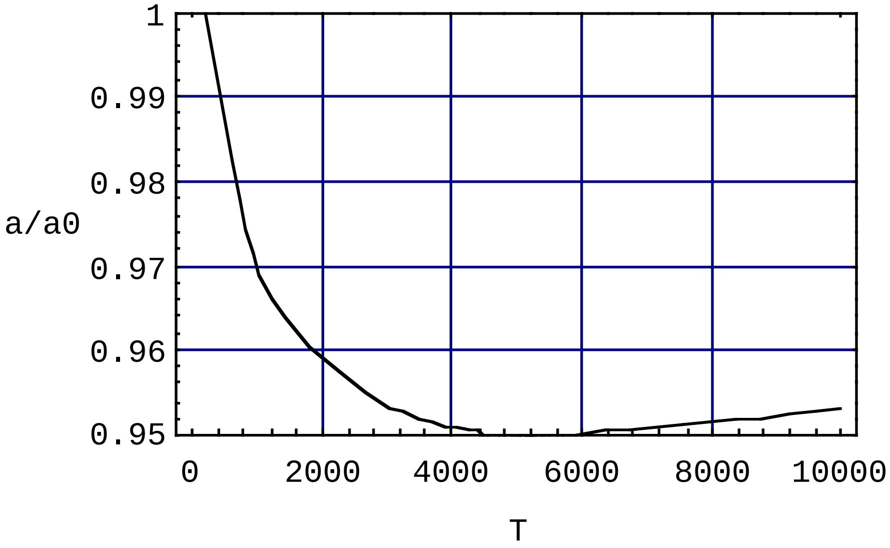

Figure 1.5. Sound speed ratio a/a_0 for calorically imperfect diatomic oxygen O_2. (Ignores dissociation effects).

One more form of the sound speed will be developed involving derivatives of $\rho = \rho(h,s)$. We begin with $p = p(h,s)$ and $h = h(\rho,s)$. Then $(\partial p/\partial\rho)_s = (\partial p/\partial h)_s(\partial h/\partial\rho)_s$. From the first law (1.8), $(\partial p/\partial h)_s = \rho$. We can obtain the derivative $(\partial h/\partial\rho)_s$ from $\rho = \rho(h,s)$ by implicit differentiation as $(\partial h/\partial\rho)_s = 1/(\partial\rho/\partial h)_s$ so that

$$a^2 = \frac{\rho}{(\partial\rho/\partial h)_s}\,. \tag{1.55}$$

1.8 Equilibrium Conditions

Considerations of equilibrium may be developed from the first and second laws of thermodynamics as described by Liepmann and Roshko (1957), §1.13. From the second law of thermodynamics, for any process $ds \geq dq/T$. Thus is we arrive at a state where any further additions of heat, δq will cause the entropy to *decrease*, $\delta s \leq \delta q/T$ then that state is said to be in *stable equilibrium*, (since no further changes will occur). From the combined first and second law, $Tds-(de+pdv)=0$. But if we arrive at a state where any virtual changes δe and δv cause the entropy to decrease, then

$$T\delta s-(\delta e+p\delta v)\leq 0\,, \tag{1.56}$$

and the system will be in stable equilibrium. Or, a system at constant internal energy and constant specific volume will be in stable equilibrium if all changes cause the entropy to decrease, $\delta s\leq 0$. Thus a system at constant e and v will be in stable equilibrium if *the entropy is a maximum.*

Similarly, from (1.8), the condition of stable equilibrium will be

$$T\delta s-\delta h+v\delta p\leq 0\,, \tag{1.57}$$

or for a constant p and h process, equilibrium will be again reached when the entropy is a maximum. We can determine some other equilibrium condition involving the free energies from (1.11) and (1.12). We see that for equilibrium

$$\delta f+s\delta T+p\delta v\geq 0\,, \tag{1.58}$$

$$\delta g+s\delta T-v\delta p\geq 0\,. \tag{1.59}$$

Thus for a constant temperature and constant volume process, stable equilibrium occurs when *the Helmholz free energy is a minimum* and for a constant temperature and constant pressure process, stable equilibrium occurs when *the Gibbs free energy is a minimum.* This condition on the Gibbs free energy will be used in §1.9 to develop the law of mass action for equilibrium chemistry.

1.9 Gas Mixtures

We will now consider mixtures of gases, which may or may not be reacting. Most of the formulas developed in the preceding sections, remain valid, but only apply to the individual species within the mixture and not to the mixture as a whole. We will now add subscripts to identify the species quantities, *e.g.*, e_i, h_i, p_i, *etc.* Quantities written from now on without subscripts will apply to properties of the mixture.

Extensive and intensive properties

For a mixture of gases, the extensive properties are additive. For example the total mass of the mixture must equal the sum of the masses of the component species

$$M=\sum_{i=1}^{N}M_i\,. \tag{1.60}$$

Similarly, the internal energy of the mixture $E=\sum E_i$, the enthalpy of the mixture, $H=\sum H_i$, and the entropy of the mixture, $S=\sum S_i$.

For an individual gas species, the internal energy is related to the internal energy per unit mass by $E_i = M_i e_i$. Summing over the i-species and dividing by the mass of the mixture gives the internal energy per unit mass of the mixture as

$$e = \frac{E}{M} = \sum_{i=1}^{N} \frac{M_i}{M} e_i \,. \tag{1.61}$$

We can introduce the *mass fraction* of species i as

$$c_i \equiv \frac{M_i}{M} \,. \tag{1.62}$$

For a gas, since each species will expand to fill the entire volume, $V_i = V$, we can introduce the species density $\rho_i = M_i/V$ so that $c_i = \rho_i/\rho$. The intensive properties of the mixture may then be written as

$$e = \sum_{i=1}^{N} c_i e_i \,, \qquad h = \sum_{i=1}^{N} c_i h_i \,, \qquad s = \sum_{i=1}^{N} c_i s_i \,. \tag{1.63}$$

The density of the mixture may be written as

$$\rho = \frac{M}{V} = \frac{1}{V} \sum_{i=1}^{N} M_i = \sum_{i=1}^{N} \rho_i \,. \tag{1.64}$$

From this relationship it is obvious that the sum of the mass fractions is unity, $\sum c_i = 1$.

Equation of state

Mixtures of gases which are in chemical and thermodynamic equilibrium have the important property that the temperature of each species is the same, or $T_i = T$. Furthermore, from the kinetic theory of gases for mixtures which are weakly interacting, the well-known Dalton's law of partial pressures says that the pressure of the gas mixture is the sum of the partial pressures of the species, $p = \sum p_i$. In this section we will be dealing with mixtures of thermally perfect gases, so that $p_i = \rho_i R_i T$. Then the pressure of the mixture becomes

$$p = \sum_{i=1}^{N} \rho_i R_i T = \rho \tilde{R} T \,, \tag{1.65}$$

where the gas constant of the mixture is defined as

$$\tilde{R} = \sum_{i=1}^{N} c_i R_i = \frac{\hat{R}}{\hat{M}} \,, \tag{1.66}$$

and the molecular mass of the mixture is defined as

$$\frac{1}{\hat{M}} = \sum_{i=1}^{N} \frac{c_i}{\hat{M}_i}\,. \tag{1.67}$$

Thus the mixture is thermally perfect if $\tilde{R}$ or equivalently $\hat{M}$ is constant. This will be the case only if the mass fractions c_i are constant. Hence, a mixture of thermally perfect gases will be thermally perfect only if the gases are not reacting.

We can determine the partial pressure of each species from the mixture pressure p by again noting that $p_i = \rho_i R_i T$ and dividing by (1.65) so that

$$\frac{p_i}{p} = \frac{\rho_i}{\rho}\frac{R_i}{\tilde{R}} = c_i \frac{\hat{M}}{\hat{M}_i}\,.$$

We can simplify the above by introducing the the number of moles of species i. which equals the mass of i divided by the mass per mole of i (the molecular mass of i), so that $\mathcal{N}_i = M_i/\hat{M}_i$. Then with the total number of moles of the mixture as $\mathcal{N} = \sum \mathcal{N}_i$ and introducing the mole fraction

$$Y_i \equiv \frac{\mathcal{N}_i}{\mathcal{N}}\,, \tag{1.68}$$

we can obtain the relationship

$$p_i = Y_i p\,. \tag{1.69}$$

From the above definitions, we can see that the mass fraction and mole fraction are related by

$$c_i = Y_i \frac{\hat{M}_i}{\hat{M}}\,. \tag{1.70}$$

First and Second Laws

In the mixture, the first and second laws apply for each species as given by (1.7) and (1.8). In terms of the species enthalpy h_i, we have $dh_i = Tds_i + v_i dp_i$. If we multiply this relationship by the mass fraction c_i and sum from $i = 1$ to N, we obtain

$$\sum_{i=1}^{N} c_i dh_i = T\sum_{i=1}^{N} c_i ds_i + v\sum_{i=1}^{N} dp_i\,.$$

From (1.63)

$$dh = \sum_{i=1}^{N} c_i dh_i + \sum_{i=1}^{N} h_i dc_i\,,$$

with similar relationships for de and ds. We then obtain the combined first and second law for a mixture of gases as

$$dh = Tds + vdp + \sum_{i=1}^{N} g_i dc_i \,, \tag{1.71}$$

or in terms of the internal energy

$$de = Tds - pdv + \sum_{i=1}^{N} g_i dc_i \,. \tag{1.72}$$

The Gibb's free energy, g_i in the above equations is sometimes called the chemical potential (per unit mass) and is given the symbol μ_i.

From (1.71) and (1.72), we see that for a gas mixture that $h = h(s, p, c_i)$ and $e = e(s, v, c_i)$. Note that the notation $h = h(s, p, c_i)$ is used as a shorthand for $h = h(s, p, c_1, c_2, \ldots, c_N)$, *etc.* We can develop Maxwell's relations for the mixture in terms of enthalpy derivatives as

$$\left(\frac{\partial h}{\partial s}\right)_{p,c_i} = T\,, \qquad \left(\frac{\partial h}{\partial p}\right)_{s,c_i} = v\,, \qquad \left(\frac{\partial h}{\partial c_i}\right)_{s,p,c_j} = g_i\,, \tag{1.73}$$

and in terms of energy derivatives as

$$\left(\frac{\partial e}{\partial s}\right)_{v,c_i} = T\,, \qquad \left(\frac{\partial e}{\partial v}\right)_{s,c_i} = -p\,, \qquad \left(\frac{\partial e}{\partial c_i}\right)_{s,v,c_j} = g_i\,. \tag{1.74}$$

Note that the subscript c_i in the above expressions means that all mass fractions for $i = 1, \ldots, N$ are held fixed and the subscript c_j indicates that all the mass fractions for $j \neq i$ are held fixed.

Reciprocity relations may be developed for gas mixtures from (1.71) and (1.72) using procedures similar to those used for a single species in (1.18) and (1.20), with all the mass fractions c_i held fixed. We obtain

$$\left(\frac{\partial e}{\partial v}\right)_{T,c_i} = -p + T\left(\frac{\partial p}{\partial T}\right)_{v,c_i}\,, \tag{1.75}$$

$$\left(\frac{\partial h}{\partial p}\right)_{T,c_i} = v - T\left(\frac{\partial v}{\partial T}\right)_{p,c_i}\,. \tag{1.76}$$

Thermodynamic Properties

The energy, enthalpy and entropy of a mixture are obtained from (1.63). We may develop an expression for the enthalpy of a mixture using $h_i \equiv e_i + p_i v_i$ so that following (1.63), we have $\sum c_i h_i = \sum c_i e_i + \sum c_i p_i v_i$. Then with the definitions $c_i = \rho_i/\rho$, $v_i = 1/\rho_i$ and $v = 1/\rho$ we may obtain that in general

$$h = e + pv\,. \tag{1.77}$$

For a mixture of thermally perfect gases, the species energy and enthalpy may be written as in (1.33) so that

$$e = \sum_{i=1}^{N} c_i \int_0^T c_{v_i}\, dT + \sum_{i=1}^{N} c_i h^0_{f_i}\,, \tag{1.78}$$

$$h = \sum_{i=1}^{N} c_i \int_0^T c_{p_i}\, dT + \sum_{i=1}^{N} c_i h^0_{f_i}\,, \tag{1.79}$$

The first summation term in each of these expressions is sometimes called the *sensible internal energy* and the *sensible enthalpy*, respectively. The second summation term is sometimes called the *chemical enthalpy.* A discussion of the chemical enthalpy for mixtures is found in Anderson (1990) pp. 550-551.

We can define the *frozen* specific heats of the mixture as

$$\tilde{c}_v \equiv \left(\frac{\partial e}{\partial T}\right)_{v,c_i} = \sum_{i=1}^{N} c_i \left(\frac{\partial e_i}{\partial T}\right)_{v,c_i} = \sum_{i=1}^{N} c_i c_{v_i}\,, \tag{1.80}$$

$$\tilde{c}_p \equiv \left(\frac{\partial h}{\partial T}\right)_{p,c_i} = \sum_{i=1}^{N} c_i \left(\frac{\partial h_i}{\partial T}\right)_{p,c_i} = \sum_{i=1}^{N} c_i c_{p_i}\,, \tag{1.81}$$

For mixtures of thermally perfect gases, $c_{v_i} = c_{v_i}(T)$, $c_{p_i} = c_{p_i}(T)$ and $R_i = c_{p_i} - c_{v_i}$, we have

$$\tilde{c}_p - \tilde{c}_v = \sum_{i=1}^{N} c_i (c_{p_i} - c_{v_i}) = \sum_{i=1}^{N} c_i R_i = \tilde{R}\,, \tag{1.82}$$

We again note that mixtures of thermally perfect gases will be **not** be thermally perfect since e, h, $\tilde{c}_p$ and $\tilde{c}_v$ will not be only functions of T since they will also depend upon c_i which, as will be shown in the next section will depend upon ρ and T for chemical equilibrium.

Frozen Sound Speed

We can define the frozen sound speed as

$$a_f^2 \equiv \left(\frac{\partial p}{\partial \rho}\right)_{s,c_i}\,. \tag{1.83}$$

This sound speed may be evaluated for any mixture, reacting or non-reacting, with equilibrium or non-equilibrium chemistry. Frozen sound speed relationships, similar to the single species results (1.51)–(1.55) may be developed from using the first and second law and related expressions for mixtures in (1.71)–(1.76). Note that we can easily switch between partial derivatives of ρ and partial derivatives of v using $v = 1/\rho$.

For example if we have an equation of state of the form $p = p(\rho, T, c_i)$ and consider $T = T(\rho, s, c_i)$ then $(\partial p/\partial \rho)_{s,c_i} = (\partial p/\partial \rho)_{T,c_i} + (\partial p/\partial T)_{\rho,c_i}(\partial T/\partial \rho)_{s,c_i}$. We can evaluate $\partial p/\partial \rho$ and $\partial p/\partial T$ from the equation of state. To find $(\partial T/\partial \rho)_{s,c_i}$ we can consider $e = e(\rho, T, c_i)$, so that $(\partial e/\partial \rho)_{s,c_i} = (\partial e/\partial \rho)_{T,c_i} + (\partial e/\partial T)_{\rho,c_i}(\partial T/\partial \rho)_{s,c_i}$. Then from (1.72), $\partial e/\partial \rho)_{s,c_i} = p/\rho^2$. Also From (1.80) $(\partial e/\partial T)_{\rho,c_i} = \tilde{c}_v$ and $(\partial e/\partial \rho)_{T,c_i}$ may be evaluated from reciprocity (1.75). Putting this together we obtain

$$a_f^2 = \left(\frac{\partial p}{\partial \rho}\right)_{T,c_i} - \frac{T}{\rho^2 \tilde{c}_v}\left(\frac{\partial p}{\partial T}\right)^2_{\rho,c_i} . \tag{1.84}$$

For a mixture of thermally perfect gases, the equation of state is $p = \rho \tilde{R} T$ where $\tilde{R} = \sum c_i R_i$. Then $(\partial p/\partial \rho)_{T,c_i} = \tilde{R}T$ and $(\partial p/\partial T)_{\rho,c_i} = \rho \tilde{R}$ and using (1.82) we obtain for a mixture of thermally perfect gases:

$$a_f^2 = \frac{\tilde{c}_p}{\tilde{c}_v}\tilde{R}T . \tag{1.85}$$

Again note that $\tilde{c}_p$, $\tilde{c}_v$ and $\tilde{R}$ are not constant, but depend upon the mass fractions.

1.10 Equilibrium Chemistry

Consider as an example an equilibrium reaction of water going to molecular hydrogen and oxygen:

$$2\,H_2O \rightleftharpoons 2\,H_2 + O_2 . \tag{1.86}$$

Suppose we begin with a mixture containing N_{1_0} molecules H_2O, N_{2_0} molecules H_2 and N_{3_0} molecules O_2. At a later instant, after changing the pressure and temperature and allowing sufficient time to come to equilibrium, we have N_1 molecules H_2O, N_2 molecules H_2 and N_3 molecules O_2. Conservation of hydrogen atoms tells us that in the mixture there will be two hydrogen atoms for every H_2O molecule and two hydrogen atoms in every H_2 molecule, so that $2N_1 + 2N_2 = 2N_{1_0} + 2N_{2_0}$ or in terms of the change of the number of molecules, $2\Delta N_1 + 2\Delta N_2 = 0$. Similarly, conservation of oxygen atoms gives $\Delta N_1 + 2\Delta N_3 = 0$. We can rearrange these two atomic conservation equations as

$$\frac{\Delta N_1}{-2} = \frac{\Delta N_2}{2} = \frac{\Delta N_3}{1} . \tag{1.87}$$

Note that for the *reactants* on the left side of (1.86), we have divided ΔN_1 by the negative of the stoichiometric coefficient of H_2O and for the *products* on the right side of (1.86), we have divided ΔN_2 and ΔN_3 by their respective stoichiometric coefficients. This relationship can be written for a general equilibrium reaction of the form

$$\alpha_1 X_1 + \alpha_2 X_2 + \ldots + \alpha_j X_j \rightleftharpoons \beta_{j+1} X_{j+1} + \ldots + \beta_n X_n \,. \tag{1.88}$$

with the reactants on the left and the products on the right. Atomic conservation will give

$$\frac{dN_1}{\nu_1} = \frac{dN_2}{\nu_2} = \cdots = \frac{dN_n}{\nu_n} \,, \tag{1.89}$$

where $\nu_i = -\alpha_i$ for the reactants and $\nu_i = \beta_i$ for the products. Note that the scheme of using the negative of the stoichiometric coefficients for the reactants is only a convention. The ultimate results will not depend upon which way the reaction in (1.88) is written.

We can write the atomic conservation equation in terms of the number of moles of each species $\mathcal{N}_i$ by recalling that $\mathcal{N}_i = N_i/\hat{N}$, where $\hat{N}$ is Avogadro's number, the constant number of of molecules or atoms per mole. We see that

$$\frac{d\mathcal{N}_1}{\nu_1} = \frac{d\mathcal{N}_2}{\nu_2} = \cdots = \frac{d\mathcal{N}_n}{\nu_n} \,. \tag{1.90}$$

We can also evaluate this relationship in terms of the mass fraction of each species $c_i = M_i/M$ with the mass of each species M_i related to the number of moles of each species by the constant atomic mass of the species $\hat{M}_i$ as $M_i = \hat{M}_i \mathcal{N}_i$. The atomic conservation relationship becomes

$$\frac{dc_1}{\hat{M}_1 \nu_1} = \frac{dc_2}{\hat{M}_2 \nu_2} = \cdots = \frac{dc_n}{\hat{M}_n \nu_n} = d\xi \,, \tag{1.91}$$

where we have introduced the quantity ξ as the degree of advancement of the reaction. We see that the mass fraction of any species depends only upon the value of ξ.

Law of Mass Action

The law of mass action may be evaluated from the condition that in an equilibrium reaction at a fixed temperature and pressure, the Gibb's free energy must be a minimum, as in (1.59). For a mixture, the Gibb's free energy has been found to be $g = \sum c_i g_i$ with $g_i = g_i(p_i, T)$ given in (1.47). From the atomic conservation equation for the equilibrium reaction, (1.91), we can see that c_i may be written as a function of a single variable ξ. The condition of equilibrium may then be expressed as

$$\left(\frac{\partial g}{\partial \xi}\right)_{p,T} = 0 = \sum_{i=1}^{n} g_i \frac{dc_i}{d\xi} + \sum_{i=1}^{n} c_i \left(\frac{\partial g_i}{\partial \xi}\right)_{p,T} \,. \tag{1.92}$$

The last summation term may be shown to be zero from the evaluation of g_i for a thermally perfect gas in (1.47) which may be written as $g_i = \omega_i(T) + R_i T \log p_i$.

Differentiating gives $(\partial g_i/\partial\xi)_{p,T} = (R_iT/p_i)(\partial p_i/\partial\xi)_{p,T}$. Multiplying by c_i and summing over all species i gives $\sum c_i(\partial g_i/\partial\xi)_{p,T} = \sum(\rho_i/\rho)(R_iT/p_i)(\partial p_i/\partial\xi)_{p,T} = (1/\rho)\sum(\partial p_i/\partial\xi)_{p,T}$, where the equation of state $p_i = \rho_iR_iT$ has been used. Now interchanging summation and differentiation and applying Dalton's law $p = \sum p_i$ gives $\sum(\partial p_i/\partial\xi)_{p,T} = (\partial/\partial\xi)(\sum p_i)_{p,T} = (\partial p/\partial\xi)_{p,T}$ which must be zero. Therefore $\sum c_i(\partial g_i/\partial\xi)_{p,T} = 0$ and the equilibrium condition (1.92) becomes $\sum g_i(dc_i/d\xi) = 0$.

From (1.91), $dc_i/d\xi = \hat{M}_i\nu_i$ and the condition of equilibrium may be stated as:

$$\sum_{i=1}^{n}\hat{M}_i\nu_ig_i = 0\,. \tag{1.93}$$

Substituting the relation for $g_i = \omega_i(T) + R_iT\log p_i$ given in (1.47) and performing some algebraic manipulation we obtain the law of mass action as:

$$\prod_{i=1}^{n}p_i^{\nu_i} = \exp\left[-\sum_{i=1}^{n}\frac{\nu_i}{R_iT}\omega_i(T)\right] = K_p(T)\,, \tag{1.94}$$

where $\omega_i(T)$ is defined in (1.48). The exponential term above defines the equilibrium constant $K_p(T)$ for a mixture of thermally perfect gases in terms of the quantity $\omega_i(T)$ defined in (1.48). For some species, it is difficult to obtain an expression for ω_i because of uncertainties in the absolute value of the entropy. Under these circumstances, an experimentally developed curve fit for K_p is used. For example, Vincenti and Kruger, (1965) discuss on page 168, some curve fit equilibrium constants. They describe the results of Wray, in terms of the equilibrium constant for concentration

$$K_c(T) = \prod_{i=1}^{n}[X_i]^{\nu_i} = C_cT^{\eta_c}e^{-\Theta/T}\,, \tag{1.95}$$

where C_c, η_c and Θ are constants for a given reaction, with values for some elementary air reactions given in Table 1.3. The units of the constants are such that the units for K_c are $kg-mole/m^3$. The concentration $[X_i]$ is the number of moles of species i per unit volume, $\mathcal{N}_i/V$. Then by definition $\rho_i = M_i/V = \hat{M}_i\mathcal{N}_i/V = \hat{M}_i[X_i]$ and $p_i = \rho_iR_iT = \hat{M}_i[X_i](\hat{R}/\hat{M}_i)T = [X_i]\hat{R}T$ so that

$$K_p(T) = (\hat{R}T)^{\sum\nu_i}K_c(T)\,. \tag{1.96}$$

Also listed in the table are the characteristic temperatures for dissociation, Θ_D, for the first 3 reactions and the characteristic temperatures for ionization, Θ_I, for the last reaction. These temperatures are given in terms of electron volts (ev), where 1ev corresponds to a characteristic temperature of $11,600\ K$. The dissociation energy per unit mass is equal to $R_i\Theta_{D_i}$ and the ionization energy per

Table 1.3 Equilibrium Constants

Reaction	$K_c = C_c T^{\eta_c} e^{-\Theta/T}$			Θ_D or Θ_I
	C_c	η_c	Θ (°K)	(ev)
$O_2 \rightleftharpoons O + O$	1.2×10^6	-0.5	59,500	5.12
$N_2 \rightleftharpoons N + N$	18×10^3	0	113,000	9.76
$NO \rightleftharpoons N + O$	4.0×10^3	0	75,500	6.49
$NO \rightleftharpoons NO^+ + e$	1.44×10^{-7}	+1.5	107,000	9.25

unit mass is equal to $R_i\Theta_{I_i}$. These energies may be used to determine the heats of formation of N, O, NO and NO^+, as described in Vincenti and Kruger (1965), pp. 170.

The law of mass action may be used in conjunction with atomic conservation to determine the mass fractions of species, given the value of two thermodynamic variables, such as p and T or ρ and T. We can indicate this procedure by replacing p_i in (1.94) with $\rho_i R_i T = c_i R_i \rho T$ so that

$$(c_1^* R_1)^{\nu_1} (c_2^* R_2)^{\nu_2} \cdots (c_n^* R_n)^{\nu_n} (\rho T)^{\sum \nu_i} = K_p(T)\,, \tag{1.97}$$

where c_i^* has been used to indicate the value of the mass fraction in chemical equilibrium. Next, from atomic conservation (1.93) we find that

$$\frac{\Delta c_i^*}{\hat{M}_i \nu_i} = \frac{\Delta c_1^*}{\hat{M}_1 \nu_1}\,, \quad i = 2, \ldots, n\,, \tag{1.98}$$

where Δc_i^* is the change in c_i^* from a known initial distribution c_{i_0}. Multiplying by the universal gas constant $\hat{R}$ and recalling that $R_i = \hat{R}/\hat{M}_i$ we find that

$$c_i^* R_i = \frac{\nu_i}{\nu_1}\left[c_1^* - (c_1)_0\right] R_1 + (c_i)_0\, R_i\,, \quad i = 2, \ldots, n\,. \tag{1.99}$$

Upon substituting (1.99) into (1.97) we obtain a single nonlinear equation involving c_1^* and the known values of ρ, T and the initial distribution of mass fractions. It may be more efficient to solve (1.97) and (1.98) as a system of N non-linear algebraic equations in N unknowns. In practice, there are some numerical issues involved in determining mass fractions from the law of mass action, and often it will be solved as an optimization problem, directly minimizing the Gibbs free energy of the mixture. A discussion of these issues may be found in Liu and Vinokur (1989).

If we wish to determine the mass fractions at a given pressure and temperature instead of density and pressure, we can use the mixture state equation (1.60) as

$$\rho T = p/\tilde{R} = p/\sum_{i=1}^{n} c_i^* R_i\,, \tag{1.100}$$

which may be substituted into (1.97).

Properties of Mixtures in Chemical Equilibrium

The energy, enthalpy and entropy for any mixture are determined from (1.62) as $e = e(\rho, T, c_i)$, $h = h(\rho, T, c_i)$ and $s = s(\rho, T, c_i)$. For a mixture in chemical equilibrium, the mass fraction $c_i = c_i^*$, the equilibrium values given in (1.97)–(1.99) as a function of ρ and T. Then again using the superscript * to indicate equilibrium mixture values, we have $e^* = e(\rho, T, c_i = c_i^*) = e[\rho, T, c_i^*(\rho, T)] = e^*(\rho, T)$, with similar relationships for h^* and s^*. Thus the values of the state variables in chemical equilibrium depend upon two thermodynamic variables, just as in the case of a single species gas. This result has an impact on the definitions of c_v, c_p and the sound speed.

We may note that the combined first and second laws for a reacting mixture of gases, given in (1.67) or (1.68) simplifies for the case of a mixture in chemical equilibrium. For this case we have shown in (1.87) that $\sum g_i dc_i = 0$, so that the combined first and second law becomes

$$dh = Tds + vdp\,, \tag{1.101}$$

or

$$de = Tds - pdv\,. \tag{1.102}$$

The above equations apply for a single species, a non-reacting mixture or a reacting mixture in chemical equilibrium.

We can define an equilibrium specific heat at constant volume, c_v^* as

$$c_v^* = \left(\frac{\partial e^*}{\partial T}\right)_\rho = \left(\frac{\partial e}{\partial T}\right)_{\rho, c_i} + \sum_{i=1}^{N} \left(\frac{\partial e}{\partial c_i}\right)_{\rho, T} \left(\frac{\partial c_i^*}{\partial T}\right)_\rho \,. \tag{1.103}$$

We have already defined a frozen c_v as $\tilde{c}_v = (\partial e/\partial T)_{\rho, c_i}$ in (1.75) and we see from (1.62) that $(\partial e/\partial c_i)_{\rho, T} = e_i$ so that

$$c_v^* = \tilde{c}_v + \sum_{i=1}^{N} e_i \left(\frac{\partial c_i^*}{\partial T}\right)_\rho \,. \tag{1.104}$$

A similar expression may be developed for c_p^* as

$$c_p^* = \tilde{c}_p + \sum_{i=1}^{N} h_i \left(\frac{\partial c_i^*}{\partial T}\right)_p \,. \tag{1.105}$$

We have determined relationships for ρ_i^*/ρ in terms of ρ and T in (1.97)–(1.99). We can determine $\partial c_i^*/\partial T$ by logarithmically differentiating (1.97) to obtain $\sum (1/c_i^*) \partial c_i^*/\partial T = -(1/T) \sum \nu_i + d(\log K_p)/dT$. Then from (1.98) $R_i dc_i^* =$

$(\nu_i/\nu_1)R_1 dc_1^*$ so that

$$\left(\frac{\partial c_i^*}{\partial T}\right)_\rho = \frac{\nu_i}{R_i}\left[-\frac{1}{T}\sum_{i=1}^{N}\nu_i + \frac{d\log K_P}{dT}\right] \Big/ \sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i}\,. \tag{1.106}$$

From the definition of K_p in (1.94) and the definition of $w_i(T)$ in (1.48) we obtain

$$\frac{d\log K_P}{dT} = \sum_{i=1}^{N}\frac{\nu_i h_i}{R_i T^2}\,. \tag{1.107}$$

Then, using $h_i = e_i + R_i T$, we may write for equilibrium mixtures of thermally perfect gases:

$$\left(\frac{\partial c_i^*}{\partial T}\right)_\rho = \frac{\nu_i}{R_i}\sum_{i=1}^{N}\frac{\nu_i e_i}{R_i T^2} \Big/ \sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i}\,, \tag{1.108}$$

We may develop the derivative of c_i^* with respect to ρ in a similar fashion as

$$\left(\frac{\partial c_i^*}{\partial \rho}\right)_T = -\frac{\nu_i}{\rho R_i}\sum_{i=1}^{N}\nu_i \Big/ \sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i}\,, \tag{1.109}$$

For the c_p^* relationship, we need the derivative of c_i^* with respect to T at constant p instead of constant ρ as in (1.108). We may proceed by considering $c_i^*(T,p)$ using (1.97)–(1.100). We obtain

$$\left(\frac{\partial c_i^*}{\partial T}\right)_p = \frac{\nu_i}{R_i}\sum_{i=1}^{N}\frac{\nu_i h_i}{R_i T^2} \Big/ \left[\sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i} - \left(\sum_{i=1}^{N}\nu_i\right)^2 \Big/ \sum_{i=1}^{N} c_i^* R_i\right]\,. \tag{1.110}$$

Note that the above equations for the derivatives of c_i^* rely on mass fractions satisfying conservation equations of the form (1.98) and (1.99) and hence are valid for a single equilibrium reaction of the form (1.88). For more complicated equilibrium chemistry, alternate relationships must be developed.

Substituting (1.108) and (1.110) into (1.104) and (1.105) we obtain the following expressions for equilibrium specific heats:

$$c_v^* = \tilde{c}_v + \frac{1}{T^2}\left(\sum_{i=1}^{N}\frac{\nu_i e_i}{R_i}\right)^2 \Big/ \sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i}\,, \tag{1.111}$$

$$c_p^* = \tilde{c}_p + \frac{1}{T^2}\left(\sum_{i=1}^{N}\frac{\nu_i h_i}{R_i}\right)^2 \Big/ \left[\sum_{i=1}^{N}\frac{\nu_i^2}{c_i^* R_i} - \left(\sum_{i=1}^{N}\nu_i\right)^2 \Big/ \sum_{i=1}^{N} c_i^* R_i\right]\,, \tag{1.112}$$

The equilibrium sound speed may be defined as

$$a_e^2 \equiv \left(\frac{\partial p}{\partial \rho}\right)_{s,c_i=c_i^*} = \left(\frac{\partial p^*}{\partial \rho}\right)_s , \tag{1.113}$$

where $p^* = p[\rho, T, c_i^*(\rho, T)] = p^*(\rho, T)$. Now, following procedures used for a single species gas, we consider $T = T(\rho, s)$ to obtain

$$a_e^2 = \left(\frac{\partial p^*}{\partial \rho}\right)_T + \left(\frac{\partial p^*}{\partial T}\right)_\rho \left(\frac{\partial T}{\partial \rho}\right)_s . \tag{1.114}$$

We can develop a relationship for $(\partial T/\partial \rho)_s$ by considering $e^* = e^*(v, T)$ and $T = T(v, s)$. Then $(\partial e^*/\partial v)_s = (\partial e^*/\partial v)_T + (\partial e^*/\partial T)_v (\partial T/\partial v)_s$. From Maxwell's relationships, (1.74) $(\partial e^*/\partial v)_s = -p$ and from (1.111) $c_v^* = (\partial e^*/\partial T)_v$. From reciprocity, (1.75), $(\partial e^*/\partial v)_T = -p^* - T(\partial p^*/\partial T)_v$. Putting this all together along with $\rho = 1/v$, gives

$$c_v^* \left(\frac{\partial T}{\partial \rho}\right)_s = \frac{T}{\rho^2} \left(\frac{\partial p^*}{\partial T}\right)_\rho . \tag{1.115}$$

Next we may write the derivatives of p^* in terms of the derivatives of p as

$$\left(\frac{\partial p^*}{\partial \rho}\right)_T = \left(\frac{\partial p}{\partial \rho}\right)_{T,c_i} + \sum_{i=1}^{N} \left(\frac{\partial p}{\partial c_i}\right)_{\rho,T} \left(\frac{\partial c_i^*}{\partial \rho}\right)_T , \tag{1.116}$$

$$\left(\frac{\partial p^*}{\partial T}\right)_\rho = \left(\frac{\partial p}{\partial T}\right)_{\rho,c_i} + \sum_{i=1}^{N} \left(\frac{\partial p}{\partial c_i}\right)_{\rho,T} \left(\frac{\partial c_i^*}{\partial T}\right)_\rho . \tag{1.117}$$

For a mixture of thermally perfect gases, $p = \rho \tilde{R} T$, so that $(\partial p/\partial \rho)_{T,c_i} = \tilde{R} T$, $(\partial p/\partial T)_{\rho,c_i} = \rho \tilde{R}$ and $(\partial p/\partial c_i)_{\rho,T} = \rho R_i T$. Substituting (1.115)–(1.117) into (1.114) yields

$$a_e^2 = \tilde{R} T + \rho T \sum_{i=1}^{N} R_i \left(\frac{\partial c_i^*}{\partial \rho}\right)_T + \frac{T}{c_v^*} \left[\tilde{R} + T \sum_{i=1}^{N} R_i \left(\frac{\partial c_i^*}{\partial T}\right)_\rho\right]^2 , \tag{1.118}$$

where the partial derivatives of c_i^* are given in (1.108) and (1.109).

Symmetric Diatomic Gas

The formulas given in the previous section simplify considerably for an equilibrium mixture of a dissociating, symmetric, diatomic gas. Consider a generic species A_2 which dissociates into A by

$$A_2 \rightleftharpoons 2A . \tag{1.119}$$

We will consider species 1 to be the diatomic molecule A_2 and species 2 to be the atom A. According to our convention, the stoichiometric coefficients are $\nu_1 = -1$ and $\nu_2 = 2$. Obviously the molecular weights of the species must be related by $\hat{M}_2 = \hat{M}_1/2$. Let us further assume that initially only A_2 is present so that $(c_1)_0 = 1$ and $(c_2)_0 = 0$. Then atomic conservation, (1.91) gives the following relationship between the equilibrium mass fractions:

$$c_2^* = 1 - c_1^* \,. \tag{1.120}$$

From the definition of K_p, (1.94)

$$p_1^{-1} p_2^2 = K_p(T) \,. \tag{1.121}$$

Assuming that each species is thermally perfect, $p_1 = c_1^* R_1 \rho T$ and $p_2 = c_2^* R_2 \rho T$. We may also note that $R_2 = \hat{R}/\hat{M}_2 = 2R_1$. Then, substituting into (1.121),

$$\frac{4(1 - c_1^*)^2}{c_1^*} \rho R_1 T = K_p(T) \,. \tag{1.122}$$

If we are given values of ρ and T, we may use (1.122) to determine c_1^*. If we know p and T, then we must use the mixture state equation $p = \rho \tilde{R} T$, where

$$\tilde{R} = (2 - c_1^*) R_1 \,. \tag{1.123}$$

Substituting $p/\tilde{R}$ for ρT in (1.122) gives

$$\frac{(1 - c_1^*)^2}{c_1^*(2 - c_1^*)} = \frac{1}{4p} K_p(T) \,. \tag{1.124}$$

Thus we may solve a quadratic equation for $c_1^*(p, T)$. One root will be non-physical with $c_1^* > 1$.

The mixture properties are now readily found by

$$\begin{aligned} e &= c_1^* e_1(T) + (1 - c_1^*) e_2(T) \,, \\ h &= c_1^* h_1(T) + (1 - c_1^*) h_2(T) \,, \\ s &= c_1^* s_1(p, T) + (1 - c_1^*) s_2(p, T) \,, \end{aligned} \tag{1.125}$$

where quantities with subscript 1 correspond to diatomic A_2 and generally include translational, rotational, vibrational and electronic excitation effects along with the heats of formation. Quantities with subscript 2 correspond to monatomic A and include translational and electronic excitation effects.

Frozen mixture values of the specific heats may be computed as

$$\tilde{c}_v = c_1^* c_{v_1}(T) + (1 - c_1^*) c_{v_2}(T) \,, \tag{1.126}$$

and

$$\tilde{c}_p = \tilde{c}_v + \tilde{R}\,, \tag{1.127}$$

and the frozen sound speed

$$a_f^2 = \frac{\tilde{c}_p}{\tilde{c}_v}\tilde{R}T\,. \tag{1.128}$$

Equilibrium values of the specific heats, c_v^*, c_p^* and the equilibrium sound speed may be computed using (1.111), (1.112) and (1.118). These relationships require the derivatives of c_1^* with respect to ρ and T found in (1.108)–(1.110). We find that

$$c_v^* = \tilde{c}_v + \frac{c_1^*(1-c_1^*)}{(1+c_1^*)}\frac{[e_2(T)-e_1(T)]^2}{R_1T^2}\,, \tag{1.129}$$

$$c_p^* = \tilde{c}_p + \frac{c_1^*(1-c_1^*)(2-c_1^*)}{2}\frac{[h_2(T)-h_1(T)]^2}{R_1T^2}\,, \tag{1.130}$$

and

$$a_e^2 = \left(\tilde{R} - \frac{c_1^*(1-c_1^*)}{(1+c_1^*)}R_1 + \frac{1}{c_v^*}\left[\tilde{R} + \frac{c_1^*(1-c_1^*)}{(1+c_1^*)}\frac{(e_2-e_1)}{T}\right]^2\right)T\,. \tag{1.131}$$

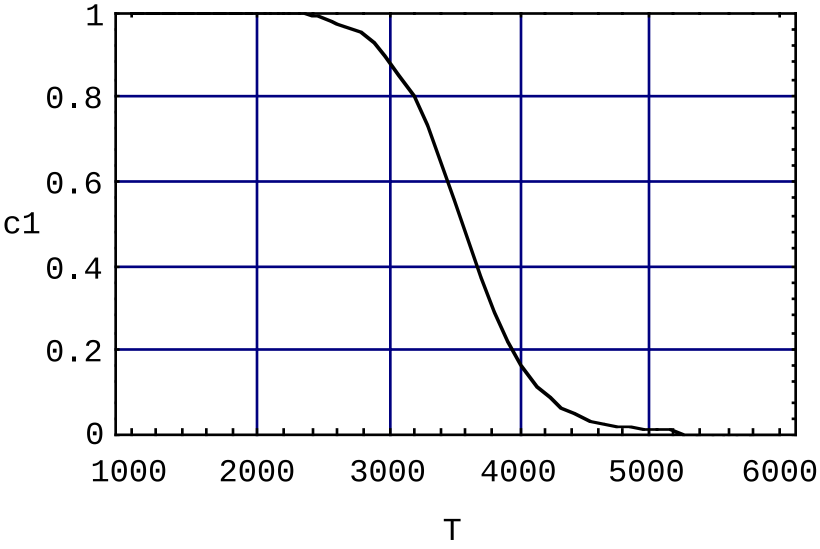

Figure 1.6. Equilibrium mass fraction distribution of dissociating oxygen O_2.

As an example, consider diatomic oxygen O_2 dissociating at a pressure of $1atm$. The mass fraction of O_2, c_1^* is plotted versus T in Fig. 1.6. We see that dissociation begins at approximately $2400K$ and is completed by approximately $5000K$. The thermal imperfection of the gas mixture is indicated in Fig. 1.7, where we plot

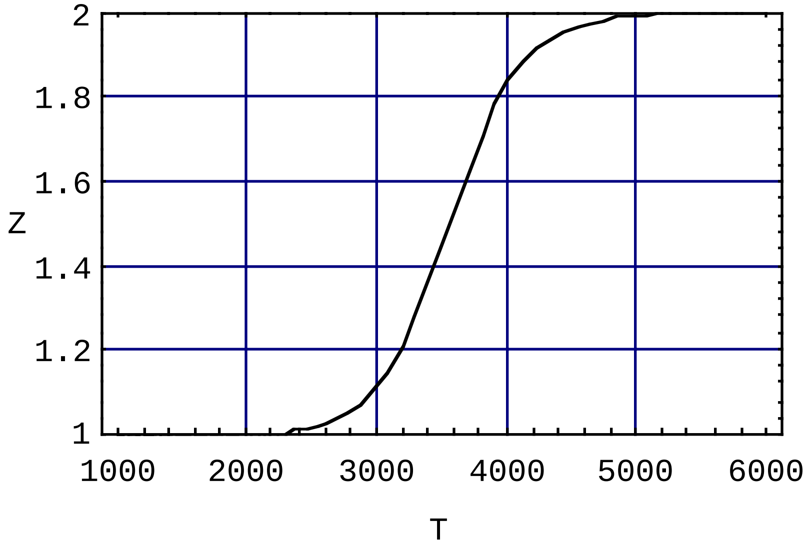

Figure 1.7. Thermal imperfection of a dissociating oxygen mixture, $Z = p/\rho R_1 T$.

$Z = p/\rho R_1 T$. Note that using the mixture state equation gives $Z = 2 - c_1^*$. The plot shows that $Z = 1$ before dissociation and $Z = 2$ after dissociation. This is consistent with the fact that $p = \rho R_1 T$ before dissociation and $p = \rho R_2 T = 2\rho R_1 T$ after dissociation.

The specific heat ratio, c_v^*/R_1 is plotted in Fig. 1.8 and the sound speed ratio, a/a_0 is plotted in Fig. 1.9, where $a_0^2 = 1.4 R_1 T$. In these plots both the equilibrium and frozen mixture values are presented, with the solid line corresponding to equilibrium and the dotted line corresponding to frozen. Only small differences in c_v values between the frozen and equilibrium cases. Small, but significant differences may be noted between the frozen and equilibrium sound speeds. In general, larger differences are seen in more complicated mixtures, such as air.

Equilibrium Air

As an example of an equilibrium gas mixture composed of a system of reactions, we consider a simplified model for air. For temperatures up to approximately $8000K$ air may be considered to be composed of O_2, N_2, O, N, NO, NO^+ and electrons e^-. The principal ionization reaction at these temperatures will involve NO. There are seven species and hence, seven unknown mass fractions. For the purpose of applying the law of mass action, we may assume the following reactions:

$$\begin{aligned}
\text{reaction1}: &\quad O_2 \rightleftharpoons O + O\,,\\
\text{reaction2}: &\quad N_2 \rightleftharpoons N + N\,,\\
\text{reaction3}: &\quad NO \rightleftharpoons N + O\,,\\
\text{reaction4}: &\quad NO \rightleftharpoons NO^+ + e^-\,.
\end{aligned}$$

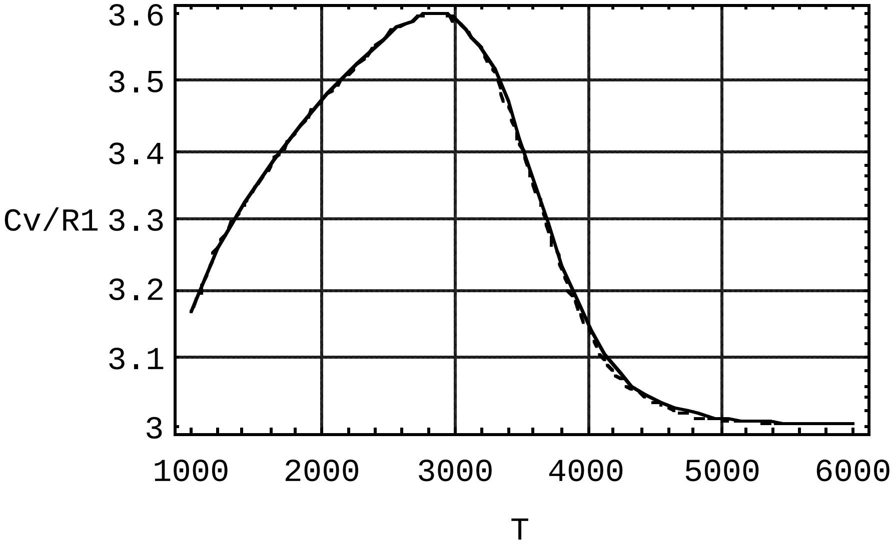

Figure 1.8. Equilibrium and frozen specific heat ratio for dissociating O_2.

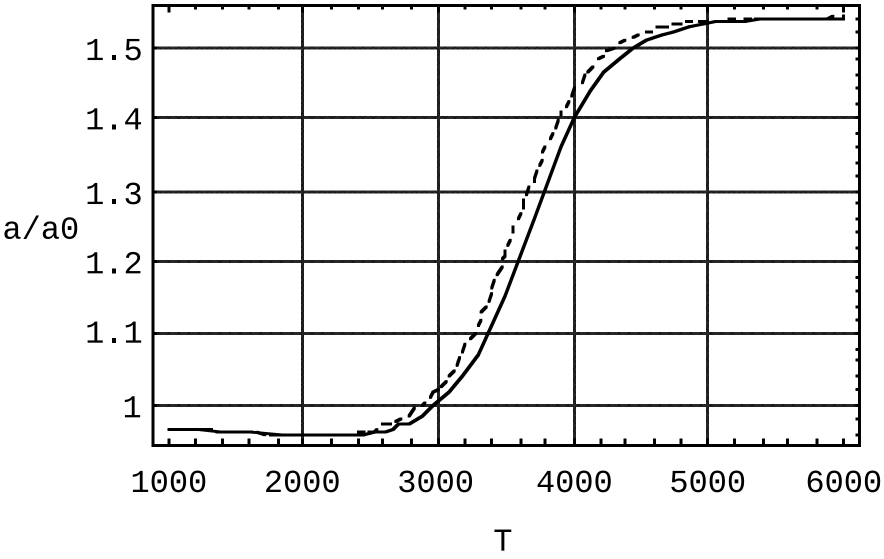

Figure 1.9. Equilibrium and frozen sound speed ratio for dissociating O_2, $a_0^2 = 1.4 R_1 T$.

Note, that the above system of reactions does not cover all the possible reactions for these species. However, for the purpose of equilibrium chemical composition, the above system is sufficient. It is shown in Vincenti and Kruger (1965), pp. 168–169, that adding additional reactions does not alter the resulting composition.

The law of mass action applied to each of these reactions gives

$$(c_{O_2} R_{O_2})^{-1} (c_O R_O)^2 = K_{p_1}(T)/\rho T \,, \qquad (1.132)$$

$$(c_{N_2}R_{N_2})^{-1}(c_N R_N)^2 = K_{p_2}(T)/\rho T\,, \tag{1.133}$$

$$(c_{NO}R_{NO})^{-1}(c_N R_N)(c_O R_O) = K_{p_3}(T)/\rho T\,, \tag{1.134}$$

$$(c_{NO}R_{NO})^{-1}(c_{NO^+}R_{NO^+})(c_{e^-}R_{e^-}) = K_{p_4}(T)/\rho T\,. \tag{1.135}$$

The remaining relationships to determine the mass fractions come from atomic and charge conservation. We cannot use the previously developed relations, (1.89)–(1.91), since these apply only to a single reaction (1.88). Instead, we can apply conservation directly to our mixture of 7 species. For the mixture, conservation of N atoms gives

$$2N_{N_2} + N_N + N_{NO} + N_{NO^+} = 2\left(N_{N_2}\right)_0\,, \tag{1.136}$$

and conservation of O atoms gives

$$2N_{O_2} + N_O + N_{NO} + N_{NO^+} = 2\left(N_{O_2}\right)_0\,, \tag{1.137}$$

where it has been assumed that the mixture initially contains only N_2 and O_2. Since the mixture was initially charge neutral, conservation of charge gives

$$N_{NO^+} = N_{e^-}\,. \tag{1.138}$$

Rewriting (1.136)–(1.138) in terms of mass fractions gives

$$2c_{N_2}R_{N_2} + c_N R_N + c_{NO}R_{NO} + c_{NO^+}R_{NO^+} = 2\left(c_{N_2}\right)_0 R_{N_2}\,, \tag{1.139}$$

$$2c_{O_2}R_{O_2} + c_O R_O + c_{NO}R_{NO} + c_{NO^+}R_{NO^+} = 2\left(c_{O_2}\right)_0 R_{O_2}\,, \tag{1.140}$$

and

$$c_{NO^+}R_{NO^+} = c_{e^-}R_{e^-}\,. \tag{1.141}$$

Equations (1.132)–(1.135) and (1.139)–(1.141) yield a system of seven nonlinear algebraic equations in seven unknowns provided that ρ and T are specified. If p and T are given, then the equation of state for a mixture of thermally perfect gases may be used to give the density in terms of the pressure. From (1.100) applied to this system, we obtain

$$\rho T = p/\left(c_{N_2}R_{N_2} + c_N R_N + c_{O_2}R_{O_2} + c_O R_O + c_{NO}R_{NO} + c_{NO^+}R_{NO^+} + c_{e^-}R_{e^-}\right)\,. \tag{1.142}$$

In general the resulting algebraic system may be solved interms of ρ and T or p and T. It turns out that this approach is generally not computationally efficient and methods which apply minimization techniques directly to the Gibbs free energy are often used, *e.g.*, White *et al.* (1958). A computer program based on this approach is by Gordon and McBride (1971). A review of the various approaches to equilibrium chemical composition are discussed in Liu and Vinokur (1989).

For dealing with thermodynamic properties of a known system, such as air in chemical equilibrium, often a curve-fitting approach is utilized. The procedure consists of computing equilibrium compositions of air over a very broad range of pressures, temperatures and densities. Then thermodynamic properties, such as internal energy, enthalpy, entropy, and sound speed are computed for every pair of values of pressure and temperature or density and temperature. Then, the thermodynamic properties are curve fit as functions of various pairs of thermodynamic state values, such as pressure and temperature. The curve fit coefficients are then stored in a computer program for the retrieval of any of the thermodynamic properties. This results in a very efficient method for obtaining thermodynamic data for a known system in chemical equilibrium. However, usually only the thermodynamic properties are curve fit and it is not possible to get the specific chemical composition. As will be seen in the next chapter, for equilibrium gas dynamic calculations, only the thermodynamic properties of the mixture are required.

An example of this curve fitting approach has been performed by Srinivasan *et al.* (1987), for equilibrium air. They presented curve fits of $p(e, \rho)$, $a(e, \rho)$, $T(e, \rho)$, $s(e, \rho)$, $T(p, \rho)$, $h(p, \rho)$, $\rho(p, s)$, $e(p, s)$ and $a(p, s)$. The range of validity of the curve fits are for temperatures up to $25,000K$ and densities from 10^{-7} to 10^3 amagats. ($1amagat = 1.292kg/m^3$, standard density for air).

The equilibrium composition of air used in the curve fits was found from the NASA program RGAS, which utilizes approaches such as that of Bailey (1967). Up to 30 species were considered for the high temperature calculations, including O_2, O, O^-, O_2^-, O^+, O_2^+, O^{++}, N_2, N, N^+, N^{++}, N_2^+, CO_2, CO, CO^+, C, C^+, C^{++}, NO_2, NO, N_2O, NO^+, A, A^+, A^{++}, Ne, Ne^+ and e^-.

The chemical composition of air varies considerably of a range of temperatures and densities. At room temperature, air consists of about 78% diatomic nitrogen, 21% diatomic oxygen, approximately 1% argon and traces of carbon dioxide. Note that these percentages are for the composition *by volume*. This means that the *mole fractions*, (1.68) of N_2, O_2 and A are, 0.78, 0.21 and 0.01, respectively. According to Srinivasan *et al.* (1987), for $10^{-2} < \rho/\rho_0 < 10$, where ρ_0 is 1 amagat, the equilibrium air composition may be classified in the following regimes:

1. $T < 2500K$. The chemically composition is approximately the same as that for room temperature.
2. $2500K < T < 4000K$. The oxygen dissociation regime; no significant nitrogen dissociation; slight NO formation.
3. $4000K < T < 8000K$. The nitrogen dissociation regime; Oxygen fully dissociated.
4. $T > 8000K$. Ionization of the atomic constituents.

An example of the chemical composition of air versus temperature at a density of 10^{-2} amagats is given in Fig. 1.12. This figure is from Vincenti and Kruger (1965), pp. 174 and is based on the calculations of Hilsenrath, Klein and Wooley.

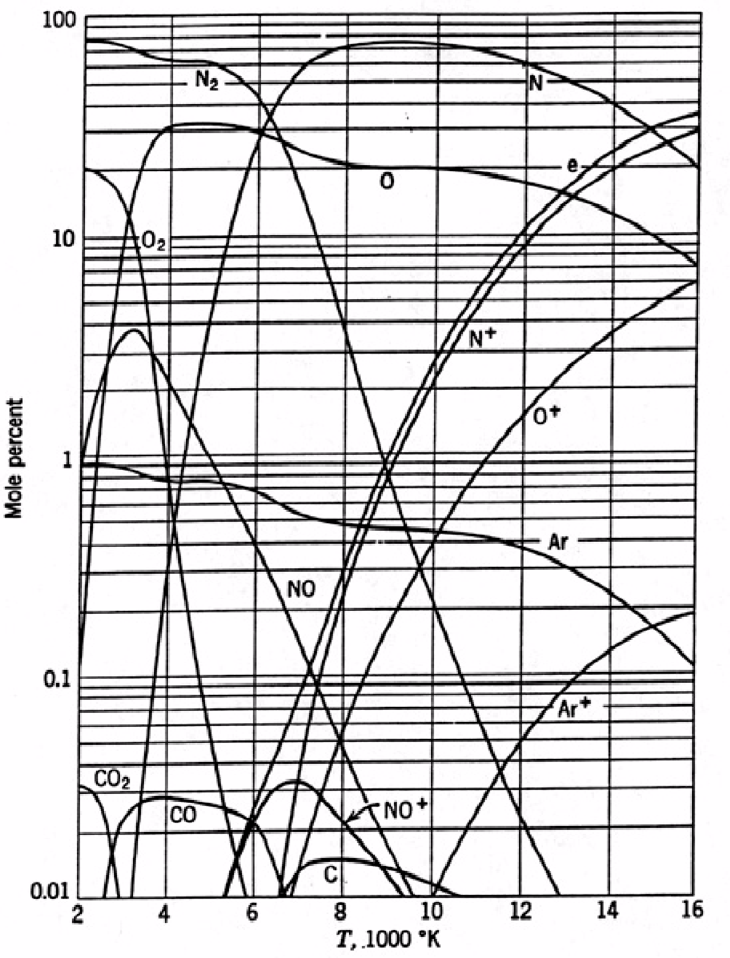

Figure 1.10. Equilibrium air composition at a density of 10^{-2} *amagats.*

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2. GOVERNING INVISCID EQUATIONS FOR EQUILIBRIUM FLOW

2.1 Continuum, Equilibrium Flow

One assumption that will be considered throughout these notes is the representation of the fluid as a continuum. We will speak of infinitesimal fluid elements or fluid particles, which are meant to contain statistically meaningful numbers of molecules. We can define macroscopic fluid properties by taking averages over the millions of molecules in our fluid element over a time, which is small compared to any characteristic flow time.

In this chapter, we will be developing the governing equations under the conditions of local thermodynamic equilibrium. We also assume that the fluid is not reacting or is in chemical equilibrium. This situation may be referred to as *equilibrium flow.* As the fluid particles move through a nonuniform flow field, it is assumed that there is sufficient time for an adequate number of molecular collisions to occur, so that the particles appear to be moving from one equilibrium state to the next. One consequence of this assumption is that the fluid may be considered inviscid. Clearly, these local equilibrium assumtions will be violated in regions of the fluid where very rapid changes occur over an extremely small distance, such as across shock waves and in boundary and shear layers. Even without such strong flow gradients, non-equilibrium vibrational energy and finite-rate chemistry effects are sometimes important. These will be discussed in a forthcoming chapter.

In dealing with equilibrium flows, we have seen in Chapter 1 that the thermodynamic state for an equilibrium mixture depends upon two state variables, §1.10. Thus we can develop the governing equations for the mixture itself, and not consider individual species conservation relations. It is important to recall that an equilibrium mixture of thermally perfect gases will not be thermally perfect.

The governing conservation laws may be directly developed in terms of a control volume which moves with a fixed group or aggregate of fluid particles. The governing conservation laws may be stated from the basic principles of conservation of mass, Newton's Second Law and the First Law of Thermodynamics as:

i. *Continuity: The time rate of change of the mass of a fixed group of fluid particles is zero.*
ii. *Momentum Conservation: The time rate of change of momentum of a fixed group of fluid particles is equal to the sum of the forces acting on the fluid particles.*
iii. *Energy Conservation: The time rate of change of total energy (internal and kinetic) of a fixed group of fluid particles is equal to the rate of heat added to the fluid particles plus the rate of work done on the fluid particles.*

The above statements utilize the particle or *Lagrangian* description of motion. However, it is often more convenient to deal with a control volume which is fixed in space, called the field or *Eulerian* description of motion. The conservation laws involve time derivatives of quantities associated with a group of fluid particles moving with the fluid. In the Eulerian description we consider a control volume which is fixed in space, with the fluid particles streaming through the volume. For a single fluid particle we can relate time derivatives in a Lagrangian frame to derivatives in an Eulerian frame through what is called the *substantial* derivative. For a group of fluid particles the relationship appears through the *Reynolds Transport Theorem.*

The rigorous, classical treatment of the relationship between the particle and field descriptions may be found in Truesdell (1964) and Serrin (1959). (It is interesting to note that the particle description is often ascribed to Lagrange. Historical evidence, as discussed by Truesdell, 1964, attributes this description to Euler.)

2.2 The Substantial Derivative

The conservation laws may be directly expressed in terms of time derivatives of mass, momentum and total energy following a fixed group of fluid particles. This derivative is often called the *substantial* or *material* derivative and is denoted as D/Dt. An expression may be derived for the substantial derivative of a property of a fluid, say $f(x, y, z, t)$. At a time t_1 a fluid particle is at a position x_1, y_1, z_1 with a property $f_1 = f(x_1, y_1, z_1, t_1)$ and at a time t_2 the same fluid particle has moved to a position x_2, y_2, z_2 with a property f_2. Expanding f_2 in a Taylor's series:

$$f_2 = f_1 + \left(\frac{\partial f}{\partial x}\right)_1 (x_2 - x_1) + \left(\frac{\partial f}{\partial y}\right)_1 (y_2 - y_1) + \left(\frac{\partial f}{\partial z}\right)_1 (z_2 - z_1) + \left(\frac{\partial f}{\partial t}\right)_1 (t_2 - t_1) + \cdots \tag{2.1}$$

The substantial derivative may then be formally written as:

$$\left(\frac{Df}{Dt}\right)_1 = \lim_{t_2 \to t_1} \left[\frac{f_2 - f_1}{t_2 - t_1}\right] = u_1 \left(\frac{\partial f}{\partial x}\right)_1 + v_1 \left(\frac{\partial f}{\partial y}\right)_1 + w_1 \left(\frac{\partial f}{\partial z}\right)_1 + \left(\frac{\partial f}{\partial t}\right)_1 , \tag{2.2}$$

where u, v and w are the velocity components in the x, y and z directions. In general:

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \boldsymbol{V} \cdot \nabla f \, . \tag{2.3}$$

We see that the substantial derivative consists of a local time derivative and a *convective* derivative associated with the motion of the fluid. Thus, even in a steady flow, where the local time derivative would be zero, the substantial derivative would, in general, not be zero.

2.3 Reynolds Transport Theorem

Here we will attempt to relate the basic conservation equations, mass, momentum and energy, to the fluid in a control volume fixed in space. The conservation laws involve the time rate change of *extensive* properties of the fixed group of fluid particles. These properties are mass, momentum and total energy, which we will denote using the generic symbol N. We can say that $N = \int \eta \, dM$ where η is the corresponding *intensive* property, (extensive property per unit mass) and M is the mass. We can then take the integral over the mass in terms of an integral over the volume τ by introducing the mass density ρ, such that $N = \iiint \rho\eta \, d\tau$. We see that for mass conservation, N corresponds to the total mass, so that $\eta = 1$. Similarly, for momentum conservation, $\eta = \boldsymbol{V}$, the velocity vector, or momentum per unit mass, and for energy conservation, $\eta = e + \boldsymbol{V}\cdot\boldsymbol{V}/2$, with e being the internal energy per unit mass and $\boldsymbol{V}\cdot\boldsymbol{V}/2$ the kinetic energy per unit mass.

A similar expression must be developed for the derivative

$$\frac{DN}{Dt} = \frac{D}{Dt} \iiint_{\mathcal{V}(t)} \rho\eta \, d\tau \,. \tag{2.4}$$

However, since the derivative follows a fixed group of fluid particles, the domain of integration, $\mathcal{V}$ is a function of time. We may recall Leibnitz' rule for differentiating a definite integral involving a parameter. If $I(t) = \int_{a(t)}^{b(t)} f(x,t)\, dx$, then the derivative

$$\frac{dI}{dt} = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}\, dt + f[b(t),t]\frac{db}{dt} - f[a(t),t]\frac{da}{dt} \,. \tag{2.5}$$

The derivative in (2.4) may be evaluated using a multi-dimensional form of Leibnitz' rule. A heuristic derivation can be simply made by considering a two-dimensional integral over a rectangular domain, sketched in Fig. 1., whose right and left sides, $x = r$ and $x = l$, and upper and bottom surfaces, $y = u$ and $y = b$, all move with the fluid and hence, vary with time. Note that we are only considering the *translation* of the fluid volume and not any *angular* or *shearing* deformations. Such deformations are due to shearing stresses acting on the control surface and are caused by viscous forces. Their contribution to the derivative in (2.4) will be negligible (in the limit as $\Delta t \to 0$).

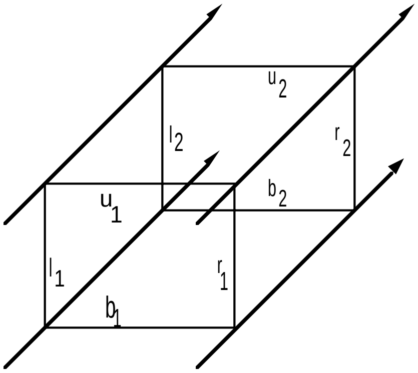

Figure 2.1. Control volume moving with the fluid.

We can define the two-dimensional counterpart of a volume integral as

$$I(t) = \int_{l(t)}^{r(t)} \int_{b(t)}^{u(t)} f(x,y,t)\, dxdy\,. \tag{2.6}$$

At a time t_1 the integral is

$$I_1 = I(t_1) = \int_{l_1}^{r_1} \int_{b_1}^{u_1} f(x,y,t_1)\, dxdy\,, \tag{2.7}$$

where $r_1 = r(t_1)$, etc. A similar formula results for I_2 evaluated at a nearby time t_2 where the fluid boundaries have moved to r_2, l_2, u_2 and b_2. (The time t_2 is taken to be *infinitesimally* close to time t_1, so that the fluid element may be assumed to remain rectangular.) By manipulating the limits of the x-integration as $\int_{l_2}^{r_2} = \int_{l_1}^{r_1} + \int_{r_1}^{r_2} - \int_{l_1}^{l_2}$ and with a similar procedure for the y-integration, we obtain

$$\begin{aligned} I_2 - I_1 = &\int_{l_1}^{r_1} \int_{b_1}^{u_1} [f(x,y,t_2) - f(x,y,t_1)]\, dydx + \int_{r_1}^{r_2} \int_{b_2}^{u_2} f(x,y,t_2)\, dydx \\ &- \int_{l_1}^{l_2} \int_{b_2}^{u_2} f(x,y,t_2)\, dydx + \int_{l_1}^{r_1} \int_{u_1}^{u_2} f(x,y,t_2)\, dydx - \int_{l_1}^{r_1} \int_{b_1}^{b_2} f(x,y,t_2)\, dydx \end{aligned} \tag{2.8}$$

Now from the mean-value theorem, $\int_{r_1}^{r_2} f(x,y,t)\, dx = (r_2 - r_1) f(\tilde{r}, y, t)$ where $r_1 \leq \tilde{r} \leq r_2$ with similar results for the integrals between l_1 and l_2, b_1 and b_2 and u_1 and u_2. Substituting these results

$$\begin{aligned} \left(\frac{DI}{Dt}\right)_1 = \lim_{t_2 \to t_1} \left[\frac{I_2 - I_1}{t_2 - t_1}\right] = \Bigg(&\int_l^r \int_b^u \frac{\partial f}{\partial t}\, dydx + \int_b^u \left[\frac{\partial r}{\partial t} f(r,y,t) - \frac{\partial l}{\partial t} f(l,y,t)\right] dy \\ &+ \int_l^r \left[\frac{\partial u}{\partial t} f(x,u,t) - \frac{\partial b}{\partial t} f(x,b,t)\right] dx \Bigg)_1 , \end{aligned} \tag{2.9}$$

where typical velocity terms are defined as $(\partial r/\partial t)_1 = (r_2 - r_1)/(t_2 - t_1)$and $(\partial b/\partial t)_1 = (b_2 - b_1)/(t_2 - t_1)$ in the limit as $t_2 \to t_1$. These velocities are the velocities normal to the boundaries. The last two integrals in the above expression correspond to the surface integral $\iint f\ \boldsymbol{V} \cdot \hat{\boldsymbol{n}}\, d\sigma$. The first term corresponds to the volume integral $\iiint (\partial f/\partial t)\, d\tau$, where the domain of integration is now the *fixed* domain $\mathcal{V}$ corresponding to volume initially occupied by the group of fluid particles. Since the domain is fixed, we may now take the derivative outside the integral. Thus

$$\frac{DN}{Dt} = \frac{d}{dt} \iiint_{\mathcal{V}} \rho\eta\, d\tau + \iint_{\mathcal{S}} \rho\eta \boldsymbol{V} \cdot \hat{\boldsymbol{n}}\, d\sigma\,, \tag{2.10}$$

where the domain $\mathcal{V}$ represents a control volume fixed in space, surrounded by a control surface $\mathcal{S}$. This is the well known *Reynolds Transport Theorem* which states that for a control volume fixed in space, the time derivative DN/Dt following a fixed group of fluid particles which initially occupy the control volume equals the time rate of change of N inside the control volume plus the net flux of N through the control surface surrounding the control volume.

2.4 Continuity

As stated in §1., the continuity equation is an expression of the conservation of mass of a fixed group of fluid particles, or $DM/Dt = 0$. Implicit here is the assumption that no mass is being created inside the fluid itself, (e.g. no mass sources). Note that we are dealing here with mass conservation of the entire mixture. If there are chemical reactions, then the mass of the individual species may be created or destroyed. However the total mass of the mixture will not change due to chemical reactions. This will be the case for reactions in or out of chemical equilibrium. For chemical equilibrium, only the global continuity equation is required, whereas for finite-rate chemistry, the individual species continuity equations are required.

Utilizing (2.10) with N taken to be the total mass and $\eta = 1$, we may express this law as:

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho\, d\tau + \iint_{\mathcal{S}} \rho \boldsymbol{V} \cdot \hat{\boldsymbol{n}}\, d\sigma = 0\,. \tag{2.11}$$

This integral form of the continuity equation which applies to any control volume fixed in space, $\mathcal{V}$, finite or infinitesimal. This equation can be put into differential form utilizing the divergence theorem (also known as Gauss's theorem). The theorem states that for a vector $\boldsymbol{A}$ which has continuous partial derivatives in a domain $\mathcal{V}$ which is bounded by a simple, piecewise smooth surface $\mathcal{S}$, then

$$\iiint_{\mathcal{V}} \nabla \cdot \boldsymbol{A}\, d\tau = \iint_{\mathcal{S}} \boldsymbol{A} \cdot \hat{\boldsymbol{n}}\, d\sigma\,. \tag{2.12}$$

Taking $\boldsymbol{A}$ in (2.12) as $\rho\boldsymbol{V}$, equation (2.11) then becomes the volume integral

$$\iiint_{\mathcal{V}} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{V})\right] d\tau = 0\,.$$

In general, the only ways that an integral expression can equal zero, is if the integrand is zero or if positive contributions in one part of the range of integration exactly cancel negative contributions in another part of the range. In this case, since expression (2.12) must be valid for any control volume $\mathcal{V}$, the only way for the integral to be zero is if the integrand is zero. Hence

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{V}) = 0\,, \tag{2.13}$$

which is the usual differential form of the continuity equation. It is important to note that the differential equation (2.13) is valid under the conditions implied by the divergence theorem. In particular the equation will be valid only in a domain where ρ and$\boldsymbol{V}$ have continuous partial derivatives. Thus the differential form of the continuity equation *will not be valid across discontinuities.* The same will be true for the differential forms of the other conservation laws. This issue has relevance in the numerical solution of the fluid dynamic equations with discontinuities, such as shock waves.

Another form of the differential continuity equation may be obtained by expanding in (2.13), $\nabla \cdot (\rho \boldsymbol{V}) = \rho(\nabla \cdot \boldsymbol{V}) + \boldsymbol{V} \cdot \nabla \rho$ and utilizing the substantial derivative (2.2), whereby

$$\frac{1}{\rho}\frac{D\rho}{Dt} + (\nabla \cdot \boldsymbol{V}) = 0\,. \tag{2.14}$$

We see that for a constant density fluid, $D\rho/Dt = 0$ and we obtain the incompressible form of the continuity equation as

$$\nabla \cdot \boldsymbol{V} = 0\,. \tag{2.15}$$

Note that this equation is valid for unsteady as well as steady incompressible flow.

2.5 Momentum

The momentum equation for fluid flow represents an expression of Newton's Second Law applied to a fixed group of fluid particles. It may be stated that the time rate of change of momentum of the fluid particles equals the sum of the forces acting on the fluid particles. Utilizing (1.10) with N representing the total momentum of the fluid particles and $\eta = \boldsymbol{V}$ we obtain

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho \boldsymbol{V}\, d\tau + \iint_{\mathcal{S}} \rho \boldsymbol{V}(\boldsymbol{V} \cdot \hat{\boldsymbol{n}})\, d\sigma = \boldsymbol{F}\,, \tag{2.16}$$

where $\boldsymbol{F}$ is the total force acting on the fluid particles. The total force may be considered to be composed of volume and surface forces. The volume forces act on each fluid particle within the control volume, and are sometimes called *body forces*. Two typical body forces are gravity forces and electromagnetic forces. We will represent the total volume force as $\iiint \rho \boldsymbol{g}\, d\tau$, where $\boldsymbol{g}$ is the body force per unit mass.

The surface forces can be considered to be composed of normal forces and tangential forces. For an inviscid fluid, where we neglect the effects of viscosity, the tangential forces will be zero and the normal forces are due only to the hydrostatic pressure and may be written as $-\iint p\hat{\boldsymbol{n}}\, d\sigma$.

The integral form of the momentum equation for an inviscid fluid becomes

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho \boldsymbol{V}\, d\tau + \iint_{\mathcal{S}} \rho \boldsymbol{V}(\boldsymbol{V} \cdot \hat{\boldsymbol{n}})\, d\sigma = -\iint_{\mathcal{S}} p\hat{\boldsymbol{n}}\, d\sigma + \iiint_{\mathcal{V}} \rho \boldsymbol{g}\, d\tau\,. \tag{2.17}$$

In order to obtain the differential equation corresponding to the above integral momentum equation it is necessary to utilize a tensor form of the divergence theorem. Using standard Cartesian tensor notation, for a second-order tensor T_{ij} then

$$\iiint_{\mathcal{V}} \partial_j T_{ij}\, d\tau = \iint_{\mathcal{S}} n_j T_{ij}\, d\sigma\,. \tag{2.18}$$

The same *caveat* about continuous partial derivatives implied in (2.12) also holds here. For the momentum equation, we may take $T_{ij} = \rho V_i V_j$ so that

$$\iiint_{\mathcal{V}} \left[\frac{\partial}{\partial t}(\rho V_j) + \partial_i(\rho V_i V_j) + \partial_j p - \rho g_j \right] d\tau = 0\,.$$

And again, as in (2.13), since the above must hold for any control volume $\mathcal{V}$, then the integrand must be zero, or

$$\frac{\partial}{\partial t}(\rho V_j) + \partial_i(\rho V_i V_j) + \partial_j p = \rho g_j\,. \tag{2.19}$$

When expanded for Cartesian coordinates, (2.19) may be recognized as the differential momentum equations in *conservation law* or *conservative* form. They may be written as

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) + \frac{\partial}{\partial y}(\rho uv) + \frac{\partial}{\partial z}(\rho uw) &= \rho g_x\,, \\ \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho uv) + \frac{\partial}{\partial y}(\rho v^2 + p) + \frac{\partial}{\partial z}(\rho vw) &= \rho g_y\,, \\ \frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial x}(\rho uw) + \frac{\partial}{\partial y}(\rho vw) + \frac{\partial}{\partial z}(\rho w^2 + p) &= \rho g_z\,. \end{aligned} \tag{2.20}$$

The above equations could have been derived using the usual vector form of Gauss' theorem (2.12) by first taking vector components of (2.18).

A convenient vector form of the differential momentum equations may be obtained by expanding the derivatives in (2.20) and utilizing continuity (2.13) such that

$$\frac{D\boldsymbol{V}}{Dt} = -\frac{1}{\rho}\nabla p + \boldsymbol{g}\,. \tag{2.21}$$

This momentum equation is in *non-conservation* form and is often referred to as *Euler's equation.*

2.6 Energy

The energy equation follows from a statement of the First Law of Thermodynamics applied to a fluid system. For a fixed group of fluid particle, this may be expressed as the time rate of change of total energy of the fluid is equal to the rate of heat added to fluid plus the rate of work done on the fluid. The rate of change of total energy may be expressed in an Eulerian frame using (2.10) with $\eta = e_0 = e + \boldsymbol{V}\cdot\boldsymbol{V}/2$, the total energy per unit mass. The rate of work done may be considered to be $\int \boldsymbol{V} \cdot d\boldsymbol{F}$ where $\boldsymbol{F}$ is the force acting on the fluid, which for an inviscid fluid, contains only pressure and body forces. Consistent with a model of an inviscid fluid we must also consider a non-heat conducting fluid since, according to equilibrium kinetic theory the coefficient of thermal conductivity is proportional to the coefficient of viscosity. Thus we obtain the integral form of the energy equation for an inviscid, non-conducting fluid

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho e_0 \, d\tau + \iint_{\mathcal{S}} \rho e_0 \boldsymbol{V} \cdot \hat{\boldsymbol{n}} \, d\sigma = \iiint_{\mathcal{V}} \rho \dot{q} \, d\tau - \iint_{\mathcal{S}} p \boldsymbol{V} \cdot \hat{\boldsymbol{n}} \, d\sigma + \iiint_{\mathcal{V}} \rho \boldsymbol{V} \cdot \boldsymbol{g} \, d\tau \, , \tag{2.22}$$

where $\dot{q}$ is the rate of heat added per unit mass. This term corresponds to heat added through internal heat sources in the fluid, such as heat released during chemical reactions. It is zero for an adiabatic fluid.

We can obtain the corresponding differential energy equation for an inviscid, non-heat conducting fluid in *conservation form* by applying the divergence theorem (2.12), and following the identical arguments made in dealing with the continuity equation (2.13) to obtain

$$\frac{\partial}{\partial t}(\rho e_0) + \nabla \cdot (\rho \boldsymbol{V} h_0) = \rho \dot{q} + \rho(\boldsymbol{V} \cdot \boldsymbol{g}) \, , \tag{2.23}$$

where the stagnation enthalpy, $h_0 = e_0 + p/\rho$. An alternative, *non-conservative form* of the differential energy equation may be obtained by expanding the derivatives in (2.23), utilizing continuity (2.13) and the substantial derivative (2.3) to obtain

$$\frac{De_0}{Dt} = \dot{q} - \frac{1}{\rho}\nabla \cdot (p\boldsymbol{V}) + \boldsymbol{V} \cdot \boldsymbol{g} \, . \tag{2.24}$$

2.7 Conservation and Non-conservation Forms

The conservation equations of fluid mechanics have been derived for an inviscid, non-heat conducting fluid. The equations have been derived in integral and differential form. The integral conservation equations, (2.11), (2.17) and (2.22) may be regarded as most general, since they apply to any control volume fixed in space. The size of the control volume may be finite or infinitesimal, and the geometry is arbitrary. The integral equations are often used in computational fluid mechanics as the starting point for the development of finite-volume or finite-element methods. However, this form of the governing equations is usually not amenable for analytic solutions. For these, we usually consider the governing partial differential equations.

Noting the previous development of the governing differential equations, it should be evident that the application of the divergence theorem required that flow properties contain continuous partial derivatives in the domain of interest. This precludes the general application of the governing differential equations in domains containing flow discontinuities. Discontinuities such as shock waves and contact surfaces are prevalent in high-speed gas dynamics. Of course, the differential equations may be used between discontinuities, just not across them.

This presents a difficulty for the numerical solution of the governing partial differential equations by finite-difference methods. One possibility is to use the method between discontinuities, with the discontinuity computed separately according to the appropriate *jump conditions*,(which are evaluated from the governing integral equations). The procedures are often referred to as *shock-fitting techniques* and are reviewed by Moretti (1986).

An alternate approach, is to apply the discretized form of the governing differential equations everywhere and to compute discontinuities as very steep, but continuous gradients through the concept of *weak solutions.* The theory of weak solutions is due to Lax (1963). In computing discontinuities in this manner, also referred to as *shock capturing*, it is imperative to use the *conservation law form* of the governing differential equations, (2.13), (2.19) and (2.23). It can be shown, e.g. Tannehill, Anderson and Pletcher (1997), that the discretized form of the conservative differential equations is consistent with the discretized form of the governing integral equations, and hence should be valid, in the sense of weak solutions, across discontinuities. For shock-fitting applications, or analytical developments, the conservative or non-conservative forms of the governing differential equations, (2.14), (2.21) and (2.24) are formally equivalent. The differential equations in conservative or conservation-law form are often written in matrix form, which for Cartesian coordinates and negligible body forces may be written as

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = 0\,, \tag{2.25}$$

where

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e_0 \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (\rho e_0 + p)u \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (\rho e_0 + p)v \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (\rho e_0 + p)w \end{pmatrix}. \tag{2.26}$$

2.8 Equation of state

The fluid dynamic equations for an inviscid, non-conducting gas in local thermodynamic and chemical equilibrium consist of a set of 5 equations in 6 unknowns, and an equation of state is needed to close the system. For example, we can consider the simplest example of solving (2.25). Typically these equations are solved by integrating or *marching* in time with spatial derivatives approximated using finite differences, finite-volume approximations or with finite elements. A simple Euler-explicit time integration would result in the semi-discrete form:

$$\frac{\mathbf{Q}^{n+1}_{i,j,k} - \mathbf{Q}^{n}_{i,j,k}}{\Delta t} + \left(\frac{\partial \mathbf{F}}{\partial x}\right)^n_{i,j,k} + \left(\frac{\partial \mathbf{G}}{\partial y}\right)^n_{i,j,k} + \left(\frac{\partial \mathbf{H}}{\partial z}\right)^n_{i,j,k} = 0\,. \tag{2.27}$$

This system would be solved from an initial value of $\mathbf{Q}^n_{i,j,k}$ specified at every mesh point (i,j,k). Then values of $\mathbf{F}^n_{i,j,k}$, $\mathbf{G}^n_{i,j,k}$, $\mathbf{H}^n_{i,j,k}$ must be evaluated along with approximations for their derivatives and finally $\mathbf{Q}^{n+1}_{i,j,k}$ is found at each (i,j,k) from (2.27).

However, in order to find the vector of fluxes $\mathbf{F}$, $\mathbf{G}$ or $\mathbf{H}$ from the vector of conserved variables $\mathbf{Q}$, an additional quantity must be specified. We can illustrate this by considering the components of $\mathbf{Q}$ to be denoted $q_1, q_2, \ldots, q_5$ so that from (2.25) $q_1 = \rho$, $q_2 = \rho u$, $q_3 = \rho v$, $q_4 = \rho w$ and $q_5 = \rho e_0$. Then if denote, for example, the elements of $\mathbf{F}$ as $f_1, f_2, \ldots, f_5$, we can easily see that $f_1 = \rho u = q_2$, $f_2 = \rho u^2 + p = q_2^2/q_1 + p$, $f_3 = \rho uv = q_2 q_3/q_1$, $f_4 = \rho uw = q_2 q_4/q_1$, $f_5 = (\rho e_0 + p)u = (q_5 + p)q_2/q_1$. Similar expressions may be written for $\mathbf{G}$ and $\mathbf{H}$. In order to close the system, we must be able to relate p to $q_1, q_2, \ldots, q_5$.

It should be clear that from the elements of $\mathbf{Q}$ we can easily determine the three velocity components $u = q_2/q_1$, $v = q_3/q_1$, $w = q_4/q_1$, the density $\rho = q_1$ and the internal energy per unit mass $e = e_0 - (u^2 + v^2 + w^2)/2 = q_5/q_1 - (q_2^2 + q_3^2 + q_4^2)/2q_1^2$. Hence, to close the system, we need to specify the value of p from values of ρ and e. This is easily accomplished for a gas which is both thermally perfect and calorically perfect. From (1.25) $p = \rho RT$ and from (1.34) $e = c_v T$, so that using $c_p - c_v = R$ and $\gamma = c_p/c_v$ we may write $p = (\gamma - 1)\rho e$. Then finally p is written in terms of $\mathbf{Q}$ as $p = (\gamma - 1)[q_5 - (q_2^2 + q_3^2 + q_4^2)/2q_1]$.

But the situation is much more complicated for a gas which is not perfect. For a case where we have a single species which is thermally perfect but calorically imperfect we would have $p = \rho RT$. But the energy relationship would be non-linear in T, such as from (1.33) as $e(T) = \int_0^T c_v(T)dT + h_f^0$. We know the value of e from $e = q_5/q_1 - (q_2^2 + q_3^2 + q_4^2)/2q_1^2$ and we have to iteratively solve for T from the equation for e and then use that value of T to find p. And this must be done at each mesh point and each time step.

It is even more complicated for a mixture of gases in chemical equilibrium. If we assume that the individual species are thermally perfect, then from (1.65) we have $p = \rho \tilde{R} T$ with $\tilde{R} = \sum c_i R_i$. But since the gas is in chemical equilibrium $c_i = c_i^*(\rho, T)$. We also have the internal energy of the mixture from (1.63) as $e = \sum c_i e_i(T)$. As we have shown above, from $\mathbf{Q}$, we know the state variables, ρ and e. In order to find p we would have to iteratively solve for T. Starting from a guessed value of $T = T^l$ and the known value of ρ, we could solve the law of mass action and atomic and charge conservation to yield the chemical composition $c_i^l = c_i^*(\rho, T^l)$ based on the assumed temperature. Then we can compute the internal energy of the mixture based on these values as $e^l = \sum c_i^l e_i(T^l)$. Then by comparing e^l to $e = q_5/q_1 - (q_2^2 + q_3^2 + q_4^2)/2q_1^2$ we can change the value of T^l based on the error $e - e^l$. We can continue iterating until e^l is close to e. When the system converges, then we have $p = \rho \tilde{R}^l T^l$. Note that each iteration involves solving for the complete chemical composition and that this must be done at each mesh point and each time step.

However the situation is considerably simplified if curve fits to the thermodynamic data are available, such as the TGAS routines for air of Srinivasan *et al.* (1987) discussed in §1.10. Then the curve fit $p = p(\rho, e)$ serves as the equation of state to close the system and does not require any iterations or calculation of the chemical composition. This is an enormous simplification.

2.9 Results from the energy equation

The energy equation for an inviscid non-heat conducting fluid has been developed in integral form, (2.22), in differential, conservation law form, (2.13), and in non-conservation form, (2.24). Other forms of (2.24) are often useful. To obtain an equation in terms of the internal energy per unit mass, $e = e_0 - \boldsymbol{V}\cdot\boldsymbol{V}/2$, we can utilize (2.14) and (2.21) to obtain

$$\frac{De}{Dt} = \dot{q} - \frac{p}{\rho}\nabla\cdot\boldsymbol{V}\,. \tag{2.28}$$

Stagnation enthalpy, stagnation temperature

We can get a useful form of the energy equation by introducing the enthalpy per unit mass, $h = e + p/\rho$, so that (2.28) becomes

$$\frac{Dh}{Dt} = \dot{q} + \frac{1}{\rho}\frac{Dp}{Dt}\,, \tag{2.29}$$

and in terms of the stagnation enthalpy per unit mass, $h_0 = h + \boldsymbol{V}\cdot\boldsymbol{V}/2$, we obtain

$$\frac{Dh_0}{Dt} = \dot{q} + \frac{1}{\rho}\frac{\partial p}{\partial t} + \boldsymbol{V}\cdot\boldsymbol{g}\,. \tag{2.30}$$

The above form of the energy equation, (2.30), is useful since it can be used to infer the conditions under which $Dh_0/Dt = 0$. Namely, for the steady flow of an adiabatic, inviscid, non-heat conducting fluid with negligible body forces, h_0 will be constant along particle paths, (or equivalently along streamlines, since the flow is steady). Furthermore, if the flow has *uniform* stagnation enthalpy upstream, then under the above conditions, the stagnation enthalpy will be constant.

Concepts involving the stagnation temperature, T_0, (also called the *total temperature*), are useful only for gases which are thermally and calorically perfect. Then $h = c_pT$ and we can define $h_0 = c_pT_0 = c_pT + \boldsymbol{V}\cdot\boldsymbol{V}/2$. From the above definition, we find that for a perfect gas,

$$\frac{T_0}{T} = 1 + \frac{\gamma - 1}{2}M^2\,, \tag{2.31}$$

where the Mach number $M = |\boldsymbol{V}|/a$ and the perfect-gas sound speed is given by (1.50). This relationship defines T_0 at a point in the flow where the temperature is T and the Mach number is M. The stagnation temperature will be constant everywhere in the flow field whenever h_0 is constant (and the gas may be considered thermally and calorically perfect). Another form of stagnation enthalpy that is used for perfect gases is $h_0 = a^2/(\gamma - 1) + \boldsymbol{V}\cdot\boldsymbol{V}/2$.

Entropy, isentropic relations and stagnation pressure

Additional forms of the energy equation can be obtained by introducing the entropy per unit mass, s. If we assume that the gas, if reacting, is in chemical equilibrium, then we have seen that the first and second laws of thermodynamics, (1.101), must apply locally as $Tds = dh - dp/\rho$. Any expression involving the total differential, such as the one above, is very general, since for $s = s(x, y, z, t)$, then $ds = (\partial s/\partial x)dx + (\partial s/\partial y)dy + (\partial s/\partial z)dz + (\partial s/\partial t)dt$ with the paths dx, dy, dz and dt, arbitrary. So that ds may be replaced by any of the partial derivatives. Then it is easy to show that

$$T\frac{Ds}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho}\frac{Dp}{Dt}\,, \tag{2.32}$$

and substituting (2.29),

$$T\frac{Ds}{Dt} = \dot{q}\,. \tag{2.33}$$

Thus we see that for any inviscid, non-heat conducting, adiabatic flow, the entropy will be constant along particle paths. Note that no assumptions regarding flow steadiness, body forces or equation of state were needed. One should recall that this relationship is not valid across discontinuities, where the entropy can jump.

Some useful relationships may be developed for isentropic flows when dealing with thermally and calorically perfect gases. Then applying (1.46) between state 1 and state 2, and using (1.25), we obtain the following isentropic relationships:

$$\frac{p_2}{p_1} = \left(\frac{\rho_2}{\rho_1}\right)^{\gamma} = \left(\frac{T_2}{T_1}\right)^{\gamma/\gamma-1}\,. \tag{2.34}$$

If the flow has constant T_0 along with constant entropy, then using (2.31),

$$\frac{p_2}{p_1} = \left(\frac{1+\frac{\gamma-1}{2}M_2^2}{1+\frac{\gamma-1}{2}M_1^2}\right)^{-\gamma/\gamma-1}\,. \tag{2.35}$$

Another useful quantity is the stagnation pressure p_0, also termed the total pressure. This quantity may be considered to be the pressure that a fluid would reach if it were brought to rest isentropically. For a perfect gas which has constant stagnation enthalpy, (2.35) applies for an isentropic process. Then dropping the subscript 2 and considering state 1 to correspond to the stagnation state we have

$$\frac{p}{p_0} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\gamma/\gamma-1}\,. \tag{2.36}$$

This equation may be considered to define p_0 for a perfect gas. But p_0 will be constant in the flow only if the flow is isentropic and has constant h_0.

The variation in p_0 for the non-isentropic flow of a perfect gas may be inferred from (1.44). Let us apply this equation to two parts of the flow denoted by subscripts 1 and 2, so that

$$\frac{s_2 - s_1}{c_v} = \log\left[\left(\frac{T_2}{T_1}\right)^{\gamma}\left(\frac{p_2}{p_1}\right)^{1-\gamma}\right]. \tag{2.37}$$

Using the definitions of stagnation temperature (2.31) and stagnation pressure (2.36) we find that

$$\frac{s_2 - s_1}{c_v} = \log\left[\left(\frac{T_{0_2}}{T_{0_1}}\right)^{\gamma}\left(\frac{p_{0_2}}{p_{0_1}}\right)^{1-\gamma}\right], \tag{2.38}$$

and if T_0 is constant in the flow, then

$$\frac{p_{0_2}}{p_{0_1}} = e^{-(s_2-s_1)/R}. \tag{2.39}$$

Thus if the entropy increases from 1 to 2, there will be a corresponding loss in stagnation pressure.

Generalized Crocco relationship

Another useful relationship regarding the entropy may be derived from (2.38). Using the preceding arguments about the total differential, it can be shown that (2.38) implies $T\nabla s = \nabla h - \nabla p/\rho$. Expressing $\nabla h = \nabla h_0 - \nabla(\boldsymbol{V}\cdot\boldsymbol{V}/2)$ and using the vector identity $\nabla(\boldsymbol{V}\cdot\boldsymbol{V}/2) = (\boldsymbol{V}\cdot\nabla)\boldsymbol{V} + \boldsymbol{V}\times(\nabla\times\boldsymbol{V})$ and the momentum equation (2.21) to obtain

$$T\nabla s = \nabla h_0 + \frac{\partial \boldsymbol{V}}{\partial t} - \boldsymbol{V}\times(\nabla\times\boldsymbol{V}) - \boldsymbol{g}. \tag{2.40}$$

This is the generalized Crocco relationship, sometimes referred to as the Crocco-Vaszonyi equation. An important result is that for a flow where h_0 is constant, (steady, inviscid, non-heat conducting, adiabatic, negligible body forces and uniform upstream h_0), then

$$T\nabla s = -\boldsymbol{V}\times\omega, \tag{2.41}$$

where the vorticity $\omega \equiv \nabla\times\boldsymbol{V}$. Thus, for the above conditions an isentropic flow will be irrotational and *vice versa.* (This excludes the pathological case of a Beltrami flow, where the vorticity is parallel to the velocity.)

We can also infer from (2.41) that for a steady, inviscid, non-heat conducting fluid with negligible body forces, that vorticity may be seen to arise due to changes in entropy and changes in stagnation enthalpy. Under these circumstances, we see that vorticity can be considered to evolve in the flow due to generation at shock waves or due to non-uniformities in entropy and stagnation enthalpy of the oncoming stream. This phenomena will be discussed in subsequent sections.

2.10 Coordinate Systems

The development of the governing equations in general coordinate systems is a formidable task, particularly when all the viscous and heat conduction terms are included. A general discussion of the problems associated with coordinate systems appears in Aris (1962) and the detailed resulting equations, with some restrictions, appears in the article by Vinokur (1974).

The transformation of the inviscid equations of gasdynamics is somewhat simpler. In the following we consider orthogonal curvilinear coordinates applied to non-conservation law equations and more general, non-orthogonal systems applied to the conservation-law form of the inviscid equations.

Orthogonal curvilinear coordinates

In dealing with theoretical results from the governing equations it is often useful to have the governing equations in other coordinate systems. The non-conservation form equations, (2.14), (2.21) and (2.24), are written in terms of vector operations, so that the task of developing the equations in other coordinate systems is simplified if we consider orthogonal curvilinear coordinates.

Consider a new coordinate system (ξ, η, ζ) which is a known function of the Cartesian coordinates (x, y, z) and that the inverse of the transformation exists such that

$$\begin{aligned} x &= x(\xi, \eta, \zeta)\,, \\ y &= y(\xi, \eta, \zeta)\,, \\ z &= z(\xi, \eta, \zeta)\,. \end{aligned} \tag{2.42}$$

For orthogonal curvilinear coordinates the unit vectors may be written as

$$\begin{aligned} \hat{\boldsymbol{i}}_\xi &= \frac{1}{h_\xi}\left(\frac{\partial x}{\partial \xi}\hat{\boldsymbol{i}} + \frac{\partial y}{\partial \xi}\hat{\boldsymbol{j}} + \frac{\partial z}{\partial \xi}\hat{\boldsymbol{k}}\right)\,, \\ \hat{\boldsymbol{i}}_\eta &= \frac{1}{h_\eta}\left(\frac{\partial x}{\partial \eta}\hat{\boldsymbol{i}} + \frac{\partial y}{\partial \eta}\hat{\boldsymbol{j}} + \frac{\partial z}{\partial \eta}\hat{\boldsymbol{k}}\right)\,, \\ \hat{\boldsymbol{i}}_\zeta &= \frac{1}{h_\zeta}\left(\frac{\partial x}{\partial \zeta}\hat{\boldsymbol{i}} + \frac{\partial y}{\partial \zeta}\hat{\boldsymbol{j}} + \frac{\partial z}{\partial \zeta}\hat{\boldsymbol{k}}\right)\,, \end{aligned} \tag{2.43}$$

where the metric terms are

$$\begin{aligned} h_\xi^2 &= \left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2\,, \\ h_\eta^2 &= \left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2 + \left(\frac{\partial z}{\partial \eta}\right)^2\,, \\ h_\zeta^2 &= \left(\frac{\partial x}{\partial \zeta}\right)^2 + \left(\frac{\partial y}{\partial \zeta}\right)^2 + \left(\frac{\partial z}{\partial \zeta}\right)^2\,. \end{aligned} \tag{2.44}$$

Consider the velocity vector which may be written in either coordinate system as

$$\boldsymbol{V} = u\hat{\boldsymbol{i}} + v\hat{\boldsymbol{j}} + w\hat{\boldsymbol{k}} = \tilde{u}\hat{\boldsymbol{i}}_\xi + \tilde{v}\hat{\boldsymbol{i}}_\eta + \tilde{w}\hat{\boldsymbol{i}}_\zeta\,. \tag{2.45}$$

The velocity components $\tilde{u}, \tilde{v}, \tilde{w}$ may be written in terms of u, v, w through the orthogonality relations $\tilde{u} = u\hat{\boldsymbol{i}} \cdot \hat{\boldsymbol{i}}_\xi + v\hat{\boldsymbol{j}} \cdot \hat{\boldsymbol{i}}_\xi + w\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{i}}_\xi$, *etc.*

For orthogonal curvilinear coordinate the vector operations *grad*, *div* and *curl* may be written in terms of the metrics as:

$$\nabla f = \frac{1}{h_\xi}\frac{\partial f}{\partial \xi}\hat{\boldsymbol{i}}_\xi + \frac{1}{h_\eta}\frac{\partial f}{\partial \eta}\hat{\boldsymbol{i}}_\eta + \frac{1}{h_\zeta}\frac{\partial f}{\partial x_\zeta}\hat{\boldsymbol{i}}_\zeta\,, \tag{2.46}$$

$$\nabla \cdot \boldsymbol{V} = \frac{1}{h_\xi h_\eta h_\zeta}\left[\frac{\partial}{\partial \xi}(h_\eta h_\zeta \tilde{u}) + \frac{\partial}{\partial \eta}(h_\zeta h_\xi \tilde{v}) + \frac{\partial}{\partial \zeta}(h_\xi h_\eta \tilde{w})\right]\,, \tag{2.47}$$

and

$$\nabla \times \boldsymbol{V} = \frac{1}{h_\xi h_\eta h_\zeta}\begin{vmatrix} h_\xi \hat{\boldsymbol{i}}_\xi & h_\eta \hat{\boldsymbol{i}}_\eta & h_\zeta \hat{\boldsymbol{i}}_\zeta \\ \partial/\partial\xi & \partial/\partial\eta & \partial/\partial\zeta \\ h_\xi \tilde{u} & h_\eta \tilde{v} & h_\zeta \tilde{w} \end{vmatrix}\,. \tag{2.48}$$

The above expressions may be used to transform most of the vector expressions in (2.14), (2.21) and (2.24) with the exception of the convective derivative of the velocity vector $(\boldsymbol{V} \cdot \nabla)\boldsymbol{V}$, (which appears in the substantial derivative terms. The derivatives must be taken of the components of $\boldsymbol{V}$ and their directions $\hat{\boldsymbol{i}}_\xi$, $\hat{\boldsymbol{i}}_\eta$, $\hat{\boldsymbol{i}}_\zeta$. These operations are best accomplished using the vector identity

$$(\boldsymbol{V} \cdot \nabla)\boldsymbol{V} = \nabla \cdot (\boldsymbol{V}\cdot\boldsymbol{V}/2) - \boldsymbol{V} \times (\nabla \times \boldsymbol{V})\,. \tag{2.49}$$

The component of the convective velocity derivative in the ξ-direction becomes

$$\begin{aligned}[(\boldsymbol{V} \cdot \nabla)\boldsymbol{V}] \cdot \hat{\boldsymbol{i}}_\xi = {} & \frac{\tilde{u}}{h_\xi}\frac{\partial \tilde{u}}{\partial \xi} + \frac{\tilde{v}}{h_\eta}\frac{\partial \tilde{u}}{\partial \eta} + \frac{\tilde{w}}{h_\zeta}\frac{\partial \tilde{u}}{\partial \zeta} \\ & + \frac{\tilde{v}}{h_\xi h_\eta}\big(\tilde{u}\frac{\partial h_\xi}{\partial \eta} - \tilde{v}\frac{\partial h_\eta}{\partial \xi}\big) + \frac{\tilde{w}}{h_\xi h_\zeta}\big(\tilde{u}\frac{\partial h_\xi}{\partial \zeta} - \tilde{w}\frac{\partial h_\zeta}{\partial \xi}\big)\,.\end{aligned} \tag{2.50}$$

The first three terms represent $\boldsymbol{V} \cdot \tilde{u}$ and the last two terms are associated with the coordinate directions not being constant. The other two components of $(\boldsymbol{V} \cdot \nabla)\boldsymbol{V}$ may be obtained from (2.50) by cyclic permutation of the indices, ($\xi \to \eta$, $\eta \to \zeta$, $\zeta \to \xi$).

Fortunately, most coordinate systems of interest have relatively simple metric terms which results in considerable simplification of the general expressions. For example, for circular cylindrical coordinates, taking $\xi = r$, $\eta = \theta$ and $\zeta = z$ with the relations $x = r\cos\theta$, $y = r\sin\theta$ and $z = z$, the metrics are simply $h_r = 1$, $h_\theta = r$ and $h_z = 1$. The relations for spherical coordinates are only slightly more complicated. Taking $\xi = r$, $\eta = \phi$ and $\zeta = \theta$ with the relations $x = r\sin\phi\cos\theta$, $y = r\sin\phi\sin\theta$ and $z = r\cos\phi$, the metrics become $h_r = 1$, $h_\phi = r$ and $h_\theta = r\sin\phi$.

Generalized conservation form

In solving the governing equations with numerical methods we often need the governing inviscid equations in conservation law form in a grid-aligned coordinate system which is not necessarily orthogonal. Let us assume that we have a new curvilinear coordinate system ξ, η, ζ given by

$$\left.\begin{aligned} \xi &= \xi(x,y,z,t)\,, \\ \eta &= \eta(x,y,z,t)\,, \\ \zeta &= \zeta(x,y,z,t)\,, \\ \tau &= t \end{aligned}\right. . \tag{2.51}$$

where the coordinates may also be a function of time.

We can express the governing Cartesian equations, (2.25) in terms of the new coordinates ξ, η, ζ, τ by applying the chain rule, whereby

$$\begin{aligned} \frac{\partial \boldsymbol{Q}}{\partial t} &= \frac{\partial \boldsymbol{Q}}{\partial \xi}\xi_t + \frac{\partial \boldsymbol{Q}}{\partial \eta}\eta_t + \frac{\partial \boldsymbol{Q}}{\partial \zeta}\zeta_t + \frac{\partial \boldsymbol{Q}}{\partial \tau}\,, \\ \frac{\partial \boldsymbol{F}}{\partial x} &= \frac{\partial \boldsymbol{F}}{\partial \xi}\xi_x + \frac{\partial \boldsymbol{F}}{\partial \eta}\eta_x + \frac{\partial \boldsymbol{F}}{\partial \zeta}\zeta_x\,, \\ \frac{\partial \boldsymbol{G}}{\partial y} &= \frac{\partial G}{\partial \xi}\xi_y + \frac{\partial \boldsymbol{G}}{\partial \eta}\eta_y + \frac{\partial \boldsymbol{G}}{\partial \zeta}\zeta_y\,, \\ \frac{\partial \boldsymbol{H}}{\partial z} &= \frac{\partial \boldsymbol{H}}{\partial \xi}\xi_z + \frac{\partial \boldsymbol{H}}{\partial \eta}\eta_z + \frac{\partial \boldsymbol{H}}{\partial \zeta}\zeta_z\,, \end{aligned} \tag{2.52}$$

where the subscripts are used here to indicate partial differentiation, *e.g.*, $\xi_t \equiv \partial\xi/\partial t$. In order to develop the equations in conservation-law form, we substitute (2.52) into (2.25) and divide by the Jacobian of the transformation, J defined by

$$J = \left|\frac{\partial(\xi,\eta,\zeta)}{\partial(x,y,z)}\right|\,. \tag{2.53}$$

Note that we must now assume that the transformation is non-singular, so that J will not be zero or infinite. Upon manipulating the resulting equation we obtain

$$\begin{aligned} \frac{\partial}{\partial \tau}\left(\frac{\boldsymbol{Q}}{J}\right) + \frac{\partial}{\partial \xi}\left(\frac{\xi_t}{J}\boldsymbol{Q} + \frac{\xi_x}{J}\boldsymbol{F} + \frac{\xi_y}{J}\boldsymbol{G} + \frac{\xi_z}{J}\boldsymbol{H}\right) + \frac{\partial}{\partial \eta}\left(\frac{\eta_t}{J}\boldsymbol{Q} + \frac{\eta_x}{J}\boldsymbol{F} + \frac{\eta_y}{J}\boldsymbol{G} + \frac{\eta_z}{J}\boldsymbol{H}\right) \\ + \frac{\partial}{\partial \zeta}\left(\frac{\zeta_t}{J}\boldsymbol{Q} + \frac{\zeta_x}{J}\boldsymbol{F} + \frac{\zeta_y}{J}\boldsymbol{G} + \frac{\zeta_z}{J}\boldsymbol{H}\right) = \boldsymbol{Q}T_1 + \boldsymbol{F}T_2 + \boldsymbol{G}T_3 + \boldsymbol{H}T_4 \end{aligned} \tag{2.54}$$

where

$$\begin{aligned}
T_1 &\equiv \frac{\partial}{\partial \xi}\left(\frac{\xi_t}{J}\right) + \frac{\partial}{\partial \eta}\left(\frac{\eta_t}{J}\right) + \frac{\partial}{\partial \zeta}\left(\frac{\zeta_t}{J}\right) + \frac{\partial}{\partial \tau}\left(\frac{1}{J}\right) \,, \\
T_2 &\equiv \frac{\partial}{\partial \xi}\left(\frac{\xi_x}{J}\right) + \frac{\partial}{\partial \eta}\left(\frac{\eta_x}{J}\right) + \frac{\partial}{\partial \zeta}\left(\frac{\zeta_x}{J}\right) \,, \\
T_3 &\equiv \frac{\partial}{\partial \xi}\left(\frac{\xi_y}{J}\right) + \frac{\partial}{\partial \eta}\left(\frac{\eta_y}{J}\right) + \frac{\partial}{\partial \zeta}\left(\frac{\zeta_y}{J}\right) \,, \\
T_4 &\equiv \frac{\partial}{\partial \xi}\left(\frac{\xi_z}{J}\right) + \frac{\partial}{\partial \eta}\left(\frac{\eta_z}{J}\right) + \frac{\partial}{\partial \zeta}\left(\frac{\zeta_z}{J}\right) \,.
\end{aligned} \tag{2.55}$$

We can simplify the above equations by introducing the inverse-transformation

$$\left.\begin{aligned}
x &= x(\xi, \eta, \zeta, \tau) \,, \\
y &= y(\xi, \eta, \zeta, \tau) \,, \\
z &= z(\xi, \eta, \zeta, \tau) \,, \\
t &= \tau
\end{aligned}\right. . \tag{2.56}$$

Taking the differential of this transformation yields

$$\begin{pmatrix} dx \\ dy \\ dz \\ dt \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta & x_\zeta & x_\tau \\ y_\xi & y_\eta & y_\zeta & y_\tau \\ z_\xi & z_\eta & x_\zeta & z_\tau \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} d\xi \\ d\eta \\ d\zeta \\ d\tau \end{pmatrix} . \tag{2.57}$$

Similarly, taking the differential of the original transformation (2.51) gives

$$\begin{pmatrix} d\xi \\ d\eta \\ d\zeta \\ d\tau \end{pmatrix} = \begin{pmatrix} \xi_x & \xi_y & \xi_z & \xi_t \\ \eta_x & \eta_y & \eta_z & \eta_t \\ \zeta_x & \zeta_y & \zeta_z & \zeta_t \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} dx \\ dy \\ dz \\ dt \end{pmatrix} . \tag{2.58}$$

Thus we see that

$$\begin{pmatrix} \xi_x & \xi_y & \xi_z & \xi_t \\ \eta_x & \eta_y & \eta_z & \eta_t \\ \zeta_x & \zeta_y & \zeta_z & \zeta_t \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta & x_\zeta & x_\tau \\ y_\xi & y_\eta & y_\zeta & y_\tau \\ z_\xi & z_\eta & x_\zeta & z_\tau \\ 0 & 0 & 0 & 1 \end{pmatrix}^{-1} . \tag{2.59}$$

Solving for the inverse of the transformation matrix results in

$$\frac{1}{J}\begin{pmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix} = \begin{pmatrix} y_\eta z_\zeta - z_\eta y_\zeta & z_\eta x_\xi - x_\eta z_\xi & x_\eta y_\zeta - y_\eta x_\zeta \\ x_\xi y_\zeta - y_\xi z_\zeta & x_\xi z_\zeta - z_\xi x_\zeta & y_\xi x_\zeta - x_\xi y_\zeta \\ y_\xi z_\eta - z_\xi y_\eta & z_\xi x_\eta - x_\xi z_\eta & x_\xi y_\eta - y_\xi x_\eta \end{pmatrix} , \tag{2.60}$$

and

$$\frac{1}{J}\begin{pmatrix}\xi_t\\ \eta_t\\ \zeta_t\end{pmatrix} = -\begin{pmatrix} x_\tau(y_\eta z_\zeta - z_\eta y_\zeta) + y_\tau(z_\eta x_\xi - x_\eta z_\xi) + z_\tau(x_\eta y_\zeta - y_\eta x_\zeta)\\ x_\tau(x_\xi y_\zeta - y_\xi z_\zeta) + y_\tau(x_\xi z_\zeta - z_\xi x_\zeta) + z_\tau(y_\xi x_\zeta - x_\xi y_\zeta)\\ x_\tau(y_\xi z_\eta - z_\xi y_\eta) + y_\tau(z_\xi x_\eta - x_\xi z_\eta) + z_\tau(x_\xi y_\eta - y_\xi x_\eta)\end{pmatrix}. \tag{2.61}$$

From (2.60) and (2.61), it can be verified that if the transformation (2.51) possesses continuous partial derivatives, the terms T_1–T_4 in (2.54) will be zero. For example, T_2 defined in (2.55), may be written as

$$T_2 = \frac{\partial}{\partial\xi}(y_\eta z_\zeta - z_\eta y_\zeta) + \frac{\partial}{\partial\eta}(x_\xi y_\zeta - y_\xi z_\zeta) + \frac{\partial}{\partial\zeta}(y_\xi z_\eta - z_\xi y_\eta)\,,$$

which will be zero if $y_{\eta\xi} = y_{\xi\eta}$, $z_{\zeta\xi} = z_{\xi\zeta}$, *etc.*

Then, from (2.54), the governing inviscid equations in conservation-law form may be written as

$$\frac{\partial\hat{\boldsymbol{Q}}}{\partial\tau} + \frac{\partial\hat{\boldsymbol{F}}}{\partial\xi} + \frac{\partial\hat{\boldsymbol{G}}}{\partial\eta} + \frac{\partial\hat{\boldsymbol{H}}}{\partial\zeta} = 0\,, \tag{2.62}$$

where

$$\begin{aligned}
\hat{\boldsymbol{Q}} &\equiv \frac{\boldsymbol{Q}}{J}\,,\\
\hat{\boldsymbol{F}} &\equiv \frac{\xi_t}{J}\boldsymbol{Q} + \frac{\xi_x}{J}\boldsymbol{F} + \frac{\xi_y}{J}\boldsymbol{G} + \frac{\xi_z}{J}\boldsymbol{H}\,,\\
\hat{\boldsymbol{G}} &\equiv \frac{\eta_t}{J}\boldsymbol{Q} + \frac{\eta_x}{J}\boldsymbol{F} + \frac{\eta_y}{J}\boldsymbol{G} + \frac{\eta_z}{J}\boldsymbol{H}\,,\\
\hat{\boldsymbol{H}} &\equiv \frac{\zeta_t}{J}\boldsymbol{Q} + \frac{\zeta_x}{J}\boldsymbol{F} + \frac{\zeta_y}{J}\boldsymbol{G} + \frac{\zeta_z}{J}\boldsymbol{H}\,.
\end{aligned} \tag{2.63}$$

For the case where the transformation does not depend upon time, the equations often are written as (2.62) with

$$\hat{\boldsymbol{F}} = \frac{h_\xi}{J}\begin{pmatrix}\rho\hat{u}\\ \rho u\hat{u}+\hat{\xi}_x p\\ \rho v\hat{u}+\hat{\xi}_y p\\ \rho w\hat{u}+\hat{\xi}_z p\\ (\rho e_0+p)\hat{u}\end{pmatrix}, \qquad \hat{\boldsymbol{G}} = \frac{h_\eta}{J}\begin{pmatrix}\rho\hat{v}\\ \rho u\hat{v}+\hat{\eta}_x p\\ \rho v\hat{v}+\hat{\eta}_y p\\ \rho w\hat{v}+\hat{\eta}_z p\\ (\rho e_0+p)\hat{v}\end{pmatrix}, \qquad \hat{\boldsymbol{H}} = \frac{h_\zeta}{J}\begin{pmatrix}\rho\hat{w}\\ \rho u\hat{w}+\hat{\zeta}_x p\\ \rho v\hat{w}+\hat{\zeta}_y p\\ \rho w\hat{w}+\hat{\zeta}_z p\\ (\rho e_0+p)\hat{w}\end{pmatrix}, \tag{2.64}$$

where the metric terms are defined by

$$h_\xi \equiv (\xi_x^2+\xi_y^2+\xi_z^2)^{1/2}\,, \qquad h_\eta \equiv (\eta_x^2+\eta_y^2+\eta_z^2)^{1/2}\,, \qquad h_\zeta \equiv (\zeta_x^2+\zeta_y^2+\zeta_z^2)^{1/2}\,, \tag{2.65}$$

the normalized transformation derivatives given as

$$\begin{pmatrix}\hat{\xi}_x\\ \hat{\xi}_y\\ \hat{\xi}_z\end{pmatrix} = \frac{1}{h_\xi}\begin{pmatrix}\xi_x\\ \xi_y\\ \xi_z\end{pmatrix}, \qquad \begin{pmatrix}\hat{\eta}_x\\ \hat{\eta}_y\\ \hat{\eta}_z\end{pmatrix} = \frac{1}{h_\eta}\begin{pmatrix}\eta_x\\ \eta_y\\ \eta_z\end{pmatrix}, \qquad \begin{pmatrix}\hat{\zeta}_x\\ \hat{\zeta}_y\\ \hat{\zeta}_z\end{pmatrix} = \frac{1}{h_\zeta}\begin{pmatrix}\zeta_x\\ \zeta_y\\ \zeta_z\end{pmatrix}, \tag{2.66}$$

and the contravariant velocity components

$$\begin{aligned}\hat{u} &= \hat{\xi}_x u + \hat{\xi}_y v + \hat{\xi}_z w\,,\\ \hat{v} &= \hat{\eta}_x u + \hat{\eta}_y v + \hat{\eta}_z w\,,\\ \hat{w} &= \hat{\zeta}_x u + \hat{\zeta}_y v + \hat{\zeta}_z w\,.\end{aligned} \tag{2.67}$$

2.11 References Chapter 2

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3. DISCONTINUITIES

3.1 General Jump Conditions

It is known that the equation of motion for inviscid fluids may contain surfaces of discontinuity in some of the flow variables. For adiabatic flows, the discontinuities correspond to shock waves and contact surfaces. For non-adiabatic fluids, which will not be discussed here, detonation discontinuities, as described in Courant and Friedrichs (1948), may exist.

As discussed in the previous section, conditions across surfaces of discontinuity are governed by the integral conservation equations. Let us assume that a surface ϑ exists across which some of the flow variables may be discontinuous. We assume that ϑ moves through the flow with a velocity $W\hat{\boldsymbol{n}}_\vartheta$, where $\hat{\boldsymbol{n}}_\vartheta$ is a unit vector normal to the ϑ surface. (If the flow were steady, ϑ would be stationary and $W = 0$.) Consider an infinitesimal control volume of dimension Δs by Δn, which is fixed in space, with the surface ϑ bisecting it at a time t. In the sketch below, we show the orientation of the control volume and discontinuity at a time t, and after a very small interval of time Δt. The control volume is so small that we may assume that conditions to the left of ϑ are nearly constant and are denoted by a subscript 1 and the nearly constant conditions to the right of ϑ are denoted by subscript 2.

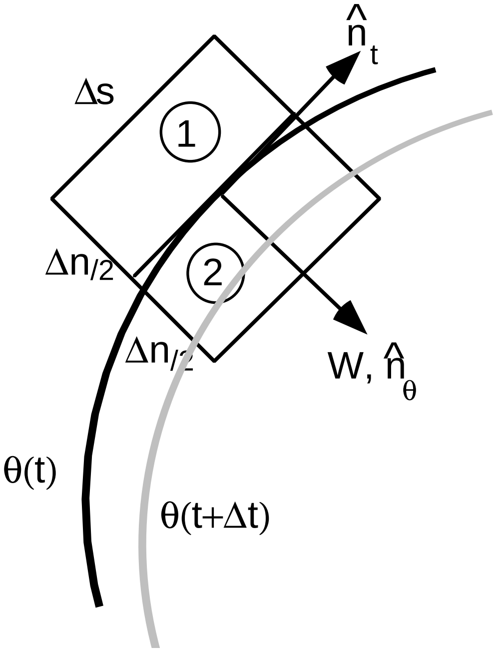

Figure 3.1. Control volume near a discontinuity.

We will apply the governing integral conservation equations across this control volume. The net flux of a generic intensive quantity η may be evaluated as

$$\begin{aligned}\iint_{\mathcal{S}} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}}\,d\sigma = \int_{\Delta s} \rho_1\eta_1(-\boldsymbol{V}_1\cdot\hat{\boldsymbol{n}}_\vartheta)\,ds + \int_{\Delta s} \rho_2\eta_2(+\boldsymbol{V}_2\cdot\hat{\boldsymbol{n}}_\vartheta)\,ds \\ + \int_{\Delta n/2} \rho_1\eta_1(+\boldsymbol{V}_1\cdot\hat{\boldsymbol{n}}_t)\,ds + \int_{\Delta n/2} \rho_1\eta_1(-\boldsymbol{V}_1\cdot\hat{\boldsymbol{n}}_t)\,ds \\ + \int_{\Delta n/2} \rho_2\eta_2(+\boldsymbol{V}_2\cdot\hat{\boldsymbol{n}}_t)\,ds + \int_{\Delta n/2} \rho_2\eta_2(-\boldsymbol{V}_2\cdot\hat{\boldsymbol{n}}_t)\,ds\end{aligned}$$

where the terms integrated over $\Delta n/2$ are seen to cancel each other. In the very small control volume, the integrands above may be assumed to be constant. Introducing the notation that $[\![f]\!]$ for the *jump in f*, where $[\![f]\!] \equiv f_2 - f_1$ we obtain

$$\iint_{\mathcal{S}} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}}\,d\sigma = (\rho_2\eta_2\boldsymbol{V}_2\cdot\hat{\boldsymbol{n}}_\vartheta - \rho_1\eta_1\boldsymbol{V}_1\cdot\hat{\boldsymbol{n}}_\vartheta)\,\Delta s = [\![\rho\eta\boldsymbol{V}\cdot\hat{\boldsymbol{n}}_\vartheta]\!]\Delta s\,.$$

The time derivative terms may be evaluated as

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho\eta\,d\tau = \lim_{\Delta t\to 0}\left[\left(\iiint \rho\eta\,d\tau\right)_{t+\Delta t} - \left(\iiint \rho\eta\,d\tau\right)_{t}\right]/\Delta t\,,$$

where it is seen that

$$\left(\iiint \rho\eta\,d\tau\right)_t = \left[\rho_1\eta_1\Delta s\Delta n/2 + \rho_2\eta_2\Delta s\Delta n/2\right]_t\ ,$$

and

$$\left(\iiint \rho\eta\,d\tau\right)_{t+\Delta t} = \left[\rho_1\eta_1\Delta s(\Delta n/2 + W\Delta t) + \rho_2\eta_2\Delta s(\Delta n/2 - W\Delta t)\right]_{t+\Delta t}\ .$$

Utilizing a Taylor's series expansion, we have $(\rho\eta)_{t+\Delta t} = (\rho\eta)_t + \partial(\rho\eta)/\partial t\,\Delta t + \cdots$. Then we find

$$\frac{d}{dt}\iiint_{\mathcal{V}} \rho\eta\,d\tau = -[\![\rho\eta]\!]W\Delta s + \frac{1}{2}\left[\frac{\partial}{\partial t}(\rho_1\eta_1) + \frac{\partial}{\partial t}(\rho_2\eta_2)\right]\Delta s\,\Delta n\,,$$

The terms containing time derivatives above are higher order than the first term and will vanish in the limit as $\Delta n \to 0$. Other terms appearing in the governing integral equations are surface integrals such as $\iint p\hat{\boldsymbol{n}}\,d\sigma = [\![p\hat{\boldsymbol{n}}_\vartheta]\!]\Delta s$ and volume terms such as $\iiint \rho\boldsymbol{g}\,d\tau = (\rho_1\boldsymbol{g}_1 + \rho_2\boldsymbol{g}_2)\Delta s\Delta n/2$. These volume terms are of higher order than the rest and will be negligible in the limit as $\Delta n \to 0$.

Using the above formulas, the conditions valid across a surface of discontinuity may be developed from the integral conservation equations, (2.1), (2.7) and (2.12). We obtain

$$[\![\rho(\boldsymbol{V}\cdot\hat{\boldsymbol{n}} - W)]\!] = 0\,, \tag{3.1}$$

$$[\![\rho \boldsymbol{V}(\boldsymbol{V}\cdot\hat{\boldsymbol{n}} - W) + p\hat{\boldsymbol{n}}]\!] = 0\,, \tag{3.2}$$

$$[\![\rho e_0(\boldsymbol{V}\cdot\hat{\boldsymbol{n}} - W) + p(\boldsymbol{V}\cdot\hat{\boldsymbol{n}})]\!] = 0\,, \tag{3.3}$$

where now $\hat{\boldsymbol{n}}$ here refers to the unit normal to the discontinuity; the subscript ϑ will no longer be used. Equations (3.1)-(3.3) are valid for any type of discontinuity.

Contact surfaces

These are surfaces where the flow is aligned with the discontinuity. They are sometimes called tangential discontinuities. There will be no flow through these surfaces so that $[\![\boldsymbol{V}\cdot\hat{\boldsymbol{n}} - W]\!] = 0$. Under this condition, it is seen that (3.1)-(3.3) will be satisfied if

$$W = \boldsymbol{V}_1\cdot\hat{\boldsymbol{n}} = \boldsymbol{V}_2\cdot\hat{\boldsymbol{n}}\,, \tag{3.4}$$

$$[\![p]\!] = 0\,. \tag{3.5}$$

As long as (3.4) and (3.5) are satisfied, all other quantities may jump arbitrarily across a contact surface. We see that for a steady flow, $W = 0$, so that the contact surface will be aligned with a stream surface. In steady or unsteady flow, the pressure is continuous across a contact surface.

Shock waves

We may develop the *jump conditions* across a shock wave from (3.1)-(3.3). Let us consider the velocity vector $\boldsymbol{V}$ to be made up of components normal to the shock wave, V_n, and in the plane tangential to the shock wave, $\boldsymbol{V}_t$, so that $\boldsymbol{V} = V_n\hat{\boldsymbol{n}} + \boldsymbol{V}_t$. Now we use the symbol $\tilde{V}_n$ for the normal component of velocity relative to the shock, $\tilde{V}_n = V_n - W$. Then, from continuity, the condition (3.1) becomes

$$[\![\rho\tilde{V}_n]\!] = 0\,. \tag{3.6}$$

The momentum jump condition becomes

$$[\![\rho\boldsymbol{V}\tilde{V}_n + p\hat{\boldsymbol{n}}]\!] = 0\,. \tag{3.7}$$

Taking components of the above yields $[\![\rho V_n\tilde{V}_n + p]\!] = 0$ and $[\![\rho\boldsymbol{V}_t\tilde{V}_n]\!] = 0$. We can simplify these expressions by using the identity $[\![fg]\!] = <f>[\![g]\!] + <g>[\![f]\!]$ and where the *average f*, is defined as $<f> \equiv (f_1 + f_2)/2$. Then utilizing (3.6) and (3.7) we obtain the *jump conditions* for the momentum equation as

$$[\![\rho\tilde{V}_n^2 + p]\!] = 0\,, \tag{3.8}$$

and

$$[\![\boldsymbol{V}_t]\!] = 0\,. \tag{3.9}$$

The *jump condition* for the energy equation follows from (3.3) as $[\![\rho e_0\tilde{V}_n + pV_n]\!] = 0$ or in terms of stagnation enthalpy, where $\rho h_0 = \rho e_0 + p$, so that $[\![\rho h_0\tilde{V}_n + pW]\!] = 0$.

A convenient form of this condition is in terms of the enthalpy itself, where here $h = h_0 - (V_n^2 + \boldsymbol{V}_t{\cdot}\boldsymbol{V}_t)/2$, so that

$$[\![h + \tilde{V}_n^2/2]\!] = 0\,. \tag{3.10}$$

The *jump conditions* for a moving shock wave are (3.6), (3.8)–(3.10).

For a steady shock wave, $W = 0$ so that $\tilde{V}_n = V_n$, and the jump conditions for a steady shock wave become

$$\begin{aligned} [\![\rho V_n]\!] &= 0\,,\\ [\![\rho V_n^2 + p]\!] &= 0\,,\\ [\![\boldsymbol{V}_t]\!] &= 0\,,\\ [\![h + V_n^2/2]\!] &= 0\,. \end{aligned} \tag{3.11}$$

The last two jump conditions above may be combined to yield $[\![h_0 = 0]\!]$, which is the well-known result that the stagnation enthalpy is continuous across a steady shock wave. Note that from (3.10), this will not be the case for an unsteady shock wave.

3.2 Normal Shocks

For the case of a normal shock, $\boldsymbol{V}_t = 0$ and we may take $V_n = u$ so that the jump conditions become:

$$\begin{aligned} [\![\rho(u-W)]\!] &= 0\,,\\ [\![\rho u(u-W) + p]\!] &= 0\,,\\ [\![h + (u-W)^2/2]\!] &= 0\,. \end{aligned} \tag{3.12}$$

For steady shock waves, $W = 0$, and the jump conditions may be written as

$$\begin{aligned} \rho_1 u_1 &= \rho_2 u_2\,,\\ \rho_1 u_1^2 + p_1 &= \rho_2 u_2^2 + p_2\,,\\ h_1 + u_1^2/2 &= h_2 + u_2^2/2\,, \end{aligned} \tag{3.13}$$

where the subscript 1 refers to conditions upstream of the shock and the subscript 2 refers to conditions downstream of the shock. If p_1, ρ_1, u_1 and h_1 are specified, then (3.13) gives 3 algebraic relations for the four unknowns p_2, ρ_2, u_2 and h_2. The system is closed with an equation of state, which we consider to be written functionally as $h = h(p, \rho)$ so that

$$h_2 = h(p_2, \rho_2)\,. \tag{3.14}$$

The specific form of (3.14) influences the way (3.13) is solved. We now consider perfect gases, calorically imperfect gases (but thermally perfect) and real gases.

Perfect gases

For a gas which is both thermally perfect and calorically perfect, the state relationship

$$h = c_p T = \frac{\gamma}{\gamma - 1} \frac{p}{\rho} \,, \tag{3.15}$$

may be used. The solution of the algebraic system (3.13) then results in the well-known Rankine-Hugoniot relations:

$$\frac{p_2}{p_1} = 1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1) \,, \tag{3.16}$$

and

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} = \frac{(\gamma + 1)M_1^2}{2 + (\gamma - 1)M_1^2} \,, \tag{3.17}$$

where the upstream Mach number $M_1 = u_1/a_1$. For a derivation of these equations consult a standard gasdynamics text such as Anderson (1990), pp. 64–69.

The remaining quantities may be directly found. The temperature ratio, from the equation of state, $p = \rho RT$, may be written as $T_2/T_1 = (p_2/p_1)(\rho_1/\rho_2)$ where the pressure and density ratios are given in terms of M_1 above. Similarly, the sound speed for a perfect gas is $a^2 = \gamma RT$ so that $(a_2/a_1)^2 = T_2/T_1$ and we obtain

$$\frac{T_2}{T_1} = \left(\frac{a_2}{a_1}\right)^2 = \left[1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1)\right] \left[\frac{2 + (\gamma - 1)M_1^2}{(\gamma + 1)M_1^2}\right] . \tag{3.18}$$

The Mach number behind the shock is found from $M_2/M_1 = (u_2/u_1)(a_1/a_2)$, so that

$$\frac{M_2}{M_1} = \left[\frac{2 + (\gamma - 1)M_1^2}{(\gamma + 1)M_1^2}\right]^{1/2} \left[1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1)\right]^{-1/2} . \tag{3.19}$$

The entropy change across the shock may be obtained from (2.36), so that after substitution we find

$$\frac{s_2 - s_1}{c_v} = \log\left(\left[1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1)\right] \left[\frac{2 + (\gamma - 1)M_1^2}{(\gamma + 1)M_1^2}\right]^{\gamma}\right) . \tag{3.20}$$

We can see from the steady jump conditions (3.13) that $h_0 = h + u^2/2$ must be constant and since we have a perfect gas, T_0 will also be constant. The loss in stagnation pressure across the shock may then be determined from (2.38) as

$$\frac{p_{0_2}}{p_{0_1}} = \left[1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1)\right]^{-1/\gamma - 1} \left[\frac{2 + (\gamma - 1)M_1^2}{(\gamma + 1)M_1^2}\right]^{-\gamma/\gamma - 1} . \tag{3.21}$$

Weak normal shocks in perfect gases

It is useful to consider the limiting case of a weak shock. The shock will have zero strength, $(p_2 - p_1)/p_1 \to 0$, as $M_1 \to 1$. We introduce a shock-strength parameter ϵ such that

$$\epsilon \equiv M_1^2 - 1 \,, \tag{3.22}$$

where from (3.16), the strength of the shock is linear in ϵ

$$\frac{p_2 - p_1}{p_1} = \frac{2\gamma}{\gamma + 1}\epsilon \,, \tag{3.23}$$

for all values of ϵ; (3.23) is exact. Next we will examine the other quantities in terms of ϵ for small values of ϵ. The density ratio will not be linear in ϵ. We can look at the leading terms of the expansion for small epsilon by using the binomial series, which may be written as

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \ldots \,, \tag{3.24}$$

which will converge for $x^2 < 1$. The leading term for the density jump (3.17) becomes

$$\frac{\rho_2}{\rho_1} = 1 + \frac{2}{\gamma + 1}\epsilon + \mathcal{O}(\epsilon^2) \,. \tag{3.25}$$

The other jump quantities may be determined in a similar fashion as

$$\frac{u_2}{u_1} = 1 - \frac{2}{\gamma + 1}\epsilon + \mathcal{O}(\epsilon^2) \,, \tag{3.26}$$

$$\frac{T_2}{T_1} = 1 + \frac{2(\gamma - 1)}{\gamma + 1}\epsilon + \mathcal{O}(\epsilon^2) \,, \tag{3.27}$$

$$\frac{a_2}{a_1} = 1 + \frac{\gamma - 1}{\gamma + 1}\epsilon + \mathcal{O}(\epsilon^2) \,. \tag{3.28}$$

and

$$\frac{M_2}{M_1} = 1 - \epsilon + \mathcal{O}(\epsilon^2) \,. \tag{3.29}$$

The last relationship is interesting in that it shows that if $M_1 > 1$ then $M_2 < 1$ and *vice versa*. This result is true for a shock of any strength.

The entropy is found by substituting ϵ into (3.20) whereby

$$\frac{s_2 - s_1}{c_v} = \log\left[1 + \frac{2}{3}\frac{\gamma(\gamma - 1)}{(\gamma + 1)^2}\epsilon^3 + \mathcal{O}(\epsilon^4)\right] \,. \tag{3.30}$$

Note that to derive the above expression the expansions must retain all terms up to $\mathcal{O}(\epsilon^4)$. For small values of x, $\log(1+x) = x - x^2/2 + x^3/3 + \ldots$, so that (3.30) becomes

$$\frac{s_2 - s_1}{c_v} = \frac{2}{3}\frac{\gamma(\gamma - 1)}{(\gamma + 1)^2}\epsilon^3 + \mathcal{O}(\epsilon^4) \,. \tag{3.31}$$

This relationship shows that for a weak shock, of strength $\Delta p/p \sim \epsilon$ the entropy jump will be essentially negligible, $\Delta s/c_v \sim \epsilon^3$. The entropy relationship (3.31) also shows that the change in entropy will be positive only if $\epsilon > 0$ or $M_1 > 1$. Thus, steady shocks will always have $M_1 > 1$ and $M_2 < 1$. These shocks will always be compressions and expansion shocks will violate the second law of thermodynamics. It should be noted that the results apply only to steady shocks in a perfect gas. Some unusual gases, which are not thermally perfect, can have expansion shocks without violating the second law. We will not consider these gases in this set of notes.

The total pressure loss through the shock is found from (3.21) whereby

$$\frac{p_{0_2}}{p_{0_1}} = 1 - \frac{2}{3}\frac{\gamma}{(\gamma+1)^2}\epsilon^3 + \mathcal{O}(\epsilon^4)\,. \tag{3.32}$$

Thus weak shocks will have a negligible total pressure loss.

Very strong normal shocks in perfect gases

We can also consider the other extreme case, that for very strong shocks where $M_1 \to \infty$. For this case we introduce a small quantity δ such that

$$\delta \equiv \frac{1}{M_1^2}\,. \tag{3.33}$$

We see that $\delta \to 0$ as $M_1 \to \infty$. Substituting into (3.16), the pressure jump across the shock becomes

$$\frac{p_2}{p_1} = \frac{1}{\delta}\frac{2\gamma}{\gamma+1}\left(1 - \frac{\gamma-1}{2\gamma}\delta\right)\,. \tag{3.34}$$

Substituting the definition of δ into (3.17) and expanding for small δ gives the following relationship for the density jump:

$$\frac{\rho_2}{\rho_1} = \frac{\gamma+1}{\gamma-1}\left(1 - \frac{2}{\gamma-1}\delta + \mathcal{O}(\delta^2)\right)\,. \tag{3.35}$$

The temperature jump, from (3.18), which after expansion yields:

$$\frac{T_2}{T_1} = \frac{1}{\delta}\frac{2\gamma(\gamma-1)}{(\gamma+1)^2}\left[1 - \frac{\gamma^2-6\gamma+1)}{2\gamma(\gamma-1)}\delta + \mathcal{O}(\delta^2)\right]\,. \tag{3.36}$$

Thus we see that as $M_1 \to \infty$, the pressure jump $p_2/p_1 \to \infty$ and the temperature jump $T_2/T_1 \to \infty$. The density jump, however, reaches a maximum value and remains fixed, $\rho_2/\rho_1 \to (\gamma+1)/(\gamma-1)$. We should remember here that the strong shock expansions are only valid for perfect gases. As M_1 becomes large, T_2/T_1 will become large and usually chemical reactions will occur so that the gas may no longer be considered perfect.

Real gases

For a steady normal shock in a real gas the jump conditions (3.12) are valid. The functional form of the equation of state is given by (3.13). For equilibrium flow, this form of the equation of state is developed by first solving for the equilibrium composition for specified values of p and ρ from the Law of Mass Action. The state equation may also be given as a curve-fit for h as a function of p and ρ for a specified gas. At any rate, we assume that no simple functional form for (3.13) exists. Without utilizing the perfect gas equation of state, (3.15), we cannot solve (3.12) in closed form and the Rankine-Hugoniot relations, (3.16) and (3.17) will not be valid. Instead we must utilize an iterative numerical procedure, such as the following:

Step 1. Starting with u_1, p_1 and ρ_1, calculate $h_1 = h(p_1, \rho_1)$ from a curve fit or equilibrium composition.
Step 2. Guess a value of $\nu = \rho_1/\rho_2$. Then $\rho_2 = \rho_1/\nu$.
Step 3. From (3.12), $u_2 = u_1\nu$, $p_2 = p_1 + \rho_1 u_1^2(1-\nu)$ and $h_2 = h_1 + (u_1^2/2)(1-\nu^2)$.
Step 4. From the equation of state (3.13) we can also determine the enthalpy which we will denote here as $\tilde{h}$ such that $\tilde{h}_2 = h(p_2, \rho_2)$.
Step 5. Does $\tilde{h}_2 = h_2$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of ν and continue from Step 3.

As an example of real gas effects on a strong normal shock, consider a re-entry vehicle traveling at 36,000 ft/sec at an altitude of 170,000 ft. Calculations have been performed for a perfect gas at $\gamma = 1.4$ and for air as a real gas using the TGAS tables and the iteration procedure described above. The results are shown in Table 3.1 below. The most significant differences are seen in the density and temperature jumps. At 170,000 ft the ambient temperature is approximately $T_1 = 283K$. A perfect gas normal shock would predict a temperature of $T_2 \approx 58,000K$ wheras the real gas calculation gives $T_2 = 11,800K$. The perfect gas temperature is clearly unrealistic. In the real gas calculation a large portion of the energy from slowing down the flow goes toward dissociating and ionizing air and exciting the molecules to higher internal energy states. None of these effects are accounted for in the perfect gas calculation.

Calorically imperfect gases

For a gas which is thermally perfect but calorically imperfect, we will have an equation of state of the form $h = h(T)$, where $T = p/\rho R$. This may be in the form for a vibrationally excited diatomic gas where e is given by (1.41) and $h = e + RT$ or by a curve fit for $c_p(T)$ with h given by (1.33). Nonetheless, again the Rankine-Hugoniot relations will not be valid and an iterative procedure must be used. A nearly identical procedure as that used for general real gases may be implemented, with the main difference being that only two upstream values are needed.

Table 3.1. Normal Shock at Nose of Re-entry Vehicle, $M \approx 32.5$

Reentry Vehicle V=36,000 ft/sec Alt.=170,000 ft	Perfect Gas γ=1.4	Equilibrium Air
p_2/p_1	1233	1387
ρ_2/ρ_1	5.972	15.19
h_2/h_1	206.4	212.8
T_2/T_1	206.4	41.6

Step 1. Starting with u_1, and T_1, calculate $h_1 = h(T_1)$.
Step 2. Guess a value of $\nu = \rho_1/\rho_2$.
Step 3. From the first and third of (3.12), $u_2 = u_1\nu$, and $h_2 = h_1 + (u_1^2/2)(1-\nu^2)$.
Step 4. From the first and third of (3.12), and the thermal equation of state $p = \rho RT$, we obtain $p_2/p_1 = 1 + (1-\nu)u_1^2/RT_1$ and $T_2/T_1 = (p_2/p_1)(\rho_1/\rho_2) = [1 + (1-\nu)u_1^2/RT_1]\nu$. Then $\tilde{h}_2 = h(T_2)$.
Step 5. Does $\tilde{h}_2 = h_2$? If not, use a root-finding procedure to modify the value of ν and continue from Step 3.

In general, we have shown that for a perfect gas, the ratio of quantities across a normal shock, such as p_2/p_1, ρ_2/ρ_1 and T_2/T_1 are a function of a single variable, the upstream Mach number M_1. For a calorically imperfect gas, the shock jumps will be a function of two quantities, the upstream velocity u_1 and the upstream temperature T_1. For real gases, the shock jumps depend on three quantities, the upstream velocity u_1 and two upstream thermodynamic variables, such as p_1 and ρ_1. We see that Mach number only plays an important role for real gases.

3.3 Oblique Shocks

An oblique shock wave is any shock wave where the component of velocity *tangential* to the shock, $\boldsymbol{V}_t$, is non-zero. As we have seen, this quantity is always conserved. The jump conditions across an oblique shock are given by (3.6), (3.8) – (3.10) for the general case and for the steady case, by (3.11). Restricting our discussion to steady, oblique shocks, we may write the jump conditions as

$$\rho_1 V_{n_1} = \rho_2 V_{n_2}\,, \tag{3.37}$$

$$\rho_1 V_{n_1}^2 + p_1 = \rho_2 V_{n_2}^2 + p_2\,, \tag{3.38}$$

$$h_1 + V_{n_1}^2/2 = h_2 + V_{n_2}^2/2\,, \tag{3.39}$$

$$\boldsymbol{V}_{t_1} = \boldsymbol{V}_{t_2}\,, \tag{3.40}$$

where again the subscript 1 refers to conditions upstream of the shock and the subscript 2 refers to conditions downstream of the shock. The first three of these relations, (3.37) – (3.39) are identical to the normal shock relations (3.13), with the exception the u is replaced by V_n. Thus we can solve (3.37) – (3.39) along with an appropriate state equation, (3.14) using the identical procedures as used for normal shocks, provided that the upstream conditions are known. But now the upstream conditions involve V_{n_1} which in general is not known.

Consider an oblique shock in two dimensions sketched below in Fig. 3.2.

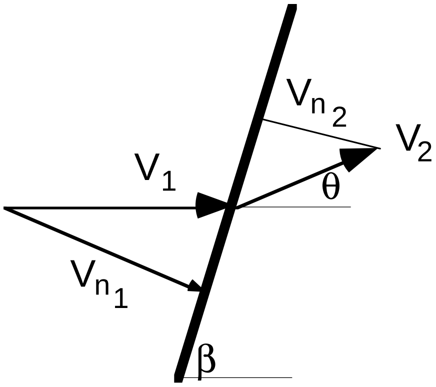

Figure 3.2. Oblique shock wave.

Relative to the upstream flow the shock wave will have an inclination angle β. Also relative to the upstream flow, the downstream flow will have an inclination angle of θ. The normal and tangential velocities upstream of the shock are

$$\begin{aligned} V_{n_1} &= V_1 \sin\beta\,, \\ V_{t_1} &= V_1 \cos\beta\,, \end{aligned} \tag{3.41}$$

and the velocity components downstream of the shock are

$$\begin{aligned} V_{n_2} &= V_2 \sin(\beta-\theta)\,, \\ V_{t_2} &= V_2 \cos(\beta-\theta)\,, \end{aligned} \tag{3.42}$$

In general we must specify one of these quantities. We usually specify θ which would be the flow angle for an oblique shock wave attached to a wedge of inclination θ. In order to find the shock angle β from a given value of θ and upstream velocity V_1 we must use the jump condition expressing continuity of tangential velocity, (3.40), which we may write as $V_1 \cos\beta = V_2 \cos(\beta-\theta)$. Replacing V_1 and V_2 by V_{n_1} and V_{n_2} by (3.41) and (3.42) we obtain

$$\frac{\tan(\beta-\theta)}{\tan\beta} = \frac{V_{n_2}}{V_{n_1}}\,. \tag{3.43}$$

Now, in principal we know V_{n_2}/V_{n_1} by the solution of (3.38) – (3.40) along with the state equation, (3.14). The procedure will be described separately for perfect and real gases in the next subsections.

Perfect gases

For oblique shocks in perfect gases, the Rankine-Hugoniot and related normal shock relations, (3.16) – (3.21) apply if the normal Mach number $M_{n_1} = M_1 \sin\beta$ is substituted for M_1. Also V_{n_2}/V_{n_1} must be substituted for u_2/u_1 in (3.17) and M_{n_2}/M_{n_1} for M_2/M_1 in (3.19). Once M_{n_2} is determined, then $M_2 = M_{n_2}/\sin(\beta - \theta)$.

We can develop an expression for β in terms of θ and M_1 by substituting $V_{n_2}/V_{n_1} = \rho_1/\rho_2$ evaluated with (3.17) into (3.43) to obtain

$$\frac{\tan(\beta-\theta)}{\tan\beta} = \frac{2+(\gamma-1)M_1^2\sin^2\beta}{(\gamma+1)M_1^2\sin^2\beta}\,. \tag{3.44}$$

This relationship may be slightly simplified using trigonometric identities as

$$\tan\theta = 2\cot\beta\left[\frac{M_1^2\sin^2\beta - 1}{M_1^2(\gamma+\cos 2\beta)+2}\right]. \tag{3.45}$$

A root-finding method must be used to determine β from θ and M_1. As is well known, two physical solutions may be obtained for this problem corresponding to *weak oblique shocks* and *strong oblique shocks*. Generally, only the weak oblique shock is stable and will occur in nature. Actually (3.45) may be written as a cubic equation in $\tan\beta$. Using standard trigonometric identities and some algebraic manipulation, (3.45) may be written as

$$\left(1+\frac{\gamma-1}{2}M_1^2\tan\theta\right)\tan^3\beta+(1-M_1^2)\tan^2\beta+\left(1+\frac{\gamma+1}{2}M_1^2\right)\tan\theta\tan\beta+1=0\,. \tag{3.46}$$

The smallest root will correspond to $\beta < \mu$ where μ is the Mach angle,

$$\sin\mu \equiv 1/M_1\,. \tag{3.47}$$

This root is not physically meaningful. The next two roots, if between μ and $\pi/2$ will be respectively the weak and strong shock solutions.

It is also well known that a solution to (3.45) may not exist. There is a maximum angle, θ_{max}, for which there will be an attached shock at a given Mach number and value of γ. The value of θ_{max} may be determined as the solution of $d\theta/d\beta = 0$. From (3.45), setting the derivative to zero yields a quadratic equation for the value of β at $\theta = \theta_{max}$. The solution for this value of β is

$$\left(\sin^2\beta\right)_{\theta_{max}} = \frac{(\gamma+1)M_1^2 - 4 + [(\gamma+1)^2M_1^4 + 8(\gamma^2-1)M_1^2 - 16(\gamma+1)]^{1/2}}{4\gamma M_1^2}\,. \tag{3.48}$$

The value of θ_{max} is found by substituting this result into (3.45).

In the limit for $M_1 \to \infty$ we can see that $\sin^2 \beta \to \gamma + 1/2\gamma$ which for $\gamma = 1.4$ corresponds to $\beta = 67.79°$. Also in the $M_1 \to \infty$ limit, (3.45) gives $\tan\theta \to \sin 2\beta/\gamma + \cos 2\beta$ which for $\gamma = 1.4$ corresponds to $\theta_{max} = 45.58°$.

Real gases

For general real gases we cannot get a closed form expression for the β, θ, M_1 relationship as was possible for the perfect gas. The continuity of tangential momentum gives (3.43), and the jump in normal velocity may be written in terms of the density jump from (3.37) as $V_{n_2}/V_{n_1} = \rho_1/\rho_2 = \nu$. Unfortunately we do not have a closed form expression for the density jump in terms of $M_1 \sin\beta$ as in the perfect gas case. However, within an iterative procedure to determine the inverse of the density jump ν, we can solve (3.43) for β. Utilizing trigonometric identities in (3.43) gives a quadratic equation for $\tan\beta$ in terms of $V_{n_2}/V_{n_1} = \nu$, whose solution is

$$\tan\beta = \frac{(1-\nu) \pm [(1-\nu)^2 - 4\nu\tan^2\theta]^{1/2}}{2\nu\tan\theta}\,. \qquad (3.49)$$

The minus sign corresponds to weak oblique shocks.

Thus an iteration procedure may be used which is only slightly more complicated than the normal shock case.

Step 1. Starting with V_1, p_1, ρ_1, and θ calculate $h_1 = h(p_1, \rho_1)$ from a curve fit or equilibrium composition.

Step 2. Guess a value of $\nu = \rho_1/\rho_2$. Then $\rho_2 = \rho_1/\nu$.

Step 3. From (3.49) solve for β corresponding to this value of ν. Then $V_{n_1} = V_1 \sin\beta$.

Step 4. From (3.37) – (3.39), $V_{n_2} = V_{n_1}\nu$, $p_2 = p_1 + \rho_1 V_{n_1}^2(1-\nu)$ and $h_2 = h_1 + (V_{n_1}^2/2)(1-\nu^2)$.

Step 5. From the equation of state (3.13) we can also determine the enthalpy which we will denote here as $\tilde{h}$ such that $\tilde{h}_2 = h(p_2, \rho_2)$.

Step 6. Does $\tilde{h}_2 = h_2$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of ν and continue from Step 3.

After convergence, with the given values of V_1, p_1, ρ_1, θ and the converged value of ν, we can compute β, V_{n_1}, V_{n_2}, p_2 and h_2. Then $V_2 = V_{n_2}/\sin(\beta - \theta)$

3.4 References Chapter 3

General References

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Courant, R. and Friedrichs, K. O. (1948). *Supersonic Flow and Shock Waves.* Interscience Publishers, New York.

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Vincenti, W. G. and Kruger, C. H. (1965). *Introduction to Physical Gas Dynamics.* J. Wiley and Sons, Inc. New York. Chapter VI.

4. ONE-DIMENSIONAL FLOW

4.1 General equations

Consider an inviscid, non-conducting flow through a duct or a streamtube. We will also assume that the flow is adiabatic and that the body forces are negligible. The unifying feature is that there is no flow through the walls. Then, under certain restrictions which we will carefully examine, the flow may be considered to depend upon one spatial coordinate. We will not initially restrict ourselves to steady flows. Let us first assume that the centerline of our duct or streamtube is straight and is aligned with the x-axis. Consider a control volume spanning the area of the tube as illustrated in Fig. 4.1, going from $x = x_1$ to $x = x_2 = x_1 + \Delta x$. The ends of the tube are selected to be perpendicular to the axis and have cross-sectional areas equal to A_1 and A_2 respectively.

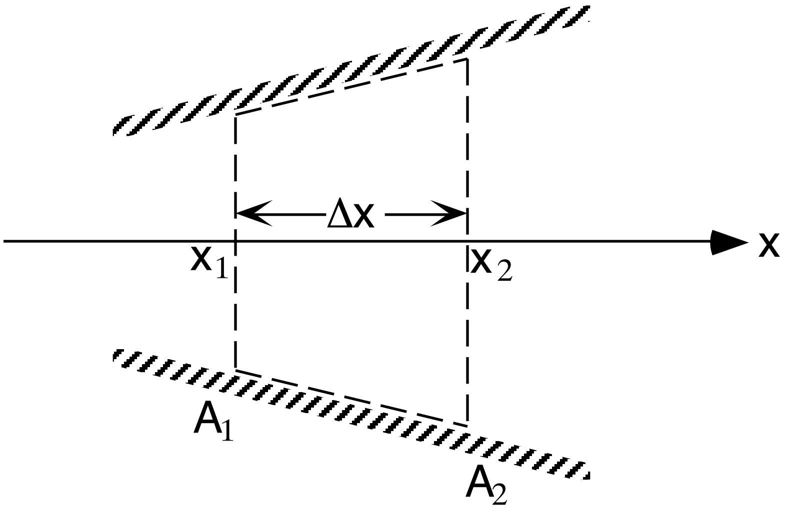

Figure 4.1. Control volume in a streamtube or duct.

The governing integral conservation equations will be continuity, (2.11), momentum, (2.17) and energy (2.22). Let us adopt our generic descriptor $N = \iiint \rho\eta \, d\tau$. The above conservation laws contain terms of the form $\partial N/\partial t$ and terms of the form $\iint \rho\eta \boldsymbol{V} \cdot \hat{\boldsymbol{n}} \, d\sigma$. The first term may be applied to the above control volume as

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} \rho\eta \, d\tau = \frac{\partial}{\partial t} \int_{x_1}^{x_2} \left(\iint \rho\eta \, dA \right) dx \, .$$

We can define a cross-sectional area average as

$$<\!\rho\eta\!> \equiv \frac{1}{A} \iint \rho\eta \, dA \, , \tag{4.1}$$

so that

$$\frac{\partial}{\partial t}\iiint_{\mathcal{V}} \rho\eta \, d\tau = \frac{\partial}{\partial t}\int_{x_1}^{x_2} <\!\rho\eta\!> A \, dx = \frac{\partial}{\partial t}(<\!\rho\eta\!> A)_1 \Delta x + \mathcal{O}(\Delta x^2)\,, \tag{4.2}$$

where we have approximated the integral between x_1 and x_2 by a simple left-endpoint rule. The surface integral term may be written as

$$\iint_{\mathcal{S}} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}} \, d\sigma = \iint_{A_1} \rho\eta(-u)\, dA + \iint_{A_2} \rho\eta(+u)\, dA + \iint_{\mathcal{S}_x} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}} \, d\sigma\,,$$

where $\boldsymbol{V}\cdot\hat{\boldsymbol{n}}$ vanishes on the surface $\mathcal{S}_x$ between A_1 and A_2. Using our definition of cross-sectional averages, (4.1), gives

$$\iint_{\mathcal{S}} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}} \, d\sigma = (<\!\rho\eta u\!> A)_2 - (<\!\rho\eta u\!> A)_1\,.$$

Now, expanding $(<\!\rho\eta u\!> A)$ at x_2 in a Taylor series about x_1 and neglecting terms of $\mathcal{O}(\Delta x^2)$ gives

$$\iint_{\mathcal{S}} \rho\eta \boldsymbol{V}\cdot\hat{\boldsymbol{n}} \, d\sigma = \frac{\partial}{\partial x}(<\!\rho\eta u\!> A)_1 \Delta x + \mathcal{O}(\Delta x^2)\,. \tag{4.3}$$

Using (4.2), (4.3) with $\eta = 1$, the continuity equation (2.11) may be applied to the specific control volume as

$$\frac{\partial}{\partial t}\left(<\!\rho\!> A\right)_1 \Delta x + \frac{\partial}{\partial x}\left(<\!\rho u\!> A\right)_1 \Delta x + \mathcal{O}(\Delta x^2) = 0\,.$$

Dividing by Δx and then taking the limit as $\Delta x \to 0$ and dropping the subscript 1 gives the general form of the streamtube continuity equation:

$$\frac{\partial}{\partial t}\left(<\!\rho\!> A\right) + \frac{\partial}{\partial x}\left(<\!\rho u\!> A\right) = 0\,. \tag{4.4}$$

Note that the above equation may be considered to be *exact* for the infitesmal control volume that we have considered. We have not neglected any terms. All that has been assumed is that the axis of the control volume is straight and that the length is infinitesmal.

Next, using (4.2) and (4.3) with $\eta = u$, we can rewrite the left-hand side of the momentum equation (2.17) in the x-direction applied to the specific control volume as

$$\frac{\partial}{\partial t}\left(<\!\rho u\!> A\right)_1 \Delta x + \frac{\partial}{\partial x}\left(<\!\rho u^2\!> A\right)_1 \Delta x + \mathcal{O}(\Delta x^2)\,.$$

Neglecting body forces, the only term on the right-hand side for an inviscid flow is the surface integral for the pressure which may be written as

$$-\iint_{\mathcal{S}} p\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{\imath}}\,d\sigma = -\iint_{A_1} p(-1)\,dA - \iint_{A_2} p(+1)\,dA - \iint_{\mathcal{S}_x} p\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{\imath}}\,d\sigma\,.$$

The first two terms may be written in terms of cross-sectional area averages and in the last term, the component of surface area $-\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{\imath}}d\sigma$ on $\mathcal{S}_x$ may be seen to be the frontal area dA. Thus

$$-\iint_{\mathcal{S}} p\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{\imath}}\,d\sigma = +\left(<\!p\!>A\right)_1 - \left(<\!p\!>A\right)_2 + \int_{x_1}^{x_2} p_w\frac{dA}{dx}\,dx\,,$$

where p_w is the average value of p taken around the surface $\mathcal{S}_x$ at a fixed location of x. The average terms at x_2 may be written in terms of the averages at x_1 using a Taylor series expansion and the integral may be approximated by left-endpoint rule so that

$$-\iint_{\mathcal{S}} p\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{\imath}}\,d\sigma = -\frac{\partial}{\partial x}(<\!p\!>A)_1\Delta x + \left(p_w\frac{dA}{dx}\right)_1\Delta x + \mathcal{O}(\Delta x^2)\,.$$

Equating the left and right hand sides of the x-momentum equation, dividing by Δx and taking the limit $\Delta x \to 0$ gives

$$\frac{\partial}{\partial t}\left(<\!\rho u\!>A\right) + \frac{\partial}{\partial x}\left(<\!\rho u^2\!>A\right) = -\frac{\partial}{\partial x}(<\!p\!>A) + p_w\frac{dA}{dx}\,. \tag{4.5}$$

Again this equation may be considered *exact* for an inviscid, adiabatic flow with negligible body forces in the specific control volume.

Finally, we can apply the same procedures for the energy equation (2.22). The process is the same as for the continuity and momentum equations and will not be repeated. The result is

$$\frac{\partial}{\partial t}\left(<\!\rho e_0\!>A\right) + \frac{\partial}{\partial x}\left(<\!\rho e_0 u\!>A\right) = -\frac{\partial}{\partial x}(<\!pu\!>A)\,. \tag{4.6}$$

Equations (4.4), (4.5) and (4.6) represent our 3 governing equations for an inviscid, non-conducting, adiabatic fluid with negligible body forces. Although only time and x-derivatives appear, there is no restriction on the variation of flow quanties in any other direction. The only assumptions are that the cross-sectional area averages are taken across a streamtube or duct in a direction perpendicular to the axis of the duct.

We will now put these equations into a form which is a bit more familiar. We will now define some flow quantities with a tilde to correspond to specific combinations of averages. Namely,

$$\begin{aligned}\tilde{\rho} &\equiv <\rho> ,\\ \tilde{p} &\equiv <p> ,\\ \tilde{u} &\equiv \frac{<\rho u>}{<\rho>} ,\\ \tilde{e}_0 &\equiv \frac{<\rho e_0>}{<\rho>} ,\\ \tilde{h}_0 &\equiv \frac{<\rho e_0 u> + <pu>}{<\rho u>} .\end{aligned} \tag{4.7}$$

With the above definitions, nearly all averaged terms of the governing equations are accounted for except $<\rho u^2>$ and the wall pressure term p_w. These terms may be approximately related to the averages defined above if we assume that the flow quantities themselves, ρ, u and p vary slowly across the duct. In particular we assume that

$$<\rho u^2> \approx \frac{<\rho u>^2}{<\rho>} = \tilde{\rho}\tilde{u}^2 , \tag{4.8}$$

and

$$p_w \approx <p> = \tilde{p} . \tag{4.9}$$

We can roughly estimate the accuracy of these expressions by assuming that ρ, u and p vary linearly across the duct from ρ_0, u_0 and p_0 to ρ_w, u_w and p_w, respectively. If the normalized variations $\epsilon_\rho = (\rho_0 - \rho_w)/\rho_0)$, $\epsilon_u = (u_0 - u_w)/u_0)$ and $\epsilon_p = (p_0 - p_w)/p_0)$ are all small, then (4.8) will be satisfied to $\mathcal{O}(\epsilon^2)$ and (4.9) will be satisfied to $\mathcal{O}(\epsilon)$, where ϵ corresponds to one of the normalized variations ϵ_ρ, ϵ_u or ϵ_p.

We can then write our "one-dimensional" governing equations as

$$\frac{\partial}{\partial t}(\tilde{\rho}A) + \frac{\partial}{\partial x}(\tilde{\rho}\tilde{u}A) = 0 , \tag{4.10}$$

$$\frac{\partial}{\partial t}(\tilde{\rho}\tilde{u}A) + \frac{\partial}{\partial x}\left[(\tilde{\rho}\tilde{u}^2 + \tilde{p})A\right] - \tilde{p}\frac{dA}{dx} = 0 , \tag{4.11}$$

$$\frac{\partial}{\partial t}(\tilde{\rho}\tilde{e}_0 A) + \frac{\partial}{\partial x}\left(\tilde{\rho}\tilde{h}_0\tilde{u}A\right) = 0 , \tag{4.12}$$

An alternate form of the equations, the non-conservation form, may be obtained by expanding the combined terms so that

$$\frac{\partial\tilde{\rho}}{\partial t} + \frac{\partial}{\partial x}(\tilde{\rho}\tilde{u}) + \frac{\tilde{\rho}\tilde{u}}{A}\frac{dA}{dx} = 0 , \tag{4.13}$$

$$\frac{\partial \tilde{u}}{\partial t} + \tilde{u}\frac{\partial \tilde{u}}{\partial x} + \frac{1}{\tilde{\rho}}\frac{\partial \tilde{p}}{\partial x} = 0\,, \tag{4.14}$$

$$\frac{\partial \tilde{h}_0}{\partial t} + \tilde{u}\frac{\partial \tilde{h}_0}{\partial x} - \frac{1}{\tilde{\rho}}\frac{\partial \tilde{p}}{\partial t} = 0\,. \tag{4.15}$$

One more assumtion that will be used with these equations concerns the definition of $\tilde{h}_0$. In general, $h_0 = h + \boldsymbol{V}\cdot\boldsymbol{V}/2$. For the one-dimensional flow equations, we assume $\tilde{h}_0 = h + \tilde{u}^2/2$ so that in two space dimensions we are assuming $\tilde{v}^2 << \tilde{u}^2$. This approximation is consistent with our previous flow assumptions of small variations across the channel. Finally, we note that from now on in this chapter, we will be dropping the tilde. We should keep in mind however that when we write, for example, u we really mean the specific cross-sectional area average $<\rho u>\ /\ <\rho>$. We also note that often these equations are called *quasi-one-dimensional* which is meant to signify allowing area variations. The original use of these equations for a steady flow is attributed to Shapiro and is described in his classic text Shapiro (1953). Other derivations are found in Liepmann and Roshko (1957) and Anderson (1990).

4.2 Steady, Constant-Area Flows

The general governing equations for an inviscid, adiabatic flow with negligible body forces and written in terms of specific cross-sectional area averages are given in the previous section. For the specific application to steady, constant area flows the *one-dimensional* equations can be written as

$$\frac{d}{dx}\left(\rho u\right) = 0\,, \tag{4.16}$$

$$\frac{d}{dx}\left(\rho u^2 + p\right) = 0\,, \tag{4.17}$$

$$\frac{d}{dx}\left(\rho h_0 u\right) = 0\,. \tag{4.18}$$

Note that we have dropped the tilda designations. Nonetheless, all the terms are still defined as if they all had tilda designations and correspond to the specific cross-sectional area averages. The above equations may be readily integrated to give $\rho u =$ constant, $\rho u^2 + p =$ constant and $h_0 =$ constant. Thus if we have a flow with conditions known at $x = x_1$, we can write the conditions at $x = x_2$ from

$$\begin{aligned} \rho_2 u_2 &= \rho_1 u_1\,, \\ \rho_2 u_2^2 + p_2 &= \rho_1 u_1^2 + p_1\,, \\ h_2 + u_2^2/2 &= h_1 + u_1^2/2\,, \end{aligned} \tag{4.19}$$

The system is closed with an equation of state of the form

$$h_2 = h(p_2, \rho_2)\,. \tag{4.20}$$

We see that the above 4 algebraic equations for the four unknowns p_2, ρ_2, h_2 and u_2 in terms of the known quatities p_1, ρ_1, h_1 and u_1 are identically the same as the normal shock jump conditions, (3.13), (3.14). Thus, the solution for the steady, inviscid, adiabatic flow in a constant area duct is that the flow at station 2 is either unchanged from the flow at station 1 or that the flow has gone through a normal shock somewhere between station 1 and station 2. No other solution is possible for this flow. A downstream condition will usually determine whether the flow passes through a shock or not. Of course, if the flow at station 1 is subsonic, then a shocked flow is impossible. Also this solution will apply for a real gas as well as a perfect gas.

4.3 Steady, Variable-Area Flows

For steady flows with variable cross-sectional area, the one-dimensional flow equations become

$$\frac{d}{dx}(\rho u A) = 0\,, \tag{4.21}$$

$$\frac{d}{dx}\left[(\rho u^2 + p)A\right] - p\frac{dA}{dx} = 0\,, \tag{4.22}$$

$$\frac{d}{dx}(\rho h_0 u A) = 0\,. \tag{4.23}$$

The first equation integrates to constant mass-flow rate, $\dot{m}$ as

$$\dot{m} = \rho u A = \text{constant}\,, \tag{4.24}$$

and the last equation can then be integrated to give constant stagnation enthalpy, h_0 as

$$h_0 = h + \frac{u^2}{2} = \text{constant}\,. \tag{4.25}$$

The momentum equation (4.22) is usually not used for solutions for these flows. Instead, the condition that entropy is constant between shocks for these flows is utilized. We have seen that for an adiabatic flow in general, that entropy will be constant along particle paths (except across shock waves). This can be verified for steady, one-dimensional flows where from (4.25) h_0 =constant so that $dh + udu = 0$ and from the non-conservative momentum equation which can be obtained by expanding the derivatives in (4.22) and utilizing continuity (4.21) to give $dp+\rho udu = 0$. Then the combined first and second law of thermodynamics for a gas in chemical equilibrium or a non-reacting gas gives $Tds = dh - dp/\rho = 0$. Thus the system will be closed with

$$s = \text{constant}\,, \tag{4.26}$$

and an equation of state

$$\rho = \rho(h, s)\,. \tag{4.27}$$

Before we discuss how to actually solve problems with these equations, some important relationships can be developed from which we can predict the qualitative behavior of steady, inviscid, adiabatic, isentropic one-dimensional flows with area change. We proceed by taking the derivative of the natural logarithm of the mass flow rate which gives $d\rho/\rho + du/u + dA/A = 0$. We have already noted that constant h_0 leads to $dh + udu = 0$ and constant entropy leads to $Tds = dh - dp/\rho = 0$. If we add the definition of the speed of sound from (1.55) as $a^2 = \rho/(\partial\rho/\partial h)_s$ which for this case is $a^2 = \rho dh/d\rho$ we can obtain the following expression:

$$(1 - M^2)\frac{du}{u} + \frac{dA}{A} = 0\,. \tag{4.28}$$

This equation indicates that for a subsonic flow $M < 1$ and a diverging area $dA > 0$ the velocity u must decrease. For a supersonic flow with a diverging area the velocity u increases. For converging areas the changes in u are opposite. The other flow quantities may be described from the following relationships:

$$\frac{du}{u} = -\frac{1}{M^2}\frac{d\rho}{\rho} = -\frac{dh}{a^2M^2} = -\frac{dp}{\rho a^2 M^2}\,. \tag{4.29}$$

Thus we see that whenever u increases, ρ, h and p will decrease and *vice versa.* Furthermore for the case of a *perfect gas* $h = C_pT$ and $a^2 = \gamma RT$ so that

$$\frac{du}{u} = -\frac{1}{(\gamma-1)M^2}\frac{dT}{T} = \frac{1}{1 + (\gamma-1)M^2/2}\frac{dM}{M}\,. \tag{4.30}$$

So that for perfect gases, whenever u increases, M will also increase and T will decrease. The qualitative behavior of these flows are summarized in Table 4.1, below.

Table 4.1 Qualitative Behavior of One-Dimensional Flows

	diverging $dA > 0$		converging $dA < 0$	
	$M < 1$	$M > 1$	$M < 1$	$M > 1$
u	decreases	increases	increases	decreases
ρ	increases	decreases	decreases	increases
p	increases	decreases	decreases	increases
h	increases	decreases	decreases	increases
$^*T$	increases	decreases	decreases	increases
$^*M$	decreases	increases	increases	decreases

* perfect gas

Equations (4.24)–(4.27) complete the system for an inviscid, adiabatic, one-dimensional steady flow (with area change and with negligible body forces). The equations are only valid for isentropic flows which will occur between discontinuities. We will illustrate the solution procedure for the case where flow conditions are known at station 1 and it is desired to determine the flow conditions at station 2. The geometry is assumed to be given so that the areas A_1 and A_2 are also known. The equations become

$$\begin{aligned} \rho_2 u_2 A_2 &= \rho_1 u_1 A_1 \,, \\ h_2 + \frac{u_2^2}{2} &= h_1 + \frac{u_1^2}{2} \,, \\ s_2 &= s_1 \,, \\ \rho_2 &= \rho(h_2, s_2) \,. \end{aligned} \tag{4.31}$$

We see that we have 4 equations in 4 unknowns. Let us first consider solving this system for a perfect gas.

Perfect gases

For a perfect gas, the condition that entropy is constant leads to $p\rho^{-\gamma}$ being constant, (2.33). Also we can write $h = C_p T$ and $p = \rho RT$ so that $h = (\gamma/\gamma - 1)p/\rho$. The equations for this flow then become

$$\begin{aligned} \rho_2 u_2 A_2 &= \rho_1 u_1 A_1 \,, \\ \frac{\gamma}{\gamma - 1}\frac{p_2}{\rho_2} + \frac{u_2^2}{2} &= \frac{\gamma}{\gamma - 1}\frac{p_1}{\rho_1} + \frac{u_1^2}{2} \,, \\ p_2 \rho_2^{-\gamma} &= p_1 \rho_1^{-\gamma} \,, \end{aligned} \tag{4.32}$$

which gives three equations for the unknowns p_2, ρ_2 and u_2. But the equations are not usually solved in this fashion. The standard procedure is to note that for an inviscid, steady, adiabatic, isentropic flow T_0 and p_0 are constant. From (2.30) and (2.35)

$$\begin{aligned} \frac{T_0}{T} &= 1 + \frac{\gamma - 1}{2} M^2 \,, \\ \frac{p}{p_0} &= \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\gamma/\gamma - 1} \,. \end{aligned}$$

We can determine T_0 and p_0 by applying the above to the known station 1. Then the unknown T_2 and p_2 may be found in terms of the Mach number M_2. We can determine M_2 from the mass-flow relationship, (4.24). We can write the mass-flow equation in terms of p, T and M using $p = \rho RT$ and $M = u/\sqrt{\gamma RT}$ so that

$$\dot{m} = \sqrt{\frac{\gamma}{RT}} p M A \,. \tag{4.33}$$

Written in terms of T_0 and p_0 from (2.30) and (2.35) gives

$$\dot{m} = \sqrt{\frac{\gamma}{RT_0}} p_0 AM \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/2-\gamma/\gamma-1} . \tag{4.34}$$

Equating $\dot{m}_1$ to $\dot{m}_2$ and noting that T_0 and p_0 are constant gives the following equation which can be used to solve for M_2 in terms of M_1 and A_1 and A_2:

$$A_2 M_2 \left(1 + \frac{\gamma - 1}{2} M_2^2\right)^{1/2-\gamma/\gamma-1} = A_1 M_1 \left(1 + \frac{\gamma - 1}{2} M_1^2\right)^{1/2-\gamma/\gamma-1} . \tag{4.35}$$

This equation is not usually solved directly in this fashion. Instead the constant mass flow condition with constant p_0 and T_0 above (4.35) is written between a general state (no subscript) and a state where the Mach number is one, designated by a superscript $*$. We obtain

$$\frac{A}{A^*} = \frac{1}{M} \left[\frac{2}{\gamma + 1} \left(1 + \frac{\gamma - 1}{2} M^2\right)\right]^{-(1/2-\gamma/\gamma-1)} . \tag{4.36}$$

To solve our problem, from M_1 and A_1 we can use (4.36) to calculate A^*. Then from A_2 and A^* we use (4.36) to calculate M_2. Once M_2 is found, the T_0 and p_0 relationships may be used to calculate p_2 and T_2. However, if we plot A/A^* versus M as shown in Fig. 4.2, we see that for a given value of A/A^* there will be two roots for M, one subsonic and one supersonic. Thus to use the equation in this fashion we will need to know whether the flow will be subsonic or supersonic. This may depend upon the geometry between station 1 and station 2. We can only go from subsonic to supersonic by passing through a throat where M will be one. In general, to pass from supersonic to subsonic flow, we will pass thru a shock and (4.36) with A^* constant will not be valid. The calculation of converging-diverging nozzle flows will be described in §4.4

We can note here the variation of A^* across a normal shock by considering a state upstream of the shock where $M = 1$ so that $A = A_1^*$ and $p_0 = p_{0_1}$. Downstream of the shock consider a state where M is also equal to one so that $A = A_2^*$ and $p_0 = p_{0_2}$. Since the mass flow (4.34) must be the same at states 1 and 2 and since T_0 does not change across a steady adiabatic shock wave, then

$$A_2^* p_{0_2} = A_1^* p_{0_1} , \tag{4.37}$$

and p_{0_2}/p_{0_1} across a shock is found from (3.21). Since p_0 *decreases* across a shock, (4.37) indicates that A^* *increases* across a shock.

Real gases

To solve a steady one-dimensional flow problem where the velocity and thermodynamic state are give at station 1 and the areas A_1 and A_2 are specified, the flow

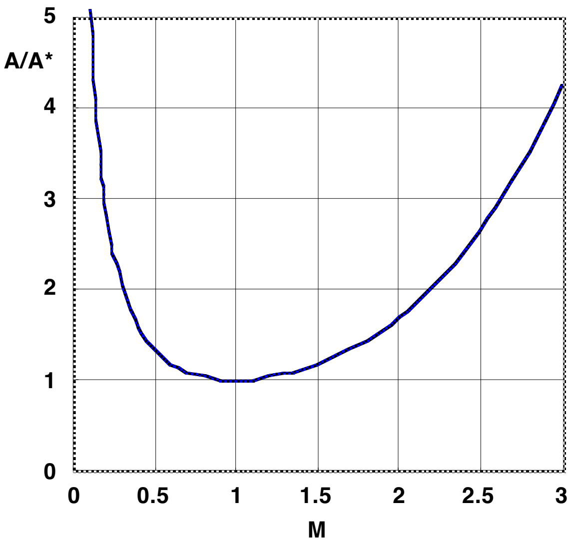

Figure 4.2. Area-Mach Number relationship for one-dimensional, steady, adiabatic, isentropic flow of a perfect gas.

conditions at station 2 may be found by applying (4.24)–(4.27). However we cannot use the perfect gas procedures of using constant T_0 and p_0 along with the A/A^* relationship. Instead we must utilize an iterative procedure. One approach is as follows:

Step 1. Starting with u_1, and the thermodynamic state, say p_1 and ρ_1, calculate $h_1 = h(p_1, \rho_1)$ and $s_1 = s(p_1, \rho_1)$ from a curve fit or equilibrium composition.

Step 2. Guess a value of u_2.

Step 3. From (4.25) $h_2 = h_1 + (u_1^2/2) - (u_2^2/2)$ and from (4.26) $s_2 = s_1$.

Step 4. From the equation of state (4.26) we can determine $\rho_2 = \rho(h_2, s_2)$ and also $p_2 = p(h_2, s_2)$.

Step 5. All the flow quantities at 2 have been determined. Then does $\rho_2 u_2 A_2 = \rho_1 u_1 A_1$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of u_2 and continue from Step 3. Note that either the subsonic or supersonic root may be found depending upon the initial guess. For subsonic root, guess a small value of u_2 and for a supersonic root guess a large value. Be careful not to exceed the theoretical maximum velocity which corresponds to $h_2 = 0$ so that $(u_2)_{max} = \sqrt{2h_0}$.

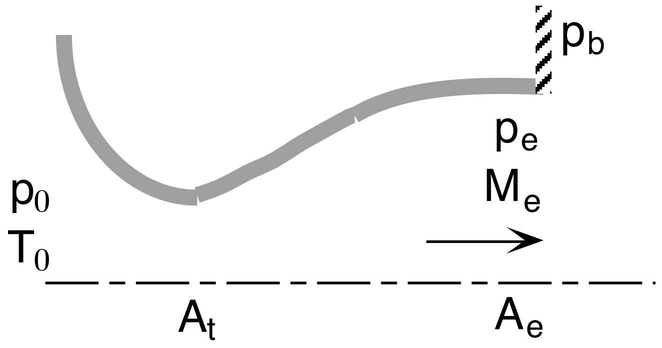

Figure 4.3. Converging-diverging nozzle.

4.4 Steady Nozzle Flows

Most nozzle flow problems consist in specifying the thermodynamic state of the chamber, *e.g.,* the stagnation conditions and one downstream condition, which is typically the back pressure p_b, for a nozzle exhausting into a constant pressure environment. The nozzle geometry is also specified. As the back pressure is decreased, the mass flow rate through the nozzle will increase until a maximum value is reached. This maximum value of mass flow will be reached when the flow in the nozzle reaches Mach 1, which will always occur at the nozzle minimum area, called the nozzle *throat.* The flow at this point is *choked* and the mass flow cannot increase any further. We can note that from (4.28) it can be seen directly that at $M = 1$, dA must equal zero and the area will be a minimum.

non-choked nozzle flows

The calculation of the flow in a nozzle which is not choked will rely on the fact that this flow will always be subsonic and hence will be isentropic (no shocks) and the pressure inside the exit plane p_e must equal the back pressure p_b. The flow will also have constant h_0. Conditions at the exit plane may be found from the known chamber conditions, h_0 and s_0 and the back pressure, so that

$$\begin{aligned} h_e + \frac{u_e^2}{2} &= h_0 \, , \\ s_e &= s_0 \, , \\ p_e &= p_b \, . \end{aligned} \tag{4.38}$$

The system is closed with an equation of state, which may be of the form

$$h_e = h(p_e, s_e) \, . \tag{4.39}$$

Once the conditions at the exit plane are determined, conditions at any other point inside the nozzle, where the area is specified, may be found using procedures outlined in the previous section.

For perfect gases, we may use constant p_0 and T_0 to simplify the calculations. From (2.35) we may write

$$\frac{p_e}{p_0} = \left(1 + \frac{(\gamma - 1)}{2} M_e^2\right)^{-\gamma/\gamma-1} , \tag{4.40}$$

and since p_0 and $p_e = p_b$ are known, (4.40) may be solved for M_e. Then (2.31) may be solved for T_e,

$$\frac{T_0}{T_e} = 1 + \frac{(\gamma - 1)}{2} M_e^2 . \tag{4.41}$$

For real gases, the exit conditions can be readily found if a curve fit to $h(p, s)$ is available. From $p_e = p_b$ and $s_e = s_0$, h_e is found from state as $h(p_e, s_e)$ and and then $u_e = \sqrt{2(h_0 - h_e)}$.

isentropic, choked nozzle flows

Choked nozzle flow calculations make use of the fact that the Mach number will be one at the throat. Then from given chamber (stagnation) conditions. the throat area A_t and $M_t = 1$, the throat conditions can be found. Then knowing all the conditions at t, the conditions at any other point in the nozzle, including the exit plane may be found using the procedures outlined in the previous section. Note that for every point in the nozzle, there will be two isentropic solutions, one subsonic and one supersonic. The flow in the converging section will be subsonic, wheras the flow in the diverging section may be subsonic or supersonic, depending upon the conditions outside the exit plane.

For perfect gases, from $M_t = 1$ we know that $A^* = A_t$. Then the Mach number at the exit plane may be found by solving (4.36) for M_e from the known value of A_e/A^*. Once M_e is found p_e/p_0 and T_e/T_0 may be found from (4.40) and (4.41) respectively. The subsonic or supersonic root must be chosen. This procedure may be repeated for any other point inside the nozzle where the area is specified.

For real gases again an iterative process must be used. First it is necessary to find the conditons at the throat from the chamber conditions and the fact that $M_t = 1$. Then the exit plane conditions and those at any other position inside the nozzle may be found using the procedures outlined in the previous section.

throat conditions:

Step 1. Starting with chamber conditons, say p_0 and T_0, calculate $h_0 = h(p_0, T_0)$ and $s_0 = s(p_0, T_0)$ from a curve fit or equilibrium composition.

Step 2. Guess a value of u_t.

Step 3. Then $h_t = h_0 - (u_t^2/2)$ and $s_t = s_0$.

Step 4. From a curve fit we determine $\rho_t = \rho(h_t, s_t)$, $p_t = p(h_t, s_t)$ and also $a_t = a(h_t, s_t)$.

Step 5. All the flow quantities at the throat have been determined. Then does $u_t = a_t$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of u_t and continue from Step 3.

exit conditions:

Step 6. Guess a value of u_e.

Step 7. Then $h_e = h_0 - (u_e^2/2)$ and $s_e = s_0$.

Step 8. From a curve fit we determine $\rho_e = \rho(h_e, s_e)$ and also $p_e = p(h_e, s_e)$.

Step 9. All the flow quantities at the exit plane have been determined. Then does $\rho_e u_e A_e = \rho_t u_t A_t$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of u_e and continue from Step 7. Note that either the subsonic or supersonic root may be found depending upon the initial guess.

4.5 Unsteady, Constant-Area Flows

We consider here an inviscid, non-conducting flow in a constant area duct. We assume that the one-dimensional averaging assumptions have been made and we further assume that the flow is adiabatic and that body forces are negligible. In this section we will consider the flow to be *unsteady.* Under these circumstances the governing equations may be developed from (4.10)–(4.12) as:

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) = 0\,, \tag{4.42}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0\,, \tag{4.43}$$

$$\frac{\partial}{\partial t}(\rho e_0) + \frac{\partial}{\partial x}\left[(\rho e_0 + p)u\right] = 0\,. \tag{4.44}$$

The non-conservation form may be obtained by expanding the combined terms as:

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0\,, \tag{4.45}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0\,, \tag{4.46}$$

$$\frac{\partial e_0}{\partial t} + u\frac{\partial e_0}{\partial x} + \frac{p}{\rho}\frac{\partial u}{\partial x} + \frac{u}{\rho}\frac{\partial p}{\partial x} = 0\,. \tag{4.47}$$

The energy equation may be written in terms of e instead of e_0 by utilizing $e_0 = e + u^2/2$. Expanding (4.47) and using (4.46) and (4.45) we obtain

$$\frac{\partial e}{\partial t} + u\frac{\partial e}{\partial x} + \frac{p}{\rho}\frac{\partial u}{\partial x} = 0\,. \tag{4.48}$$

It turns out to be convenient to use an equation of this form with p as the dependent variable instead of e. For a general gas which, if reacting was in chemical equilibrium we can assume $p = p(\rho, e)$. Then $dp = p_\rho d\rho + p_e de$. Thus

$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} = \left(\frac{\partial p}{\partial \rho}\right)_e \left(\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x}\right) + \left(\frac{\partial p}{\partial e}\right)_\rho \left(\frac{\partial e}{\partial t} + u\frac{\partial e}{\partial x}\right)\,,$$

Substituting (4.46) and (4.48) gives

$$\begin{aligned}\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} = &= -\rho\frac{\partial u}{\partial x}\left[\left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho\right] \\ &= -\rho a^2\frac{\partial u}{\partial x}\,, \end{aligned} \tag{4.49}$$

where we have used the general expression (1.51) for the speed of sound.

The governing equations are now (4.45), (4.46) and (4.49) and may be written in matrix form as

$$\frac{\partial \mathbf{W}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{W}}{\partial x} = 0\,, \tag{4.50}$$

where

$$\mathbf{W} = \begin{pmatrix}\rho\\ u\\ p\end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} u & \rho & 0\\ 0 & u & 1/\rho\\ 0 & \rho a^2 & u\end{pmatrix}. \tag{4.51}$$

Before attempting to solve this system of first-order partial differential equations, it is useful to consider how to solve a single, first-order partial differential equation, for a generic variable $f(x,t)$,

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0\,, \tag{4.52}$$

where c is the constant wave speed. This equation is sometimes called the *linear advection* equation. If we subject f to the initial condition

$$f(x,0) = g(x)\,, \tag{4.53}$$

the initial value problem will be called a Cauchy problem. One can proceed with the solution by first noting that for $f(x,t)$, an exact differential is

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt}\,. \tag{4.54}$$

By comparing (4.54) to (4.53) we may note whenever $dx/dt = c$, (4.54) will give $df/dt = 0$. We further note that any line in x, t space, defined by $x - ct =$ *constant* will have a slope $dx/dt = c$ and that the complete solution to $df/dt = 0$ is $f =$ *constant*. Thus for our Cauchy problem f will be constant along lines where $x - ct =$ *constant*. Thus the value of f at (x_1, t_1) will be the same as the value of f anywhere along the curve $x - ct = x_1 - ct_1$ and in particular along the initial data line $t = 0$ at $(x_0, 0)$ such that $x_0 = x_1 - ct_1$. Or $f(x_1,t_1) = f(x_0,0)$ and from the initial condition (4.53), $f(x_0,0) = g(x_0)$, so that $f(x_1,t_1) = g(x_0) = g(x_1 - ct_1)$.

Thus the general solution of the Cauchy problem is that $f(x,t) = g(x - ct)$ for $t \geq 0$.

Now we wish to apply procedures such as the above to the solution to our system of three equations, (4.50). However complications arise because our equations are non-linear and coupled. For the above system of first-order partial differential equations whose specific non-linearity is termed quasi-linear, since it is linear in the highest derivative, a solution is available by the *method of characteristics.* We will not attempt to develop the method of characteristics for a general system of first-order partial differential equations, but refer the reader to the developments found for example in Chester (1971) or Garabedian (1986). We will instead develop less rigorously the method of characteristics for our specific set of equations.

A key part of solving (4.50) by this approach involves the eigenvalues of the matrix $\mathbf{A}$, which may be found to be u, $u + a$ and $u - a$. The are called the *characteristic velocities* or *characteristic wave speeds* and their role in the solution will become evident. We begin by seeking linear combinations of our three equations (4.45), (4.46) and (4.49) which in some sense appear to have the form of our Cauchy problem (4.52).

Adding (4.45) and (4.49) and reorganizing some terms yields

$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} - a^2\left(\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x}\right) = 0\,. \tag{4.55}$$

This equation may be interpreted as

$$\frac{dp}{dt} - a^2\frac{d\rho}{dt} = 0\,, \tag{4.56}$$

along curves in x, t space where $dx/dt = u$. Thus we see that the partial differential equation reduces to an ordinary differential equation along characteristic lines. We may then write

$$dp - a^2 d\rho = 0 \quad on \quad \frac{dx}{dt} = u\,. \tag{4.57}$$

There will be some circumstances, where we can integrate (4.57) in closed form and we will discuss this shortly. First we can consider two other characteristic directions by adding and subtracting (4.46) and (4.49) to yield:

$$\frac{\partial p}{\partial t} + (u \pm a)\frac{\partial p}{\partial x} \pm \rho a\left[\frac{\partial u}{\partial t} + (u \pm a)\frac{\partial u}{\partial x}\right] = 0\,. \tag{4.58}$$

So that we may interpret these equations as

$$dp \pm \rho a du = 0 \quad on \quad \frac{dx}{dt} = u \pm a\,. \tag{4.59}$$

Thus we have reduced our system of three first-order partial differential equations to three first order ordinary differential equations (4.57) and (4.59) along three characteristic directions.

The first characteristic equation, may be rewritten to be $dp/d\rho = a^2$ on $dx/dt = u$. We note that the general definition of the sound speed is $a^2 = (\partial p/\partial \rho)_s$ and that in a one-dimensional flow the trajectory of a particle path is $dx/dt = u$. In general $p = p(\rho, s)$ so that $dp = (\partial p/\partial \rho)_s d\rho + (\partial p/\partial s)_\rho ds$. Then for $ds = 0$, $dp = a^2 d\rho$. Thus the characteristic equation is equivalent to the statement that the entropy is a constant along particle paths. We have found this to be true for an inviscid, non-conducting, adiabatic flow in the absence of shocks. The consequence of this for our one-dimensional flow is that the flow must be isentropic if we are to use the characteristic relationships.

The second and third characteristic relationships governed by (4.59) represent waves traveling at $u \pm a$ which implies they are right running acoustic waves and left running acoustic waves whose wave speeds are the sound speed relative to the flow velocity. The characteristic equations may be written as $dp/\rho a \pm du = 0$ on $dx/dt = u \pm a$

$$du \pm \frac{dp}{\rho a} = 0 \quad on \quad \frac{dx}{dt} = u \pm a\,. \tag{4.60}$$

may be integrated in closed form for the case of a perfect gas.

Perfect gases

For the isentropic flow of a perfect gas we can use $a^2 = dp/d\rho = \gamma p/\rho$. Then $2da/a = dp/p - d\rho/\rho$ and $d\rho = (d\rho/dp)dp = dp/a^2$. Using these relationships we can show that $dp/\rho a = 2da/(\gamma - 1)$. Then the characteristic relationships (4.60) for a perfect gas become

$$du \pm \frac{2da}{\gamma - 1} = 0 \quad on \quad \frac{dx}{dt} = u \pm a\,. \tag{4.61}$$

This can be readily integrated to yield

$$u \pm \frac{2a}{\gamma - 1} = constant \quad on \quad \frac{dx}{dt} = u \pm a\,. \tag{4.62}$$

The relationships $u \pm 2a/(\gamma - 1)$ are the well known *Riemann invariants.* For a one-dimensional isentropic flow, (4.62) represents the complete solution to the problem. This can be best seen graphically from Fig. 4.4 below.

In Fig. 4.4 we illustrate two characteristic waves originating from the initial data line $t = 0$. Along this line the values of u and a are known as a function of x. The right-running wave, originating at $(x_1, 0)$ follows a path given by $dx/dt = u + a$ and the left-running wave, originating at $(x_2, 0)$ follows a path given by $dx/dt =$

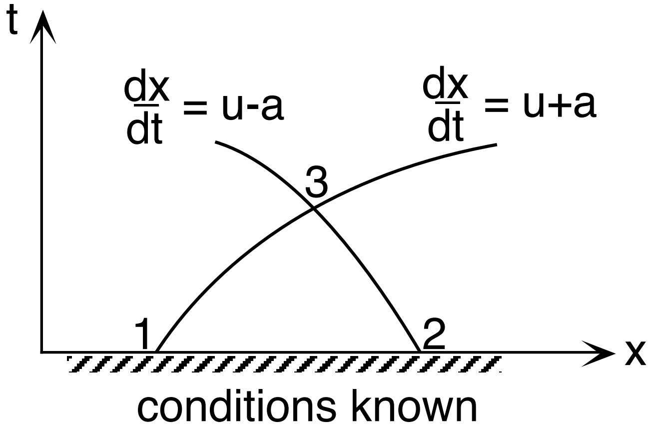

Figure 4.4. Riemann invariants for a one-dimensional, unsteady, adiabatic, isentropic flow of a perfect gas.

$u - a$. The waves intersect at (x_3, t_3). The values of u_1, a_1, u_2 and a_2 are known from the initial data. The solution at point 3 is given by the solution of

$$u_3 + \frac{2a_3}{\gamma - 1} = u_1 + \frac{2a_1}{\gamma - 1}\,, \tag{4.63}$$

$$u_3 - \frac{2a_3}{\gamma - 1} = u_2 - \frac{2a_2}{\gamma - 1}\,. \tag{4.64}$$

So that

$$u_3 = \frac{1}{2}\left[u_1 + u_2 + \frac{2}{\gamma - 1}(a_1 - a_2)\right]\,, \tag{4.65}$$

$$a_3 = \frac{1}{2}\left[a_1 + a_2 + \frac{\gamma - 1}{2}(u_1 - u_2)\right]\,. \tag{4.66}$$

In this manner the solution for u and a may be determined for any point (x, t) which is at the intersection of two characteristics which originate at the initial data line.

The solution for the other flow variables may be found from the isentropic, perfect gas relations so that

$$\frac{p_3}{p_1} = \left(\frac{a_3}{a_1}\right)^{2\gamma/(\gamma-1)}\,, \tag{4.67}$$

$$\frac{T_3}{T_1} = \left(\frac{a_3}{a_1}\right)^{2}\,. \tag{4.68}$$

The only remaining question now that we know the solution at point 3 is, where is point 3? If the characteristics were straight, then $(dx/dt)_{1-3} = u_1 + a_1$

and $(dx/dt)_{1-2} = u_2 - a_2$. Integrating gives

$$\frac{x_3 - x_1}{t_3} = u_1 + a_1 \,, \tag{4.69}$$

$$\frac{x_3 - x_2}{t_3} = u_2 - a_2 \,, \tag{4.70}$$

which may be solved for x_3 and t_3 as

$$x_3 = \frac{x_2(u_1 + a_1) - x_1(u_2 - a_2)}{(u_1 + a_1) - (u_2 - a_2)} \,, \tag{4.71}$$

$$t_3 = \frac{x_2 - x_1}{(u_1 + a_1) - (u_2 - a_2)} \,. \tag{4.72}$$

However, in general the characteristics will not be straight. In order for this to occur $u_1 + a_1$ would have to be equal to $u_3 + a_3$ and $u_2 - a_2$ would have to be equal to $u_3 - a_3$. From (4.67) and (4.68) we see that this can only occur if we have uniform conditions $u_1 = u_2$, $a_1 = a_2$ so that $u_3 = u_1 = u_2$ and $a_3 = a_1 = a_2$. For the general case we can find better approximations for x_3 and t_3 by averaging the slopes $u + a$ at 1 and 3 and $u - a$ at 2 and 3. We can do this since we can find the values u_3 and a_3 from (4.67) and (4.68) without first determining x_3 and t_3. We can use

$$\frac{x_3 - x_1}{t_3} = \frac{1}{2}\left[(u_1 + a_1) + (u_3 + a_3)\right] \,, \tag{4.73}$$

$$\frac{x_3 - x_2}{t_3} = \frac{1}{2}\left[(u_2 - a_2) + (u_3 - a_3)\right] \,, \tag{4.74}$$

which may be solved to give a better approximation for x_3 and t_3. This procedure is equivalent to using a trapezoidal rule to integrate the characteristic slopes.

Next we consider a situation where the flow conditions are uniform on at least part of the initial-data line $t = 0$. This situation is depicted in Fig. 4.5 below. First, let us consider point 3 which is formed by the intersection of two opposite family characteristic lines emanating from the uniform flow part of the initial-data line. The two characteristic relationships, (4.64), evaluated along 1–3 and 1–2 respectively are

$$u_3 + \frac{2a_3}{\gamma - 1} = u_1 + \frac{2a_1}{\gamma - 1} = u_0 + \frac{2a_0}{\gamma - 1} \,,$$

$$u_3 - \frac{2a_3}{\gamma - 1} = u_2 - \frac{2a_2}{\gamma - 1} = u_0 - \frac{2a_0}{\gamma - 1} \,.$$

The solution is obviously $u_3 = u_1 = u_2 = u_0$ and $a_3 = a_1 = a_2 = a_0$. Flow conditions have not changed and the characteristic lines will be straight since $u_3 + a_3 = u_1 + a_1 = u_0 + a_0$ and $u_3 - a_3 = u_2 - a_2 = u_0 - a_0$. This situation with

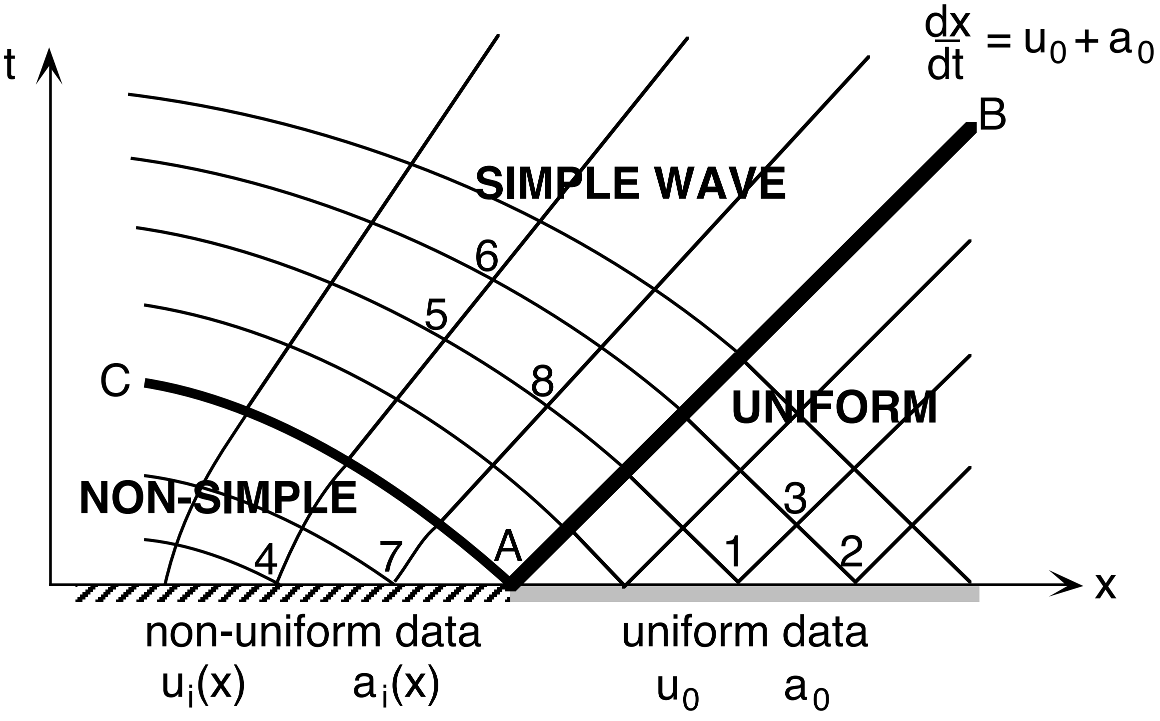

Figure 4.5. Wave diagram with uniform flow conditions on a portion of the intial data line.

uniform flow and straight characteristics will occur for any point which is found by the intersection of two characteristics lines emanating from the uniform flow part of the initial data line. Thus from Fig. 4.5, all points to the right of the heavy line A–B with slope $dx/dt = u_0 + a_0$ will have uniform flow. This is called a *uniform flow region* and generally only the waves at the boundaries of the region are drawn.

Next consider point 5. The characteristic relationships are

$$\begin{aligned} u_5 + \frac{2a_5}{\gamma - 1} &= u_4 + \frac{2a_4}{\gamma - 1}\,, \\ u_5 - \frac{2a_5}{\gamma - 1} &= u_1 - \frac{2a_1}{\gamma - 1} = u_0 - \frac{2a_0}{\gamma - 1}\,. \end{aligned}$$

We see that $u_5 \neq u_0$ and $a_5 \neq a_0$, so that the flow is not uniform. Now consider point 6 which is on the same right running characteristic as point 5. The characteristic relationships for point 6 are

$$\begin{aligned} u_6 + \frac{2a_6}{\gamma - 1} &= u_4 + \frac{2a_4}{\gamma - 1}\,, \\ u_6 - \frac{2a_6}{\gamma - 1} &= u_2 - \frac{2a_2}{\gamma - 1} = u_0 - \frac{2a_0}{\gamma - 1}\,. \end{aligned}$$

We see that point 6 does not have uniform conditions but we do see that the solution for point 6 must be identical to the solution to point 5 or $u_6 = u_5$ and $a_6 = a_5$. We can see that this will be true for any points on the right-running characteristic originating from point 4 which have a left-running characteristic originating from the uniform data line. This will occur for all points above the heavy curved line A–C which is a left-running characteristic coming from the boundary between uniform conditions and non-uniform conditions on the initial data line. Now on each right-running characteristic coming from the non-uniform data and above curve A–C will have the same conditions and that part of the characteristic will be straight, *e.g.,* $u_6 + a_6 = u_5 + a_5$. We see that on another right running characteristic, 7–8, conditions will be different since

$$\begin{aligned} u_8 + \frac{2a_8}{\gamma - 1} =& u_7 + \frac{2a_7}{\gamma - 1}\,, \\ u_8 - \frac{2a_8}{\gamma - 1} =& u_1 - \frac{2a_1}{\gamma - 1} = u_0 - \frac{2a_0}{\gamma - 1}\,. \end{aligned}$$

Since $u_7 \neq u_4$ and $a_7 \neq a_4$, then $u_7 \neq u_6 = u_5$ and $a_7 \neq a_6 = a_5$. Thus we see that this region will have one family of characteristics which are straight and have constant conditions along it. It is called a *one-wave flow region* or a *simple wave region.* Finally the region to the left of the left-running characteristic A–B coming from the boundary between uniform conditions and non-uniform conditions on the initial data line will be called a *non-simple region* because in general both families of characteristics will be curves. This can be seen because all points in this region are formed by the intersection of characteristics emanating from the non-uniform initial-data line.

Unsteady expansions and compressions

Now we will consider a long constant area tube, which has an internal piston inside the tube. At $t = 0$, the piston is located at $x = 0$. Then with an external mechanism, the piston slowly begins moving to the right at a speed of $u_p(t)$. The trajectory of the piston is the heavy line in Fig. 4.6. We will be interested in the properties of the gas to the left of the piston. Initially the fluid is at rest with a velocity u_0 and a sound speed of a_0. Throughout this section we will be assuming that the fluid behaves as a perfect gas. As the piston begins moving to the right, the fluid particles immediately adjacent to the piston must move with the same velocity as the piston $u_p(t)$. Since the flow is at rest for $t = 0$ and $x \leq 0$, then we will have a uniform region with $u = u_0 = 0$ and $a = a_0$ for everywhere to the left of the line $x = (u_0 - a_0)t = -a_0 t$ as shown in the sketch in Fig. 4.6.

Consider a point in the fluid just adjacent to the piston denoted by the point w in the figure. From the no penetration condition, $u_w = u_p(t)$. Then a right-running characteristic from the initial data line will reach the piston so that

$$u_w + \frac{2a_w}{\gamma - 1} = 0 + \frac{2a_0}{\gamma - 1}$$

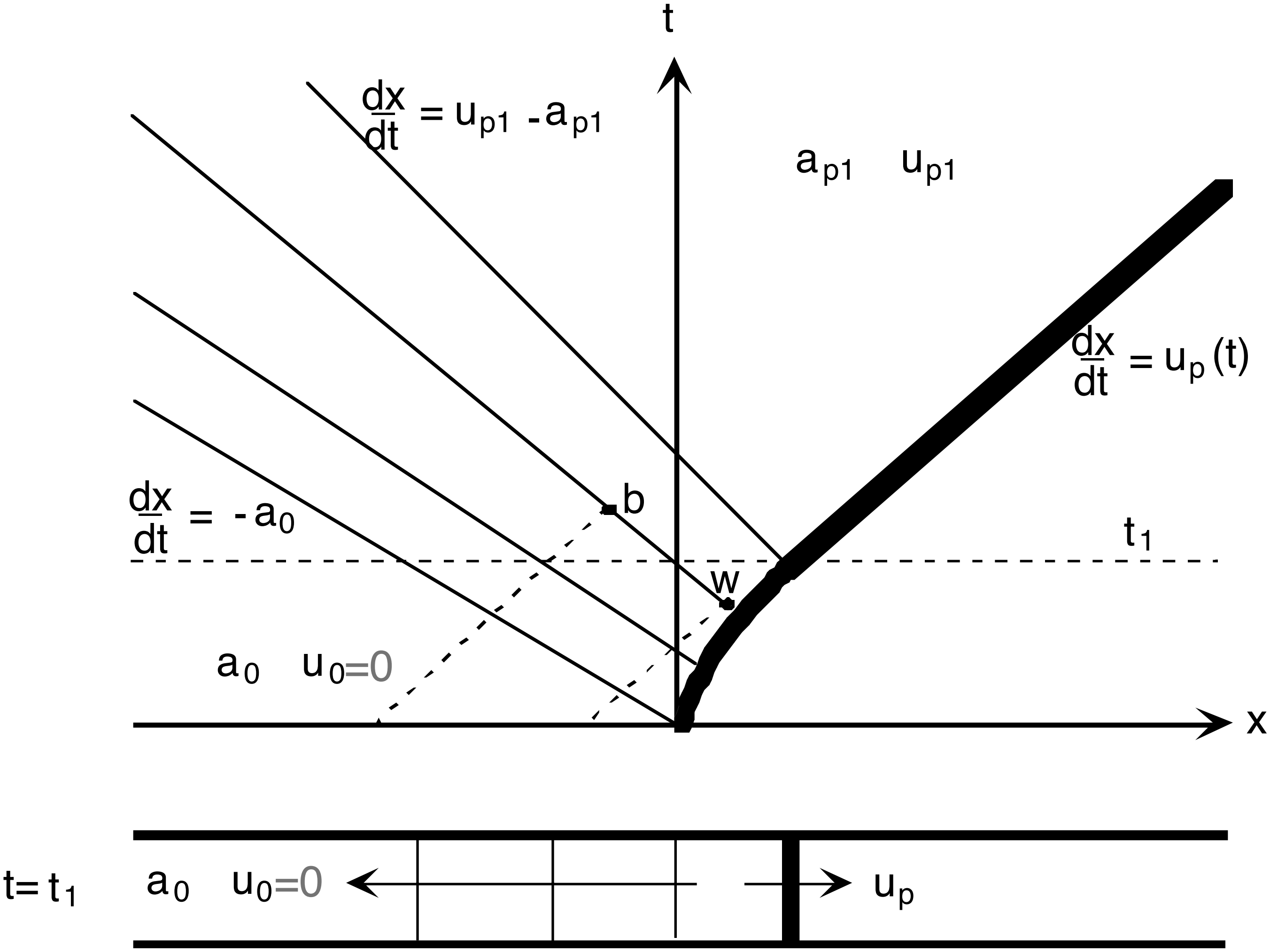

Figure 4.6. Unsteady piston creating expansion waves.

so that

$$a_w = a_p = a_0 - \frac{\gamma - 1}{2} u_p \,. \tag{4.75}$$

We see that $a_w = a_p < a_0$. Next we consider a point b on the same left-running characteristic as w. The Riemann invariants are:

$$\begin{aligned} u_b + \frac{2a_b}{\gamma - 1} &= 0 + \frac{2a_0}{\gamma - 1} \,, \\ u_b - \frac{2a_b}{\gamma - 1} &= u_w - \frac{2a_w}{\gamma - 1} = u_p - \frac{2a_p}{\gamma - 1} \,. \end{aligned}$$

We see that $u_b = u_w = u_p$ and $a_b = a_w = a_p$. Thus the characteristic line between w and b is straight and has a slope of $dx/dt = u_p - a_p$. Since $u_p > 0$ and $a_p < a_0$, the wave $w - b$ will travel to the left more slowly than the initial wave at

$dx/dt = -a_0$. We can generalize the picture by noting that for a piston whose speed is monotonically increasing, all left-running characteristics will be straight and each succeeding wave in time will travel more slowly to the right. This is an example of a simple wave region, discussed previously and sometimes called one-wave flow.

Now let us assume that at time $t = t_1$ that the piston attains a speed u_{p_1} and that the speed of sound in the gas adjacent to the piston is $a_{p_1} = a_0 - (\gamma - 1)u_{p_1}/2$. Furthermore we assume that $u_p = u_{p_1}$ for $t \geq t_1$. Then as indicated on Fig. 4.6 we have a uniform region with $u = u_{p_1}$ and $a = a_{p_1}$ to the right of the left-running characteristic $dx/dt = u_{p_1} - a_{p_1}$.

The left-running characteristics for this situation are called *expansion waves*, since as they pass over a fluid particle, the induce an increased velocity to the right (opposite to the direction of wave propagation) and they decrease the speed of sound of the fluid. A decrease in speed of sound means a decreased temperature, and for isentropic flow, a decreased pressure and density. We can describe an unsteady expansion process by following a fluid particle initially at rest in the tube some distance to the left of the piston. As the piston begins moving, the fluid particle senses no change until the first sound wave $dx/dt = -a_0$ passes over the particle. This first wave infinitesimally induces a velocity in the particle to the right and infinitesimally lowers the temperature and pressure. From that point on a continuous series of waves passes over the particle, each one speeding up the particle (to the right) and lowering the temperature and pressure until the constant values of $u = u_{p_1}$ and $a = a_{p_1}$ are reached.

Next, suppose we are somehow able to accelerate the piston to a constant speed almost instantly. Then the x–t diagram would be as indicated in Fig. 4.7. The expansion waves all appear to be emanating from the origin. This situation is called a *centered expansion* or an *expansion fan*. Note that in the figure, we are calling the constant piston speed u_p and the sound speed in the gas adjacent to the piston as a_p. Also note that the number of waves indicated is arbitrary. In reality there are an infinite number of waves within the expansion fan.

Now lets look on the other side of the piston. First we consider a piston slowly accelerating from rest and moving from towards the right at velocity $u_p(t)$ as indicated in Fig. 4.8. We see that we have a uniform region to the right of the sound wave emanating from the origin at a speed of $dx/dt = a_0$. Consider a point w in the fluid adjacent to the surface of the piston. From the no penetration condition $u_w = u_p(t)$. Taking a left running characteristic from the initial data line to point w we have

$$u_w - \frac{2a_w}{\gamma - 1} = 0 - \frac{2a_0}{\gamma - 1}$$

so that

$$a_w = a_p = a_0 + \frac{\gamma - 1}{2} u_p \,. \tag{4.76}$$

We see that $a_w = a_p > a_0$. Next we consider a point b on the same right-running

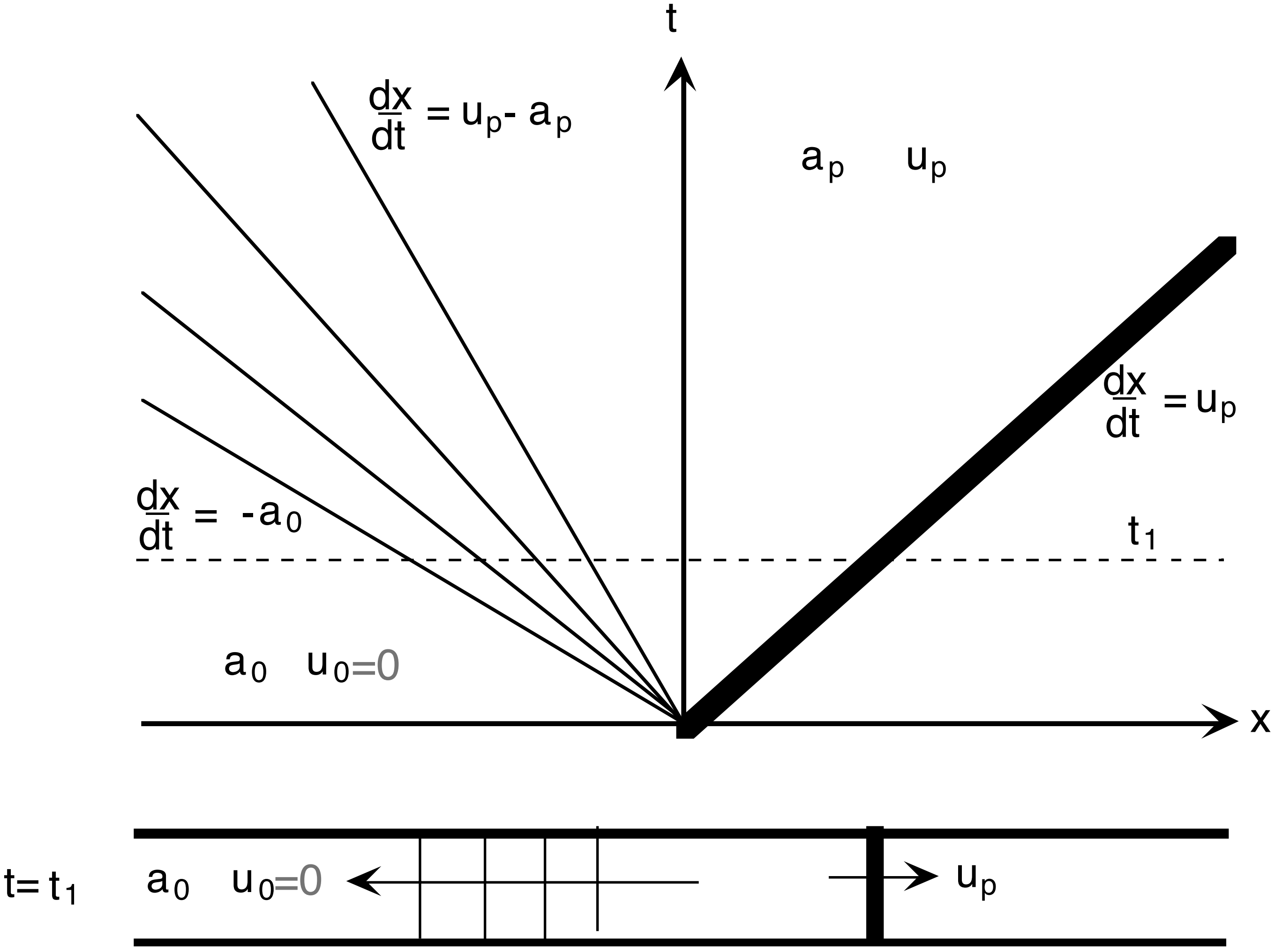

Figure 4.7. Constant speed piston creating centered expansion.

characteristic as w. The Riemann invariants are:

$$u_b - \frac{2a_b}{\gamma-1} = 0 - \frac{2a_0}{\gamma-1}\,,$$
$$u_b + \frac{2a_b}{\gamma-1} = u_w + \frac{2a_w}{\gamma-1} = u_p + \frac{2a_p}{\gamma-1}\,.$$

We see that $u_b = u_w = u_p$ and $a_b = a_w = a_p$. Thus, the characteristic line between w and b is straight and has a slope of $dx/dt = u_p + a_p$. Since $u_p > 0$ and $a_p > a_0$, the wave $w - b$ will travel to the right more quickly than the initial wave at $dx/dt = a_0$. We can see more evidence of this phenomena by considering points w' and b'. We can go through the same procedure as was done for w and b to get $u_{w'} = u_p(t')$, $a_{w'} = a_0 + (\gamma-1)u_p(t')/2$ and $u_{b'} = u_{w'}$ and $a_{b'} = a_{w'}$. Since $t' > t$, $u_p(t') > u_p(t)$ and $a_p(t') > a_p(t)$. Thus the wave $w' - b'$ will be traveling faster than $w - b$. We

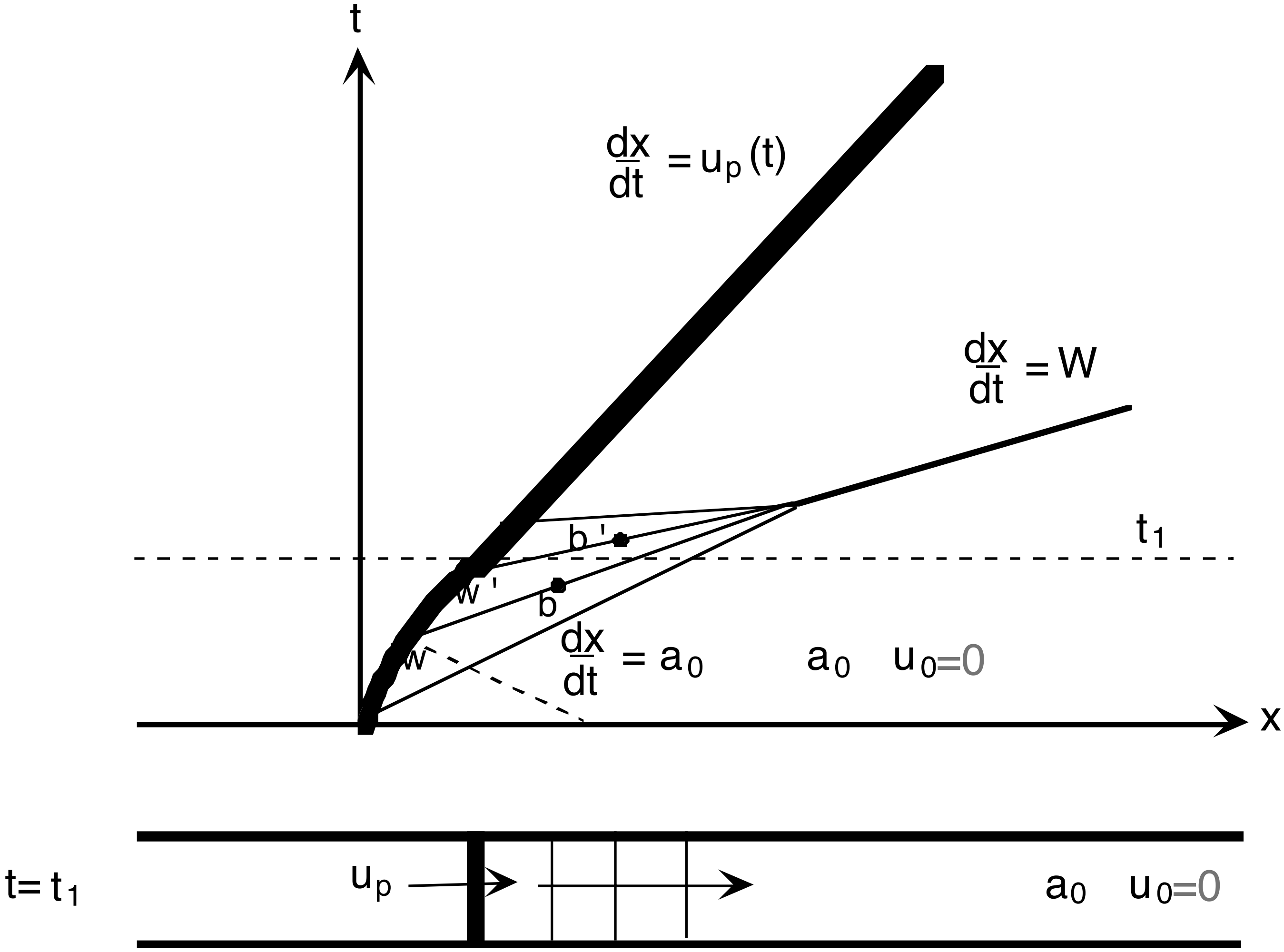

Figure 4.8. Unsteady piston creating compression waves.

can generalize the picture by noting that for a piston whose speed is monotonically increasing, all right-running characteristics will be straight and each succeeding wave in time will travel more quickly to the right. These waves pass over fluid particles inducing an increased motion to the right (in the same direction as wave propagation) and increasing the temperature and pressure. Hence they are called *compression waves.* Since succeeding waves travel faster and faster, eventually this leads to a situation where the characteristics catch up to each other. We note that it can be proven that characteristic lines of the same family cannot cross each other so that our isentropic solutions will be no longer valid once the characteristics begin to coalesce. What occurs is that the characteristic coalesce to form a non-isentropic moving shock wave. The speed of the shock wave W will be faster than the that of the initial compression wave $dx/dt = a_0$.

If we were to accelerate the piston to a constant speed u_p instantaneously,

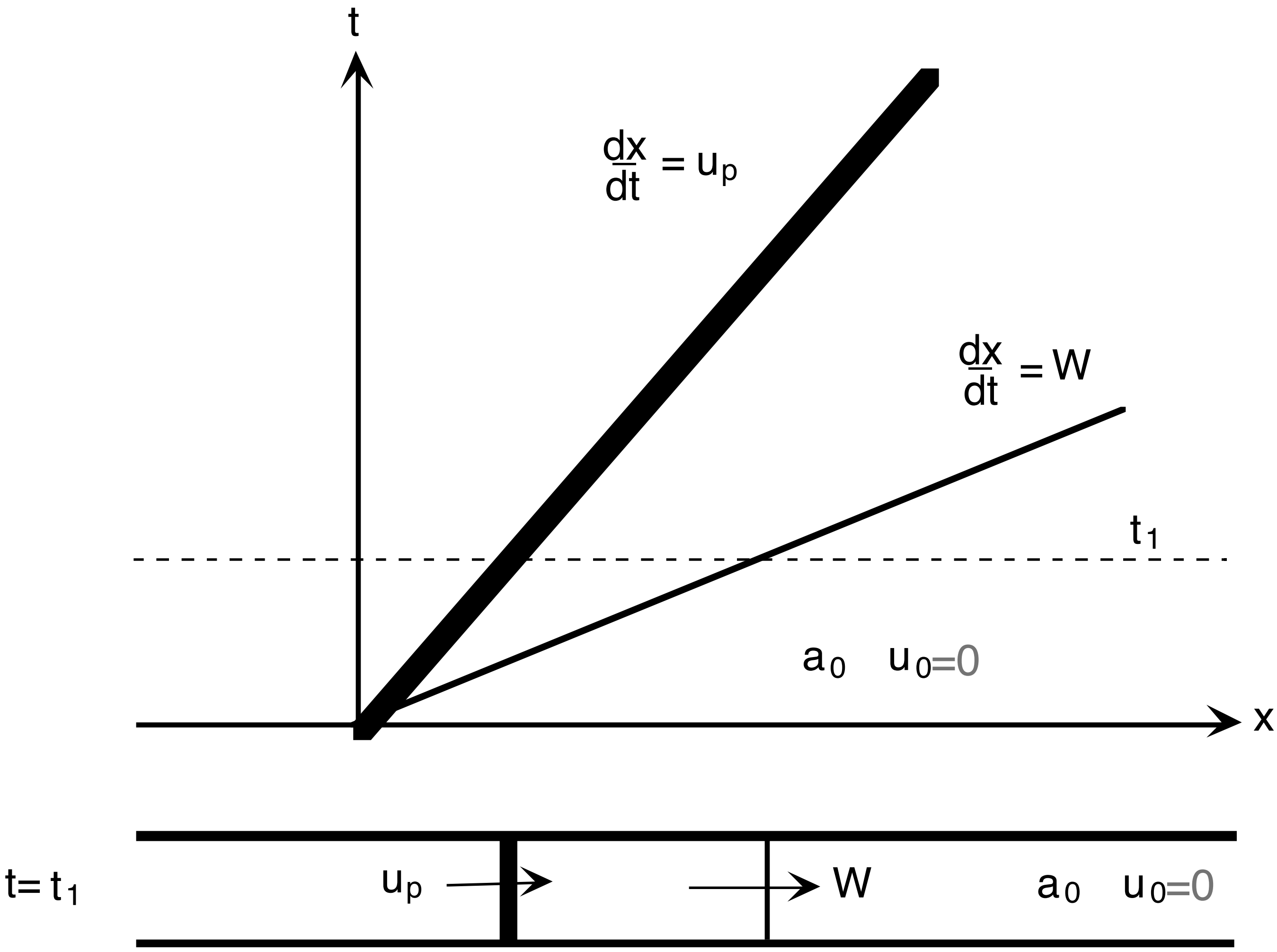

Figure 4.9. Constant speed piston creating moving shock.

then the characteristics would coalesce instantaneously as shown in Fig. 4.9. This situation would result in a shock moving at constant velocity W. Behind the shock the fluid will all be traveling at constant velocity u_p. It will be easy to show that $W > u_p$. So for a compression of this type, a fluid particle initially to the right of the piston will remain at rest until a shock moving at speed W passes over it. Then instantly the particle accelerates to velocity u_p and its sound speed increases to a_p and its pressure and temperature increase accordingly. However this process is non-isentropic.

In the next subsection we will discuss how to handle moving shock waves formed by the coalescence of compression waves. Before that, we may note some interesting properties of unsteady characteristic waves. As we have seen, these waves travel at a speeds of $u \pm a$. Thus they are traveling at the local speed of sound $\pm a$ relative to the local fluid particle velocity u. We see that compression waves will tend to coalesce since each succeeding wave is moving in a region of fluid with higher sound speed. The opposite effect occurs for expansion waves which will spread out because each succeeding wave lowers the sound speed which slows the following wave.

Shocks moving at a steady speed

Consider a shock formed from the instantaneous acceleration of a piston to velocity u_p. The shock will move at a constant speed W and the fluid behind the shock will be at a velocity u_p. The fluid in front of the shock will be at rest. This situation is illustrated in the top sketch in Fig. 4.10.

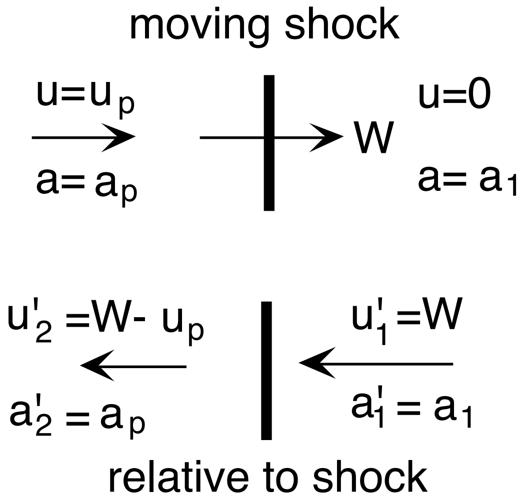

Figure 4.10. Shock wave moving at constant speed.

In this situation we know a_1 and u_p. We do not know a_p (or the corresponding pressure p_p) or the shock speed W. Note that we cannot determine a_p by taking a left-running characteristic from the initial data line to the piston because this would involve crossing the shock wave. The characteristic relationships are not valid across a shock.

One solution to this unsteady shock problem is to use the unsteady shock jump relationships developed in Chapter 3. But for the case of constant u_p and hence constant W, there is a simpler solution. We can look at the flow situation *relative to the shock*, as illustrated in the lower sketch of Fig. 4.10. An observer moving with the shock, sees a flow going from right to left, into the shock wave at a speed W and sees behind the shock, a flow going from right to left at a speed $W - u_p$. But what about the thermodynamic state, such as the temperature, pressure, sound speed, etc.? Recall that the *static* thermodynamic quantities are the values which would be measured by a probe normal to the flow *moving with the fluid particles.* Hence in the upper sketch, the fluid in front of the shock has a static pressure p_1 as measured by a probe which is not moving (since $u_1 = 0$). In the lower sketch, relative to the shock, the fluid appears to be moving at a speed W into the shock.

The pressure in front of the shock would again be p_1 as measured by a probe moving towards the shock at speed W. Since in both sketches the actual fluid velocity (in a absolute coordinate frame) is the same, the static quantities would be exactly the same. The *static* flow quantities are independent of the reference frames. Note this is definitely not true for *stagnation* quantities which most certainly depend on the reference frame.

Now in the lower sketch of Fig. 4.10, we have a steady shock with $u'_1 = W$, a'_1 and p'_1 entering the shock and $u'_2 = W - u_p$, $a'_2 = a_p$ and $p'_2 = p_p$ leaving the shock. Note we will adopt the convention that $'1$ refers to quantities entering a stationary shock (supersonic side) and $'2$ refers to quantities leaving the shock (subsonic side). The Mach number $M'_1 = W/a_1$. We know that from the Second Law of Thermodynamics, that the Mach number in front of a normal shock must be supersonic, and hence $W > a_1$, which we have already seen in our discussion of the coalescence of compression waves. For the steady shock problem in the relative coordinate frame, knowing M'_1, p'_1, T'_1 would be sufficient to determine M'_2, p'_2, T'_2 from the Rankine-Hugoniot relationships. Note Eqs. (3.16) – (3.20) apply with subscripts 1 and 2 replaced by $'1$ and $'2$. But in this problem here we know p'_1 and T'_1 but we do not know M'_1. We do know one more piece of information, u_p. We have $u'_2 = u_p - W = u_p - u'_1$. We can use this information to solve the problem.

From (3.17), after adding the $'$ notation we have

$$\frac{\rho'_2}{\rho'_1} = \frac{u'_1}{u'_2} = \frac{(\gamma+1){M'}_1^2}{2+(\gamma-1){M'}_1^2} \,. \tag{4.77}$$

Substituting $u'_1 = W$, $M'_1 = W/a_1$ and $u'_2 = W - u_p$, yields

$$\frac{W}{W-u_p} = \frac{(\gamma+1)W^2}{2a_1^2+(\gamma-1)W^2} \,. \tag{4.78}$$

Since u_p and a_1 are known, this results in a quadratic equation for W:

$$W^2 - \frac{\gamma+1}{2}u_p W - a_1^2 = 0 \,, \tag{4.79}$$

which may be solved as

$$W = \frac{\gamma+1}{4}u_p + \left[\left(\frac{\gamma+1}{4}\right)^2 u_p^2 + a_1^2\right]^{1/2} \,. \tag{4.80}$$

Once W is found, we know $M'_1 = W/a_1$ and we can use the Rankine-Hugoniot relationship for pressure, (3.16) to obtain

$$\frac{p'_2}{p'_1} = \frac{p_p}{p_1} = 1 + \frac{2\gamma}{\gamma+1}\left(\frac{W^2}{a_1^2} - 1\right) \,. \tag{4.81}$$

We then use (3.17) and (3.18) to obtain

$$\frac{\rho_2'}{\rho_1'} = \frac{\rho_p}{\rho_1} = \frac{u_1'}{u_2'} = \frac{W}{W - u_p}\,, \tag{4.82}$$

and

$$\frac{T_2'}{T_1'} = \frac{T_p}{T_1} = \frac{a_p^2}{a_1^2} = \frac{p_2'/p_1'}{\rho_2'/\rho_1'}\,. \tag{4.83}$$

Sometimes, instead of knowing u_p and p_1 and a_1, we wish to solve the problem knowing p_p and p_1 and a_1. Then since $p_2' = p_p$ and $p_1' = p_1$, we will know p_2'/p_1' and it is straightforward to use the Rankine-Hugoniot relations to get $M_1' = W/a_1$. From (4.81), we can solve for W/a_1 as

$$\frac{W}{a_1} = \left[1 + \frac{\gamma+1}{2\gamma}\left(\frac{p_p}{p_1} - 1\right)\right]^{1/2}\,. \tag{4.84}$$

Then from (4.77) we can solve for $\rho_2' = \rho_p$ and $u_2' = W - u_p$.

Shock tubes

We consider a shock tube which consists of a long constant area duct which initially contains gases at two different states separated by a diaphragm. On one side, the gas is at a high pressure and this side is called the *driver.* On the other side, the gas is at a low pressure and this side is called the *driven.* In the sketch in Fig. 4.11, the driver is on the left side of the tube and the high pressure gas is initially at rest at state 4. The driver and the driven often contain different gases. The initial conditions in the driver are p_4, T_4, a_4, γ_4 with $u_4 = 0$. The initial conditions in the driven are p_1, T_1, a_1, γ_1 with $u_1 = 0$. Often in addition to $p_4 >> p_1$ the driver is heated so that $T_4 > T_1$. At $t = 0$ the diaphragm is broken using an external mechanism. (The diaphragm material may be mylar or brass or steel depending upon the size of the tube and the pressure ratio p_4/p_1.) When the diaphragm is burst, there will be an interface between the two gas states which travels down the tube from left to right at a speed u_p. This interface acts like a massless piston and is actually a contact surface. The movement of the interface generates a shock moving to the right at a speed of W and expansion waves moving to the left into region 4. The shock raises the pressure from a low pressure of p_1 to a higher pressure p_2. The expansion waves lower the pressure from p_4 to p_3. Since the interface is a massless piston, there can be no force across it, so that

$$p_2 = p_3\,. \tag{4.85}$$

Also since there is no flow across the interface, we must have

$$u_2 = u_3 = u_p\,. \tag{4.86}$$

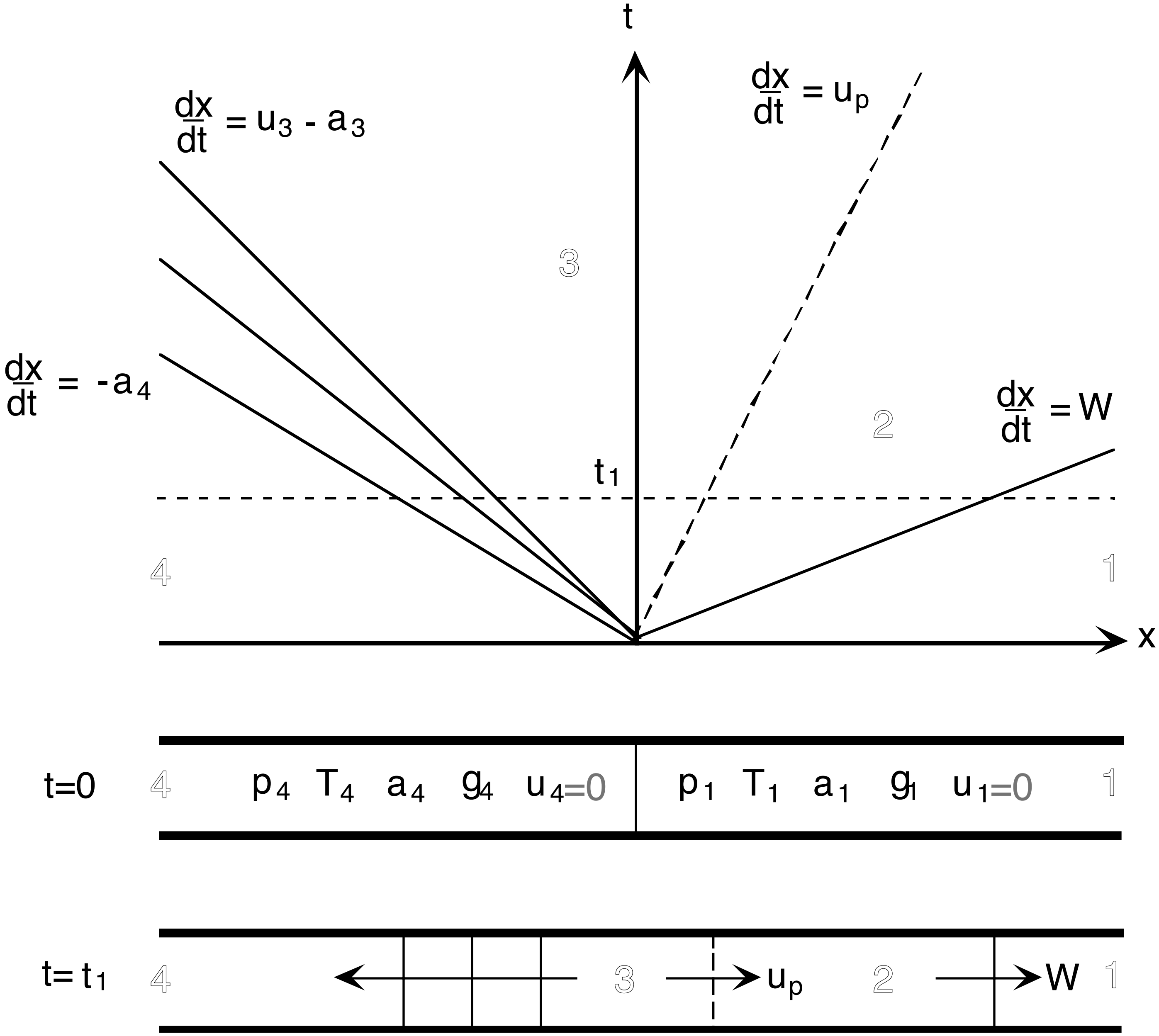

Figure 4.11. Open-ended shock tube.

This situation is illustrated in x–t diagram in Fig. 4.11. We can solve for the flow in the entire tube by using characteristic relationships across the expansion fan, the Rankine-Hugoniot relationships across the shock and the interface conditions (4.85), (4.86). Note that the gas in regions 3 and 4 is at γ_4 and the gas in regions 1 and 2 is at γ_1. In solving shock tube problems, conditions in regions 1 and 4 are generally known.

Considering a right-running characteristic going from region 4 to region 3 gives

$$u_3 + \frac{2a_3}{\gamma_4 - 1} = 0 + \frac{2a_4}{\gamma_4 - 1}\,,$$

which may be solved for a_3 as

$$\frac{a_3}{a_4} = 1 - \left(\frac{\gamma_4 - 1}{2}\right)\frac{u_3}{a_4}\,. \tag{4.87}$$

The pressure p_3 may be found from the isentropic relationships, such as used in (4.67), to give

$$\frac{p_3}{p_4} = \left[1 - \left(\frac{\gamma_4 - 1}{2}\right)\frac{u_3}{a_4}\right]^{2\gamma_4/(\gamma_4 - 1)}\,. \tag{4.88}$$

Note that in (4.87) and (4.88), the quantity u_3 has not yet been found.

Next we consider the shock wave. We can determine the shock velocity W in terms of the piston velocity $u_p = u_2$ from (4.84) as

$$\frac{W}{a_1} = \left[1 + \left(\frac{\gamma_1 + 1}{2\gamma_1}\right)\left(\frac{p_2}{p_1} - 1\right)\right]^{1/2}\,. \tag{4.89}$$

We can then solve for $u_2 = u_p$ from (4.78) as

$$\frac{u_2}{a_1} = \frac{2(W^2 - a_1^2)}{(\gamma_1 + 1)W}\,. \tag{4.90}$$

Substituting (4.89) into (4.90) gives

$$u_2 = \frac{1}{\gamma_1}\left(\frac{p_2}{p_1} - 1\right)\left[1 + \left(\frac{\gamma_1 + 1}{2\gamma_1}\right)\left(\frac{p_2}{p_1} - 1\right)\right]^{-1/2}\,. \tag{4.91}$$

We can solve for p_2/p_1 from (4.88), (4.91) and the two interface conditions (4.85) and (4.86). Eq. (4.88) gives $p_3/p_4 = f(u_3/a_1)$ and (4.91) gives $u_2/a_1 = g(p_2/p_1)$. Using $p_2 = p_3$ and $u_2 = u_3$ we can write $p_3/p_4 = (p_2/p_1)(p_1/p_4)$ and $u_3/a_4 = (u_2/a_1)(a_1/a_4)$ and substitute into (4.88) to obtain

$$\frac{p_2}{p_1}\frac{p_1}{p_4} = \left[1 - \left(\frac{\gamma_4 - 1}{2}\right)\frac{u_2}{a_1}\frac{a_1}{a_4}\right]^{2\gamma_4/(\gamma_4 - 1)}\,. \tag{4.92}$$

And substituting (4.91) for u_2/a_1 gives the following equation involving p_2/p_1 as the only unknown:

$$\frac{p_2}{p_1} = \frac{p_4}{p_1}\left[1 - \left(\frac{\gamma_4 - 1}{2}\right)\frac{a_1}{a_4}\frac{1}{\gamma_1}\left(\frac{p_2}{p_1} - 1\right)\left[1 + \left(\frac{\gamma_1 + 1}{2\gamma_1}\right)\left(\frac{p_2}{p_1} - 1\right)\right]^{-1/2}\right]^{2\gamma_4/(\gamma_4 - 1)}\,. \tag{4.93}$$

Given p_4/p_1, a_4/a_1 and γ_4 and γ_4, (4.93) may be iteratively be solved for p_2/p_1. Eq. (4.93) is sometimes referred to as the *shock tube equation*.

Once p_2/p_1 has been found we can use (4.89) to determine W/a_1 and (4.90) to find u_2/a_1. Then from the Rankine-Hugoniot relation (4.77) we have

$$\frac{\rho_2}{\rho_1} = \frac{\rho_2'}{\rho_1'} = \frac{u_1'}{u_2'} = \frac{W}{W - u_2}\,. \tag{4.94}$$

And from the thermal equation of state $T_2/T_1 = (p_2/p_1)/(\rho_2/\rho_1)$ and $a_2/a_1 = \sqrt{T_2/T_1}$. For region 3, we can use the interface conditions $p_3 = p_2$ and $u_3 = u_2$ and (4.87) to find a_3/a_4 and then $T_3/T_4 = (a_3/a_4)^2$. This completes the solution to the shock tube problem.

Some applications of shock tubes are for short duration aerodynamic testing. An illustration of this application is illustrated in Fig. 4.12. There will be a relatively uniform flow over the model between the time the shock passes over the model and the contact surface reaches the model. The time may also be shortened if wave reflections from the downstream end of the tube reach the model. We will discuss shock reflections at the end of this subsection.

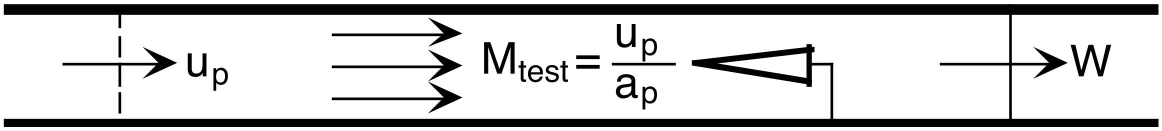

Figure 4.12. Shock tube as a test facility.

In general if the diaphragm is located at $x = 0$ and the model is located at x_t then the run time Δt is

$$\Delta t = \left(\frac{1}{u_p} - \frac{1}{W}\right) x_t\,. \tag{4.95}$$

The Mach number of the test will be

$$M_t = \frac{u_p}{a_2} = \frac{u_p}{a_1}\frac{a_1}{a_2}\,, \tag{4.96}$$

where u_p/a_1 is given in (4.91) and $a_2/a_1 = \sqrt{(p_2/p_1)/(\rho_2/\rho_1)}$ with p_2/p_1 given in (4.93) and ρ_2/ρ_1 given in (4.94).

One question that we might ask is how large can we make the test Mach number M_t. Our intuition tells us that the stronger the shock the high the value of M_t. Let us assume that we can strengthen the shock without bound, *e.g.*, $p_2/p_1 \to \infty$. Then from (4.91) we can see that

$$\frac{u_p}{a_1} \to \left[\frac{2}{\gamma_1(\gamma_1+1)}\frac{p_2}{p_1}\right]^{1/2} \quad \text{as } p_2/p_1 \to \infty\,,$$

and after some manipulation of (4.94), we can show that

$$\frac{a_2}{a_1} \to \left[\frac{(\gamma_1 - 1)}{(\gamma_1 + 1)}\frac{p_2}{p_1}\right]^{1/2} \qquad \text{as } p_2/p_1 \to \infty\,,$$

and finally

$$M_t \to \left[\frac{2}{\gamma_1(\gamma_1 + 1)}\right]^{1/2} \qquad \text{as } p_2/p_1 \to \infty\,.$$

For $\gamma_1 = 1.4$, $M_t \approx 1.89$. Thus, for a perfect gas with $\gamma_1 = 1.4$, no matter how strong we make the shock, the maximum value of test Mach number will be 1.89.

In order to strengthen the shock (increase p_2/p_1), from (4.92) we see that we can increase p_4/p_1 and we can decrease a_1/a_4. Thus we will usually want to make a_4 as large as possible. Since $a_4^2 = \gamma_4 R_4 T_4$ we can achieve high sound speeds by increasing T_4, increasing γ_4 and increasing R_4. We can increase γ_4 by using a monatomic gas in the driver such as helium. We can increase R_4 by decreasing the molecular weight of the driver gas. Helium accomplishes this and so does hydrogen. Sometimes hydrogen is heated and raised to a high temperature causing ignition which further increases the temperature and pressure of the driver gases. This is sometimes called a combustion tube.

One application for shock tubes is to generate high enthalpy flows to simulate reentry conditions. For example a reentry vehicle at $M = 30$ at an altitude of 60 km where the sound speed is $a_\infty \approx 372\ m/sec$ has a stagnation enthalpy $h_0 = a_\infty^2/(\gamma - 1) + U_\infty^2/2 \approx 6.26 \times 10^7\ m^2/sec^2$. If we use a wind tunnel with unheated air ($T_0 = 300K$) has a $h_0 = c_p T_0 \approx 3.01 \times 10^5\ m^2/sec^2$. For a wind tunnel with air heated to $T_0 = 1200K$ gets only $h_0 \approx 1.20 \times 10^6\ m^2/sec^2$. Somewhat higher values can be achieved in shock tunnels as shown in the following table:

Table 4.1 Shock Tube Use to Generate High Stagnation Enthalpy

p_4/p_1	T_4/T_1	p_2/p_1	u_p/a_1	T_2/T_1	W/a_1	$h_0(m^2/sec^2)$
10	1	2.848	0.821	1.393	1.61	4.6×10^5
100	1	6.595	1.660	2.047	2.41	7.8×10^5
100	10	21.99	3.440	4.629	4.36	2.1×10^6
100	30	33.22	4.302	6.504	5.35	3.1×10^6
100	50	39.14	4.694	7.492	5.80	3.6×10^6
300	1	29.23	4.017	5.839	5.02	2.7×10^6
300	10	92.15	7.319	16.328	8.89	8.1×10^6

Higher values of test Mach numbers M_t can be generated using shock tunnels. A shock tunnel is a shock tube followed by a diverging nozzle as shown in Fig. 4.13

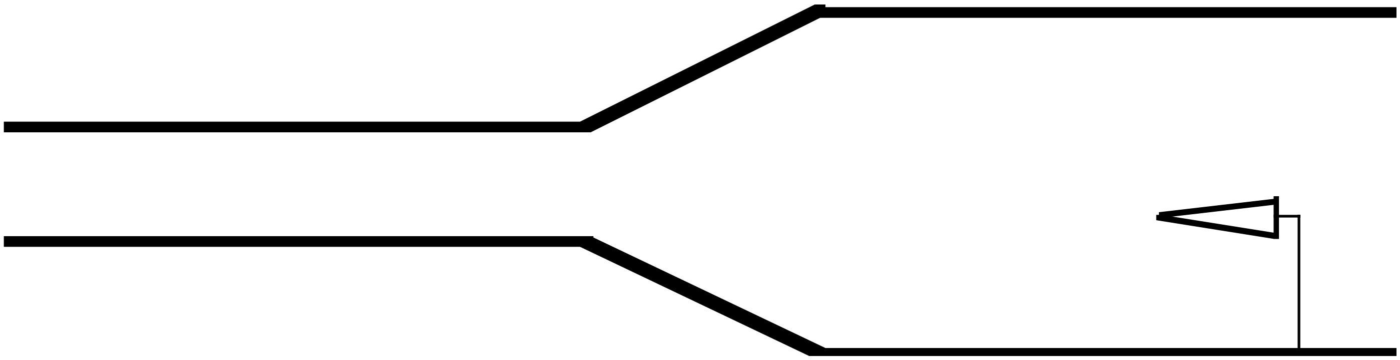

Figure 4.13. Shock tunnel.

The final part of our discussion on shock tubes consists of developing methods of treating wave reflections from closed ends of tubes. Consider a shock tube with closed ends on both the driver and driven side as sketched in Fig. 4.14. On the driver side we have reflections of the expansion fan from the wall and on the driven side we consider the shock reflection.

For the reflection of the expansion fan, the region after the reflected waves is region 6. In this region, since we must have no penetration through the walls, $u_6 = 0$. The other condition in region 6 can be determined from a left-running characteristic passing from region 3 to 6 such that

$$u_6 - \frac{2a_6}{\gamma_4 - 1} = u_3 - \frac{2a_3}{\gamma_4 - 1} \, ,$$

so that

$$a_6 = a_3 - \frac{(\gamma_4 - 1)}{2} u_3 \, , \tag{4.97}$$

and from the isentropic relationship

$$\frac{p_6}{p_3} = \left(\frac{a_6}{a_3} \right)^{2\gamma_4/(\gamma_4 - 1)} \, . \tag{4.98}$$

Since $a_6 < a_3$ and $p_6 < p_3$ we see that the reflected waves are expansions. It is generally true that unsteady expansion waves reflecting from a solid surface will reflect as expansion waves. (Also unsteady, isentropic compression waves will reflect from a solid surface as compression waves).

Next we consider the reflected shock. The region after the reflected shock we call region 5. Again, because the wall is solid, $u_5 = 0$. The situation for the shock before reflection is given in Fig. 4.10. The situation after reflection is shown in Fig. 4.15, where W_r is the velocity of the reflected shock wave.

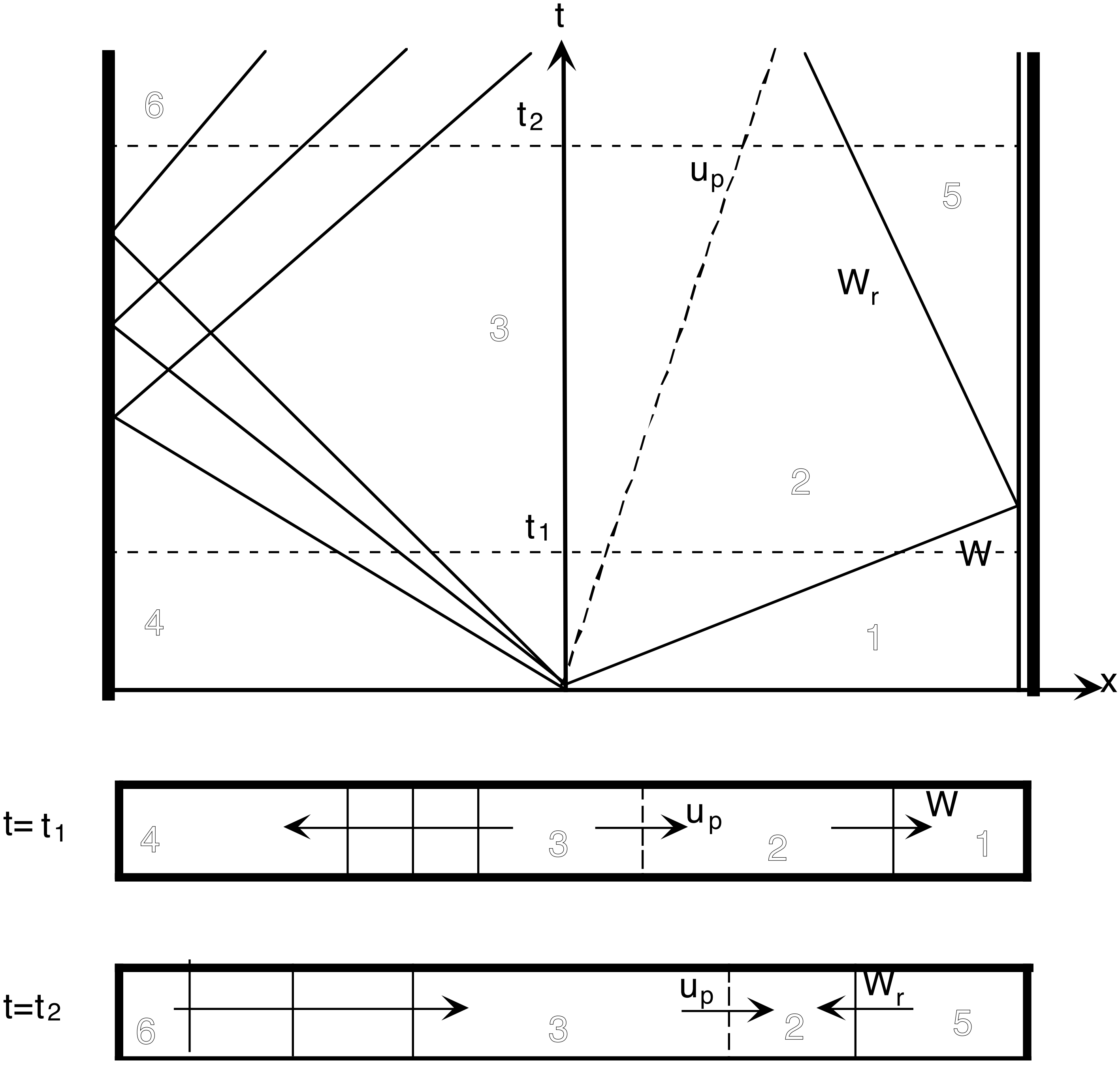

Figure 4.14. Closed-ended shock tube.

We see that region $1'$ is region 2 with the relative flow into the reflected shock at $u_1' = W_r + u_2$ and the relative flow leaving the reflected shock at $u_2' = W_r$. Then

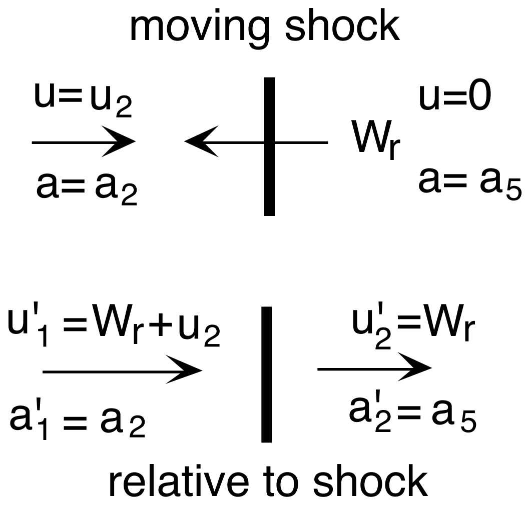

Figure 4.15. Reflected shock wave.

from the Rankine-Hugoniot condition (4.77) we see that

$$\frac{W_r+u_2}{W_r}=\frac{(\gamma_1+1)(W_r+u_2)^2}{2a_2^2+(\gamma_1-1)(W_r+u_2)^2}\,,$$

which results in

$$W_r^2+\frac{(3-\gamma_1)}{2}u_2W_r-\frac{(\gamma_1-1)}{2}u_2^2-a_2^2=0\,, \tag{4.99}$$

and may be solved for W_r. A neater form of this equation may be developed using the definitions $M_2=u_2/a_2$ and $M_r=(W_r+u_2)/a_2$. Then from (4.99) we obtain

$$M_r^2-\frac{(\gamma_1+1)}{2}M_2M_r-1=0\,, \tag{4.100}$$

which may be solved as

$$M_r=\frac{(\gamma_1+1)}{4}M_2+\left[\left(\frac{\gamma_1+1}{4}\right)^2M_2^2+1\right]^{1/2}\,. \tag{4.101}$$

After determining M_r and hence $W_r=a_2M_r-u_2$ we can use the Rankine-Hugoniot relations to find $p_5/p_2=p_2'/p_1'$ and $a_5/a_2=a_2'/a_1'$.

We have not discussed wave reflections from open ended tubes. In these situations waves will generally as waves of the *opposite* sense. Expansions will reflect as compressions and shocks will reflect as expansions. This case is discussed in Anderson as well as other references.

4.6 References Chapter 4

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5. METHOD OF CHARACTERISTICS

5.1 Second-Order PDE in 2 Independent Variables

Consider a second-order, *quasi-linear* partial differential equation in two independent variables,

$$A_1\frac{\partial^2\phi}{\partial x^2}+A_2\frac{\partial^2\phi}{\partial x\partial y}+A_3\frac{\partial^2\phi}{\partial y^2}+A_4=0\,, \tag{5.1}$$

where for a quasi-linear equation, the coefficients may depend upon the independent variables, the dependent variable and first derivatives of the dependent variable as

$$A_i=A_i(x,y,\phi,\partial\phi/\partial x,\partial\phi/\partial y)\,. \tag{5.2}$$

If the A_i were dependent upon the highest derivatives, the equation would be *nonlinear.*

Now, let us consider the conditions for which a solution $\phi(x,y)$ will be *analytic.* By this we mean that suppose ϕ and some of its derivatives are known along a certain line in space. Can we always determine a solution in the neighborhood of that line by expanding in a Taylor's series. This process is sometimes called *analytic continuation* and if this is possible, we call the solution analytic.

As a first example, suppose we know the solution ϕ along a line $x=x_0$. We call this line an *initial-data line.* Also assume that we are given the normal derivative $\partial\phi/\partial x$ along that line. Expanding in a Taylor's series we have

$$\phi(x_0+\Delta x,y)=\phi(x_0,y)+\Delta x\frac{\partial\phi(x_0,y)}{\partial x}+\frac{(\Delta x)^2}{2!}\frac{\partial^2\phi(x_0,y)}{\partial x^2}+\ldots\,. \tag{5.3}$$

So that obviously we will need the second derivative $\partial^2\phi/\partial x^2$ and all the higher derivatives evaluated along $x=x_0$. From the partial differential equation (5.1) we find

$$\frac{\partial^2\phi(x_0,y)}{\partial x^2}=-\frac{A_2}{A_1}\frac{\partial^2\phi(x_0,y)}{\partial x\partial y}-\frac{A_3}{A_1}\frac{\partial^2\phi(x_0,y)}{\partial y^2}-\frac{A_4}{A_1}\,, \tag{5.4}$$

where the coefficients A_i, $i=1,\ldots,4$ are evaluated at (x_0,y). Now, if along the line $x=x_0$, $\phi(x_0,y)=f_1(y)$ and $\partial\phi(x_0,y)/\partial x=f_2(y)$ where f_1 and f_2 are specified, then

$$\begin{aligned}\frac{\partial^2\phi(x_0,y)}{\partial x\partial y}&=\frac{df_2}{dy}\,,\\ \frac{\partial^2\phi(x_0,y)}{\partial y^2}&=\frac{d^2f_1}{dy^2}\,,\end{aligned} \tag{5.5}$$

so that the second x-derivative may be found from (5.4). The higher x-derivatives may be found by differentiating the governing equation (5.1) with respect to x

and differentiating the data f_1 and f_2 with respect to y. Thus we see that a solution for $\phi(x, y)$ with data given along a line $x = x_0$ will be analytic unless the differential equation has the property that $A_1 = 0$ along $x = x_0$. If $A_1 = 0$, then we cannot evaluate the second x-derivative of ϕ from (5.4). For example, a solution to $\phi_{yy} + 2\phi_{xy} = f(x, y)$ will not be analytic about $x = x_0$

Before we ponder the implications of *non-analyticity*, let us consider a more general situation. Consider an arbitrary initial-data line whose slope is given by $dy/dx = \lambda(x, y)$. We can consider a solution to be the line in space given by $y = y_\lambda(x)$. Suppose we are given the values of ϕ and the normal derivative $\partial\phi/\partial n$ on λ. It is then straight forward to develop relationships for the first derivatives $\partial\phi/\partial x$ and $\partial\phi/\partial y$ on λ. Equivalently, we can assume that the first derivatives are prescribed directly as a function of x on λ as

$$\begin{aligned} \frac{\partial\phi[x, y_\lambda(x)]}{\partial x} &= f_1(x)\,, \\ \frac{\partial\phi[x, y_\lambda(x)]}{\partial y} &= f_2(x)\,. \end{aligned} \tag{5.6}$$

We can determine higher derivatives of ϕ by differentiating these expressions with respect to x. For example, from the first of (5.6)

$$\frac{d}{dx}\frac{\partial\phi[x, y_\lambda(x)]}{\partial x} = \frac{\partial^2\phi[x, y_\lambda(x)]}{\partial x^2} + \frac{\partial^2\phi[x, y_\lambda(x)]}{\partial x\partial y}\frac{dy_\lambda}{dx} = \frac{df_1}{dx}\,,$$

or, since $dy_\lambda/dx = \lambda$,

$$\frac{\partial^2\phi(x, y_\lambda)}{\partial x^2} + \lambda\frac{\partial^2\phi(x, y_\lambda)}{\partial x\partial y} = \frac{df_1}{dx}\,. \tag{5.7}$$

Similarly, from the second of (5.6)

$$\frac{\partial^2\phi(x, y_\lambda)}{\partial x\partial y} + \lambda\frac{\partial^2\phi(x, y_\lambda)}{\partial y^2} = \frac{df_2}{dx}\,. \tag{5.8}$$

Thus we have two equations for the three unknown second derivatives $\partial^2\phi/\partial x^2$, $\partial^2\phi/\partial x\partial y$ and $\partial^2\phi/\partial y^2$ at (x, y_λ). The third equation can be the original partial differential equation (4.1) evaluated at (x, y_λ) such that

$$A_1\frac{\partial^2\phi(x, y_\lambda)}{\partial x^2} + A_2\frac{\partial^2\phi(x, y_\lambda)}{\partial x\partial y} + A_3\frac{\partial^2\phi(x, y_\lambda)}{\partial y^2} = -A_4\,, \tag{5.9}$$

where the coefficients A_i, $i = 1, \ldots, 4$ are evaluated at the initial-data line (x, y_λ). Equations (5.7), (5.8) and (5.9) form a linear system for the second derivatives. Thus we can see that we will not be able to determine these second derivatives under conditions when the determinant of the coefficients of the linear system is zero. Thus the solution will be indeterminate when

$$\begin{vmatrix} 1 & \lambda & 0 \\ 0 & 1 & \lambda \\ A_1 & A_2 & A_3 \end{vmatrix} = 0\,. \tag{5.10}$$

Expanding (5.10) gives the following quadratic equation for λ:

$$A_1\lambda^2 - A_2\lambda + A_3 = 0\,, \tag{5.11}$$

which has two solutions, λ_1 and λ_2 given by

$$\lambda_{1,2} = \frac{A_2 \pm \sqrt{A_2^2 - 4A_1A_3}}{2A_1}\,, \tag{5.12}$$

where λ_1 corresponds to the plus sign and λ_2 corresponds to the minus sign.

Thus, if we are given initial data along either line $dy/dx = \lambda_1$ or $dy/dx = \lambda_2$, then we cannot determine the higher derivatives from the initial data and governing equation and we cannot solve the problem by analytic continuation. Under these circumstances the lines are called *characteristic lines* of the partial differential equation.

From the solution (5.12), the slopes of these lines depend on the specific partial differential equation that we wish to solve. For example, if we were solving $\phi_{xx} - \phi_{yy} = 0$, then $A_1 = 1$, $A_2 = 0$ and $A_3 = -1$. The characteristic directions would then be lines where $dy/dx = \pm 1$. On the other hand, if we were solving LaPlace's equation, $\phi_{xx} + \phi_{yy} = 0$, so that $A_1 = 1$, $A_2 = 0$ and $A_3 = 1$. The characteristic directions would then be complex, with $dy/dx = \pm i$. So that for solving Laplace's equation, no (real) characteristic lines exist.

This property of whether or not characteristic lines exist is used as a basis to classify quasi-linear, second-order partial differential equations in two independent variables. The equation is said to be *hyperbolic* when $A_2^2 - 4A_1A_3 > 0$ so that 2 (real) characteristics exist. On the other hand, the equation is said to be *elliptic* when $A_2^2 - 4A_1A_3 < 0$ so that no (real) characteristics exist. The case where $A_2^2 - 4A_1A_3 = 0$, leads to one (real) characteristic and the equation is said to be *parabolic*.

Now let's go back and examine the implications of having the initial data specified on a characteristic line $dy/dx = \lambda$. We see that when λ is given by (5.12), the solution to the linear system for the second derivatives, (5.7)–(5.9) will be indeterminate and the determinant (5.10) will be zero. If we try solve for say $\partial^2\phi/\partial x^2$ by say Cramer's rule, we obtain

$$\frac{\partial^2\phi(x, y_\lambda)}{\partial x^2} = \frac{\begin{vmatrix} df_1/dx & \lambda & 0 \\ df_2/dx & 1 & \lambda \\ -A_4 & A_2 & A_3 \end{vmatrix}}{\begin{vmatrix} 1 & \lambda & 0 \\ 0 & 1 & \lambda \\ A_1 & A_2 & A_3 \end{vmatrix}}\,. \tag{5.13}$$

Since the denominator is zero, the solution will be infinite unless the numerator is simultaneously zero. If we have a physical problem where we do not expect to find infinite values of the flow derivatives, then we would expect that

$$\begin{vmatrix} df_1/dx & \lambda & 0 \\ df_2/dx & 1 & \lambda \\ -A_4 & A_2 & A_3 \end{vmatrix} = 0\,, \tag{5.14}$$

along a characteristic. Expanding the determinant leads to

$$(A_3 - \lambda A_2)\frac{df_1}{dx} - \lambda A_3 \frac{df_2}{dx} - \lambda^2 A_4 = 0\,,$$

which, after rearranging and using (5.12) leads to

$$\frac{df_1}{dx} + \lambda_{2,1}\frac{df_2}{dx} + \frac{A_4}{A_1} = 0\,, \tag{5.15}$$

where $\lambda_{2,1}$ is given by (5.12) with the ± signs reversed. Thus, along an initial data line which is a characteristic line, the initial data cannot be prescribed arbitrarily, but must satisfy the relationship (5.15) if the solution and its derivatives are to remain finite. (Note that we have determined this relationship from the requirement that $\partial^2\phi/\partial x^2$ remain finite. Equivalent expressions would have been obtained by requiring the other second derivatives to be finite.)

Since along the initial-data line $\partial\phi/\partial x = f_1(x)$ and $\partial\phi/\partial y = f_2(y)$ we can write (5.15) as

$$\frac{d}{dx}\frac{\partial\phi}{\partial x} + \lambda_{2,1}\frac{d}{dx}\frac{\partial\phi}{\partial y} + \frac{A_4}{A_1} = 0\,, \tag{5.16}$$

This expression, valid along a characteristic line is often called the *characteristic compatibility relation*. We see that the governing partial differential equation reduces to an ordinary differential equation along a characteristic line. (Actually, the number of independent variables reduces by one along a characteristic). In the present situation, with two independent variables, the equation will reduce to an ordinary differential equation along a characteristic. Under certain circumstances the compatibility relation can be integrated to provide an algebraic equation valid on characteristics. This will provide a general solution to the governing equations. Of course this procedure, called the *method of characteristics* can only be used when (real) characteristics exist, so that the governing equation must be hyperbolic or parabolic. The method works best for second-order equations in two independent variables (or equivalently a system of two first-order equations in two independent variables). For higher-order systems with more than two-independent variables the method becomes quite complicated and is rarely used. You may wish to consult a book on partial differential equations such as Garabedian (1964) for example.

5.2 Governing Equations for Steady, Isentropic Flow

Let us consider inviscid flows where the stagnation enthalpy is constant. From the energy equation, as discussed in §2.8, the flow must be steady and adiabatic with negligible body forces and uniform h_0 upstream. Under this circumstance, the Crocco relationship (2.40) states that an isentropic flow will be irrotational. Irrotationality provides a tremendous simplification to the governing equations, since if $\nabla \times \boldsymbol{V} = 0$ then a velocity potential $\boldsymbol{V} = \nabla\phi$ will exist, since the identity $\nabla \times \nabla\phi = 0$ must always be satisfied. Thus for irrotational flows, we can solve for a single potential function instead of three velocity components.

If we restrict ourselves to flows where h_0 is constant and entropy is constant, then the governing equations will include the continuity equation:

$$\boldsymbol{V} \cdot \nabla\rho + \rho\nabla \cdot \boldsymbol{V} = 0\,, \tag{5.17}$$

the irrotationality condition:

$$\nabla \times \boldsymbol{V} = 0\,, \tag{5.18}$$

the energy equation for constant h_0:

$$h_0 = h + \frac{\boldsymbol{V} \cdot \boldsymbol{V}}{2}\,, \tag{5.19}$$

and an equation of state which may be written as

$$\rho = \rho(h, s)\,. \tag{5.20}$$

This form of the equation of state will be valid for frozen or equilibrium flow. Note that in the above system, the irrotationality condition replaces the momentum equation. We also specify that the flow is isentropic, so that the entropy is known.

Since $\rho = \rho(h, s)$ and s is constant, $d\rho = (\partial\rho/\partial h)_s dh$ and from (1.55), $a^2 = (\partial p/\partial\rho)_s = \rho/(\partial\rho/\partial h)_s$, then $\nabla\rho = (\rho/a^2)\nabla h$. From (5.19) $\nabla h = -\nabla(\boldsymbol{V} \cdot \boldsymbol{V}/2)$ and substituting into (5.17) we obtain

$$a^2\nabla \cdot \boldsymbol{V} - \boldsymbol{V} \cdot \nabla\left(\frac{\boldsymbol{V} \cdot \boldsymbol{V}}{2}\right) = 0\,, \tag{5.21}$$

for a steady isentropic flow with uniform h_0. In two-dimensional Cartesian coordinates, the equation may be written as

$$(a^2 - u^2)\frac{\partial u}{\partial x} - uv\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) + (a^2 - v^2)\frac{\partial v}{\partial y} = 0\,. \tag{5.22}$$

Since the flow is irrotational, $\boldsymbol{V} = \nabla\phi$ with $u = \partial\phi/\partial x$ and $v = \partial\phi/\partial y$ so that

$$(a^2 - u^2)\frac{\partial^2\phi}{\partial x^2} - 2uv\frac{\partial^2\phi}{\partial x\partial y} + (a^2 - v^2)\frac{\partial^2\phi}{\partial y^2} = 0\,. \tag{5.23}$$

The system is closed with an equation of state of the form $a = a(h, s)$ where $h = h_0 - (u^2 + v^2)/2$. For a perfect gas, $h = a^2/(\gamma - 1)$ so that from (5.19) after evaluating h_0 in the free stream, we obtain

$$\frac{a^2}{\gamma - 1} + \frac{u^2 + v^2}{2} = \frac{a_\infty^2}{\gamma - 1} + \frac{U_\infty^2}{2}\,. \tag{5.24}$$

5.3 Characteristic Relations for Steady, Isentropic Flow

We now consider the development of the characteristic relations for a two-dimensional inviscid flow with constant stagnation enthalpy and constant entropy. We have seen that constant h_0 requires the flow to be steady, and adiabatic with negligible body forces and uniform h_0 upstream. Constant entropy under these conditions occurs when there are no shocks and the entropy is uniform upstream. We have seen in §4.2 that the flow will be irrotational and that the governing equation for the velocity potential is given by (4.23).

The governing equation for the velocity potential is in the form of a quasi-linear, second-order partial differential equation in two independent variables, (4.1), with the coefficients given as

$$\begin{aligned} A_1 &= a^2 - u^2\,, \\ A_2 &= -2uv\,, \\ A_3 &= a^2 - v^2\,, \\ A_4 &= 0\,. \end{aligned} \tag{5.25}$$

The characteristic directions, given in general by (4.12), may be written for this case as

$$\lambda_{1,2} = \frac{-2uv \pm 2a\sqrt{u^2 + v^2 - a^2}}{2(a^2 - u^2)}\,. \tag{5.26}$$

Thus we see that two real characteristics will exist when $u^2 + v^2 > a^2$ or the equation is hyperbolic when the flow is supersonic. When the flow is subsonic, the equation is elliptic and real characteristic lines will not exist. Thus, in order to apply the method of characteristics to this steady isentropic flow, the flow must be supersonic.

We can simplify the equation for the characteristic directions by introducing streamline variables, the velocity magnitude V and local flow angle θ such that

$$\begin{aligned} V^2 &= u^2 + v^2\,, \\ \tan\theta &= v/u\,, \end{aligned} \tag{5.27}$$

which is equivalent to $u = V\cos\theta$ and $v = V\sin\theta$. Then, introducing the Mach number $M = V/a$, (5.26) becomes

$$\lambda_{1,2} = \frac{-M^2 \sin\theta\cos\theta \pm \sqrt{M^2 - 1}}{1 - M^2\cos^2\theta}\,. \tag{5.28}$$

Next, introducing the definition of the *Mach angle* μ as

$$\sin \mu \equiv \frac{1}{M}\,, \tag{5.29}$$

after some trigonometric manipulations, the characteristic directions are seen to be

$$\lambda_{1,2} = \tan(\theta \pm \mu)\,. \tag{5.30}$$

The characteristic directions are the Mach lines measured with respect to the local flow angle. This result is for a real gas as well as a perfect gas.

The characteristic compatibility relations are given in general by (4.16) in general and for the present case, reduce to

$$\frac{du}{dx} + \tan(\theta \mp \mu)\frac{dv}{dx} = 0\,, \tag{5.31}$$

along the characteristics $dy/dx = \tan(\theta \pm \mu)$. This relationship is simplified by introducing (V, θ) from (5.27) and utilizing the Mach angle definition to obtain

$$\frac{1}{V}\frac{dV}{d\theta} = \pm \tan \mu\,, \tag{5.32}$$

which with (5.29) reduces to the characteristic relationship

$$\pm d\theta = \sqrt{M^2 - 1}\frac{dV}{V}\,, \tag{5.33}$$

on the characteristics $dy/dx = \tan(\theta \pm \mu)$. We will show in the next subsection that for a perfect gas, (5.33) may be integrated and algebraic compatibility relationship will follow. For a real gas we will indicate a numerical procedure to solve (5.33).

Supersonic flow of a perfect gas

For a perfect gas we can express dV/V in terms of dM/M so that (5.33) may be integrated. From the definition of Mach number, $dM/M = dV/V - da/a$. From the relationship for h_0 of a perfect gas given in (4.24) we have $da/a = -(\gamma - 1)(M^2/2)dV/V$ so that

$$\frac{dV}{V} = \frac{1}{1 + \frac{\gamma-1}{2}M^2}\frac{dM}{M}\,. \tag{5.34}$$

Substituting (5.34) into (5.33) gives the characteristic relationship

$$\pm d\theta = \frac{\sqrt{M^2 - 1}}{1 + \frac{\gamma-1}{2}M^2}\frac{dM}{M}\,. \tag{5.35}$$

The right-hand side is seen to be $d\nu$ where ν is the Prandtl-Meyer function defined by

$$\nu \equiv \sqrt{\frac{\gamma+1}{\gamma-1}}\tan^{-1}\sqrt{\frac{\gamma-1}{\gamma+1}(M^2-1)} - \tan^{-1}\sqrt{M^2-1}\,. \tag{5.36}$$

Thus the characteristic compatibility relationship becomes

$$\theta \mp \nu = constant\,, \tag{5.37}$$

along $dy/dx = \tan(\theta \pm \mu)$. The two relationships given in (5.37) may be used to determine a characteristic net to find θ and ν everywhere in the flow field. From ν as defined by (5.36) it is possible to determine the Mach number M. Then knowing M we can determine p and T from (2.35) and (2.30) since p_0 and T_0 will be constant for this flow.

As a simple illustration, consider a wall where the flow inclination angle abruptly changes from $\theta_1 = 0$ to $\theta_2 = -\Delta\theta$ as shown in the sketch below in Fig. 1. A centered expansion will occur. The solution for the flow in region 2 is determined from a characteristic relation written along $dy/dx = \tan(\theta - \mu)$ where $\theta_1 + \nu_1 = \theta_2 + \nu_2$ so that with θ_2 given as $-\Delta\theta$ we have $\nu_2 = \nu_1 + \Delta\theta$. Then M_2 can be found along with p_2 and T_2.

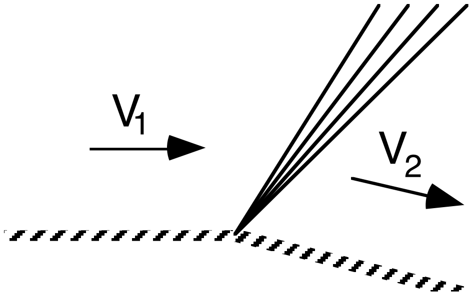

Figure 1. Centered expansion.

Supersonic flow of a real gas

For a real gas the characteristic relationships given in (4.33) must be integrated numerically. In addition to the characteristic relationships, we will have that the stagnation enthalpy $h_0 = h + V^2/2$ and the entropy s will be constant and for equilibrium chemistry, equations of state of the form $a = a(h,s)$, $p = p(h,s)$, $\rho = \rho(h,s)$, $T = T(h,s)$ will be available.

As an example of a procedure which may be used, consider the Prandtl-Meyer expansion sketched in Fig. 1. Across the expansion fan, along a characteristic $dy/dx = \tan(\theta - \mu)$, the following relationship must be satisfied:

$$d\theta = \sqrt{M^2-1}\frac{dV}{V}\,, \tag{5.38}$$

An iterative procedure to satisfy this relationship now follows:

Step 1. Starting with V_1, p_1 and ρ_1, calculate $h_1 = h(p_1, \rho_1)$ and $s_1 = s(p_1, \rho_1)$ from a curve fit or equilibrium composition.

Step 2. Guess a value of V_2.

Step 3. Then $h_2 = h_1 + (V_1^2 - V_2^2)/2$ and $s_2 = s_1$.

Step 4. Numerically integrate (5.38) using for example a trapezoidal rule so that

$$\theta_2 - \theta_1 = \frac{1}{2}\left[I(V_1) + 2\sum_{i=1}^{N} I(V_i) + I(V_2)\right] ,$$

where

$$\begin{aligned}
\Delta V &= \frac{V_2 - V_1}{N+1} , \\
V_i &= V_1 + i\Delta V , \\
h_i &= h_1 + \frac{V_1^2}{2} - \frac{V_i^2}{2} , \\
s_i &= s_1 , \\
a_i &= a(h_i, s_i) , \\
I(V_i) &= \frac{1}{V_i}\sqrt{\frac{V_i^2}{a_i^2} - 1} .
\end{aligned}$$

Step 5. Does $\theta_2 - \theta_1$ equal the prescribed $\Delta\theta$? If not, use a root-finding procedure such as a bracketing method or a secant method to modify the value of V_2 and continue from Step 3.