3. Hypersonic Aerothermodynamics

To understand these effects and how they affect hypersonic vehicle design and performance, we must consider:

- thermodynamics
- fluid dynamics
- aerodynamics

as applied under hypersonic conditions

Here, we review basic ideas from thermodynamics and fluid dynamics most needed to analyze hypersonic flows. Our ultimate goal is to determine the aerodynamic forces/moments and surface heating on the vehicle

3.1.1 Thermodynamics

State variables: Thermodynamic state of a medium is described by its state variables. For gas:

$$X = X(Y, Z) \tag{3.1}$$

where X, Y, Z are state variables

We often work with x = specific (per unit mass) form of X

Common state variables:

- $\rho = 1/v$ = mass density (v = specific volume)
- p = pressure
- T = temperature
- e = specific internal energy
- $h = \text{specific enthalpy} = e + p/\rho$
- $a = \text{speed of sound} = \left[\left(\frac{\partial p}{\partial \rho} \right)_s \right]^{1/2}$
- $c_v = \text{specific heat at constant volume} = \left(\frac{\partial e}{\partial T}\right)_v$
- c_p = specific heat at constant pressure = $\left(\frac{\partial h}{\partial T}\right)_p$

Relations between state variables of the form X = X(Y, Z) are called equations of state

Volumetrically perfect gas (ideal gas)

$$p = \rho RT = nkT$$
 (3

where

- $ightharpoonup R = \operatorname{ordinary} \operatorname{gas} \operatorname{constant} = \check{R}/W \operatorname{in} J/\operatorname{kg-K}$
- \check{R} = universal gas constant = 8314 J/kg-mol-K
- W = molecular weight in g/mol
- n = number density (another state variable)
- k = Boltzmann's constant = 1.38E-23 J/K

Thermally perfect gas (no chemistry)

$$e = e(T) \rightarrow de = c_v(T)dt$$
 $h = h(T) \rightarrow de = c_p(T)dt$

$$(3.3)$$

Calorically perfect gas

- constant c_v and c_p
- a subset of thermally perfect

$$e = c_v T$$

$$e = c_v T$$
$$h = c_p T$$

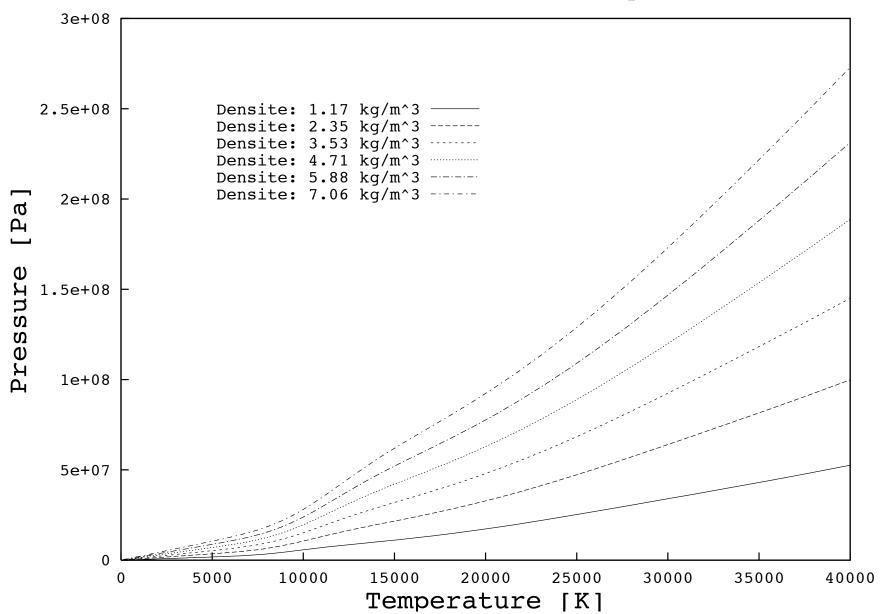
(3.4)

Temperature variation in air of c_v and c_p begins at about M=3 and air chemistry at about M=6. These real gas effects are important in hypersonic flows.

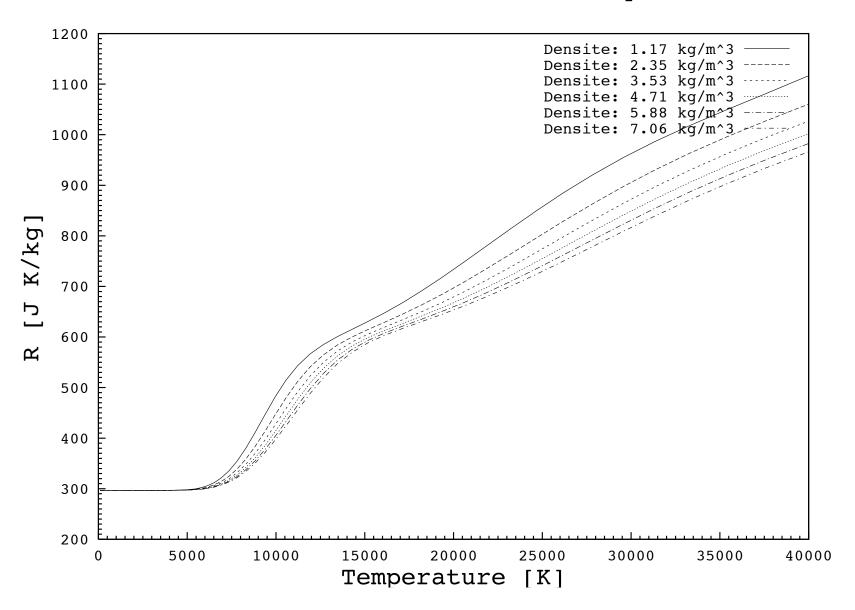
Introducing the ratio of specific heats γ :

- $\gamma = constant$ for calorically perfect
- $\gamma = \gamma(T)$ for thermally perfect
- $\gamma = \gamma(T, p)$ for real gas

Note:
$$c_p = \frac{\gamma R}{\gamma - 1}$$
 $c_v = \frac{R}{\gamma - 1}$ $c_p = c_v + R$



Pressure as a function of temperature and density for Nitrogen



R as a function of temperature and density for Nitrogen

Entropy

State variable that measures irreversible processes that represent loss mechanisms in gas dynamics. Combined forms of Ist and 2nd Laws of Thermodynamics gives:

$$Tds = de + pdv = dh - vdp (3.6)$$

For a calorically perfect gas, the change in entropy between two points is:

$$\Delta s_{21} = s_2 - s_1 = c_p \ln \left(\frac{T_2}{T_1}\right) - R \ln \left(\frac{p_2}{p_1}\right)$$

$$= c_v \ln \left(\frac{T_2}{T_1}\right) - R \ln \left(\frac{\rho_2}{\rho_1}\right) \quad (3.7)$$

$$= c_v \ln \left(\frac{p_2}{p_1}\right) - c_p \ln \left(\frac{\rho_2}{\rho_1}\right)$$

An **isentropic flow** has no change in entropy: $\Delta s_{12} = 0$

Entropy increases are caused by

- viscosity, thermal conductivity (shock waves)
- heat addition (combustion = Rayleigh flow)
- surface friction (boundary layers = Fanno flow)

For isentropic conditions, Eq. (3.7) become the isentropic relations:

$$\frac{p_2}{p_1} = \left(\frac{\rho_2}{\rho_1}\right)^{\gamma} = \left(\frac{T_2}{T_1}\right)^{\gamma/(\gamma-1)} \tag{3.8}$$

Speed of sound

$$a^{2} = \left(\frac{\partial p}{\partial \rho}\right)_{s \text{ (thermally)}\atop perfect} \frac{\gamma p}{\rho} = \gamma RT$$

(3.9)

Stagnation properties

Conservation of energy at a point in a flow

where subscript "0" is
$$h_0 = h + \frac{1}{2}u^2$$

- the stagnation value (or total value)
- ▶ the value obtained by bringing the flow isentropically to rest

For a calorically perfect gas

$$c_p T_0 = c_p T + \frac{1}{2} u^2$$

$$\frac{T_0}{T} = 1 + \frac{u^2}{2c_p T} = 1 + \frac{\gamma - 1}{2} \frac{u^2}{\gamma RT} = 1 + \frac{\gamma - 1}{2} M^2$$

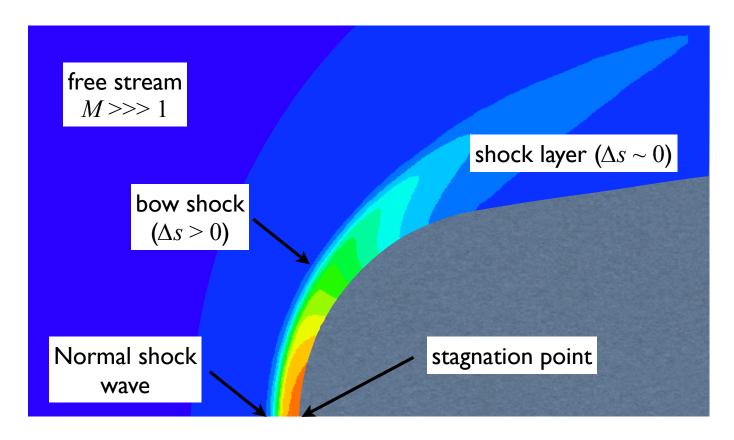
(3.10)

So, for a thermally perfect gas, the isentropic relations (Eq. 3.8) may be written as

$$\frac{T_0}{T} = \left(\frac{P_0}{P}\right)^{(\gamma-1)/\gamma} = \left(\frac{\rho_0}{\rho}\right)^{\gamma-1} = 1 + \frac{\gamma - 1}{2}M^2$$

(3.11)

In hypersonics flows M>>>1, and shock waves are formed whenever a body is placed in supersonic (M>1) flow. The following figure illustrates some of the gas dynamic phenomena for hypersonic flow over a blunted cone



To review gas dynamics, we consider flow along the stagnation streamline using continuum analysis. This approach is valid when the collision rates of the molecules in the gas are large enough to maintain thermodynamic equilibrium. The approach fails at low density (high altitude) and/or small length scales (sharp edges on the vehicle). Validity of continuum approach is assessed using the **Knudsen number**:

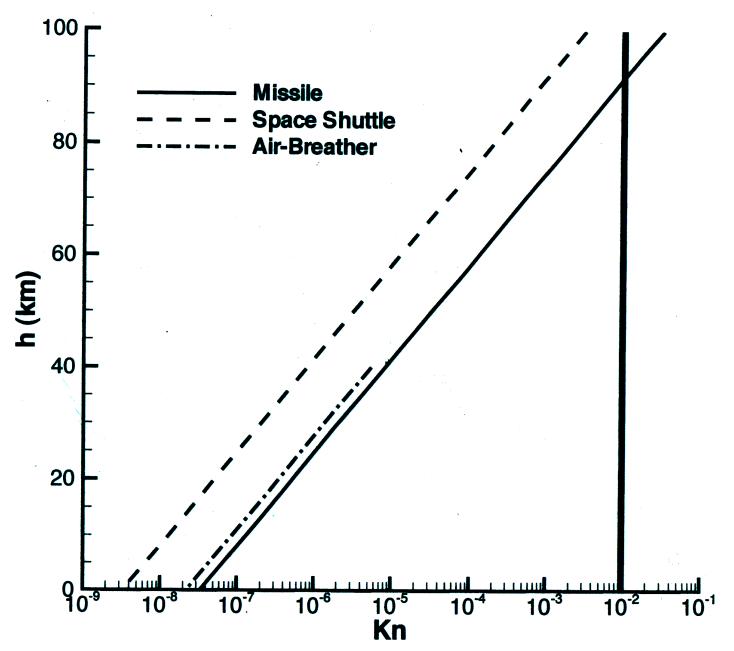
$$K_{\rm n} = rac{\lambda}{L}$$
 (3.12)

where

$$\lambda$$
 = the mean free = $\left(\sqrt{(2)n\sigma}\right)^{-1}$ (3.13)

- σ = collision cross section \approx 50 × 10⁻²⁰ m²
- ightharpoonup L = characteristic length scale

Generally, continuum analysis is valid for Kn < 0.01, which occurs for altitudes less that 85 km for L=1 m



Normal Shock waves

Hypersonic vehicles generate different types of shock waves

- normal (easiest to analyze)
- oblique
- bow

Flow along the stagnation streamline of a blunt body involves a normal shock (NS)

Application of conservation laws of mass, momentum, and energy to a control volume around a stationary NS yields:

Mass flux:
$$G = \rho_1 u_1 = \rho_2 u_2 = \text{const}$$

Impulse function: $F = p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2 = \text{const}$ (3.14)
Stagnation enthalpy: $h_0 = h_1 + \frac{1}{2}u_1^2 = h_2 + +\frac{1}{2}u_2^2 = \text{const}$

From these equations and earlier thermodynamics relations, we can derive the NS relations:

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

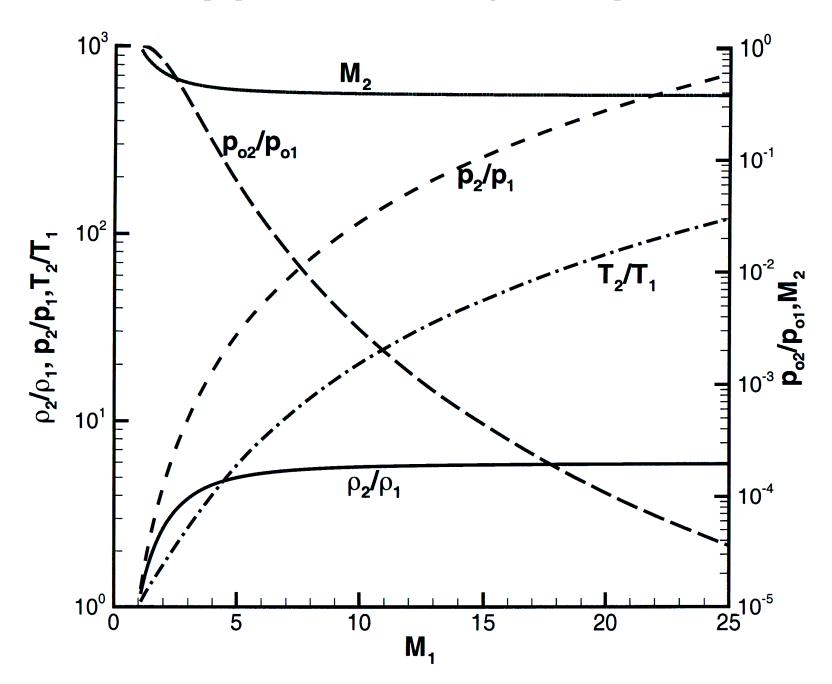
$$\frac{p_2}{p_1} = \frac{2\gamma M_1^2 - (\gamma-1)}{(\gamma+1)}$$

$$M_2^2 = \frac{2 + (\gamma-1)M_1^2}{2\gamma M_1^2 - (\gamma-1)}$$

$$T_{02} = T_{01}$$
(3.15)

From these, T_2/T_1 and p_{02}/p_{01} can be obtained

Also note that
$$\Delta s_{21} = s_2 - s_1 = -R \ln(p_{02}/p_{01})$$



Comments on the Fig. 3.1:

 $M_2 < 1$: Mach number decreases across a shock wave is always subsonic behind a NS

 $\rho_2/\rho_1 > 1 \rightarrow (\gamma+1)/(\gamma-1)$: Density increases across a shock wave approaching an asymptote at high M_I

 T_2/T_1 and p_2/p_1 continually increase across a shock as M_1 increases: hypersonic shock waves create large increases in temperature and pressure

 $p_{02}/p_{01} < 1 \Rightarrow \Delta s > 1$ Decrease in total pressure represents potential loss mechanism for air-breathing propulsion systems

While these comments are qualitatively correct, there are several complicating issues:

- High T_2 leads to real gas effects (changes in c_p , c_v , γ and chemistry)
- NS relations. Generally, we must consider shock waves generated by sharp objects. Bow shocks are even more complex.

3.2 Real Gas Effects

Previously, we saw that high temperatures and pressures are created behind shock waves formed around hypersonic vehicles

One of the important consequences is the generation of real gas effects:

- $ightharpoonup c_p$, c_v and γ vary with $T \Rightarrow$ not calorically perfect
- \blacktriangleright chemical composition varies with $T, p \Rightarrow$ not thermally perfect

Therefore, we will quantify these effects

Molecules and atoms have several forms of energy:

- \blacktriangleright kinetic= $\frac{1}{2}mu^2$
- potential, due to force field
- internal, of which there are several forms (modes)

a) Translational

For both atoms and molecules: arises from random motion

From statistical mechanics and kinetic theory:

> specific internal energy due to translational motion

$$e_{tr} = \frac{3}{2}RT\tag{3.16}$$

From thermodynamics:

$$(c_v)_{tr} = \left(\frac{\partial e_{tr}}{\partial T}\right)_v = \frac{3}{2}R$$
 for noble gas (Ar, He, Xe, etc.)
$$(c_p)_{tr} = (c_v)_{tr} + R = \frac{5}{2}R$$

$$\gamma \equiv c_p/c_v = 5/3$$
 (3.17)

b) Rotational

Exists for molecules only

Statistical mechanics shows

$$e_{rot} = \frac{\chi}{2}RT$$
 (3.18a)

where $\chi = 2$ for linear molecules (diatomic, CO₂)

= 3 for non-linear molecules (H₂O, NH₃, etc.)

Thus:

$$(c_v)_{rot} = \frac{\chi}{2}R$$
 (3.18b)

Internal energy is an additive property, so a gas with translational and rotational energies has:

$$e=rac{3+\chi}{2}RT$$
 $c_v=rac{3+\chi}{2}R$
$$c_p=rac{5+\chi}{2}R$$
 $\gamma=rac{5+\chi}{3+\chi}$ (3.19)

Therefore, for air at room temperature (mainly composed of N_2 and O_2):

$$e = \frac{5}{2}RT$$

$$c_v = \frac{5}{2}R$$

$$c_p = \frac{7}{2}R$$

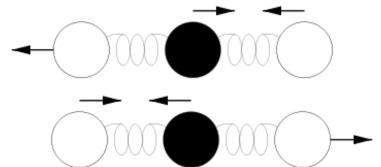
$$\gamma = \frac{7}{5} = 1.40$$

c) Vibrational

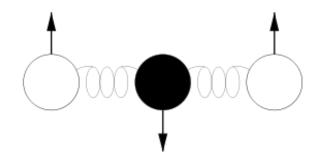
Exists for molecules only in two forms

oscillation





bending



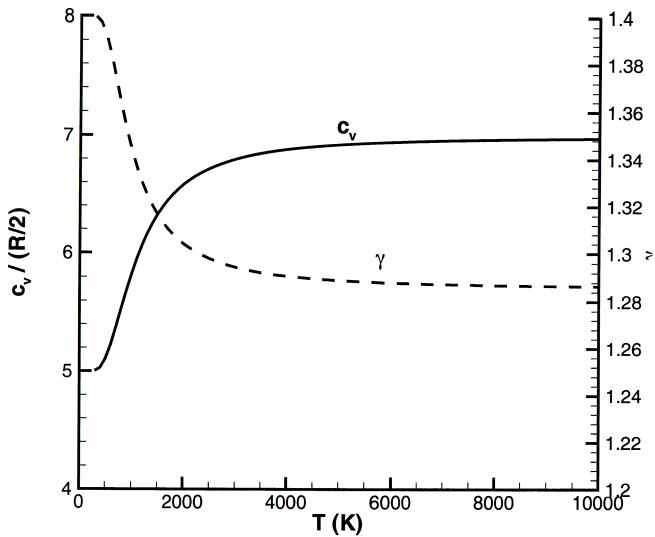
Each mode can be approximated as a harmonic oscillator for which:

$$e_{vib} = rac{R heta_v}{\exp(heta_v/T) - 1}$$
 (3.20a)

where θ_v is the characteristic temperature (or frequency) for the vibration of the chosen mode, and is different for each chemical species

Differentiation gives

$$(c_v)_{vib} = R \left(\frac{\theta_v}{T}\right)^2 \frac{\exp(\theta_v/T)}{\left[\exp(\theta_v/T) - 1\right]^2}$$
 (3.20b)



Variation of $c_v/(R/2)$ and γ as a function of T for N₂ (θ_v = 3390 K) (no chemistry)

Comments:

- At low temperature, $c_v = 5R/2$ and $\gamma = 7/5$, which means that there is rotation but no vibration
- As T increases, both c_v increases and γ decreases
- Both quantities approach asymptotically a value of $c_v = 7R/2$ and $\gamma = 9/7$, which means that the vibrational mode is fully activated

Example

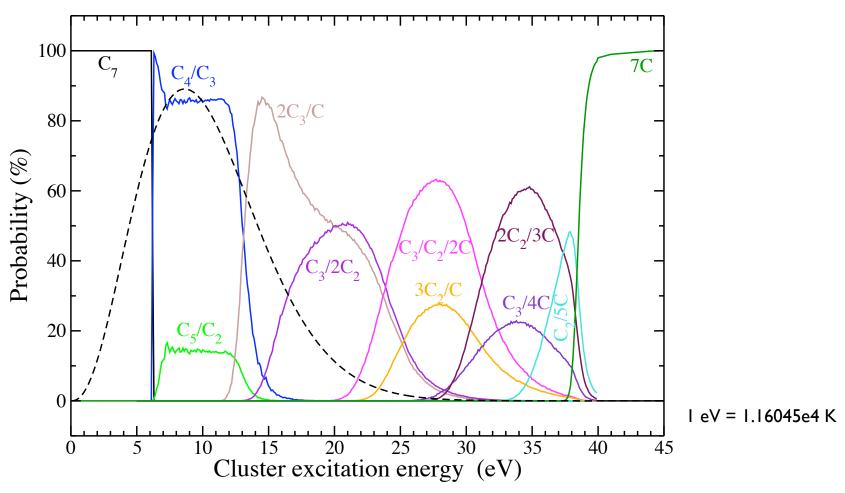
Carbon vibrational energy

The heat shield of re-entry capsules are usually made of ablative carbon-based material.

It has been shown that the carbon released into the flow field is formed of molecules C, C_2 , C_3 , C_5 and C_7

Once this material is released into the flow field, the high temperature breaks the long carbon molecules into smaller molecules

For instance, C₇ mainly dissociates into C₄ and C₃ clusters:



Source: S. Diaz-Tendero, G. Sanchez, P.-A. Hervieux, M. Alcami, and F. Martin. Ionization potentials, dissociation energies and statistical fragmentation of neutral and positively charged small carbon clusters. *Brazilian Journal of Physics*, 36:529 – 533, 06 2006.

Because of that, C₄ must also be considered, but not C₆

C5:
$$|C = C = C = C|$$
 D_{osh}

C6: $|C = R_1 = C = C = C|$
 D_{osh}
 $C_{6} : D_{osh}$
 $C_{6} : D_{osh}$
 $C_{6} : D_{osh}$
 $C_{6} : D_{osh}$

Source: J. M. L. Martin, J. P. Francois, and R. Gijbels. A critical comparison of MINDO/3, MNDO, AM1, and PM3 for a model problem: Carbon clusters C2 –C 10. An Ad Hoc reparametrization of MNDO well suited for the accurate prediction of their spectroscopic constants. Journal of Computational Chemistry, 12(1):52–70, 1991.

D∞h

```
4.3
        1648i,1286,1743
 6.0
        383(2),1301,2104
Jahn–Teller distortion to C_{2v} structure
 5.7
        1051,1218,1722
 8.5
        274,384,927,1057,1371,1933
 8.5
        200(2),447(2),966,1541,2171
 8.3
        296,383,852,1157,1536,1551
12.8
        151(2),370(2),689(2),813,1528,2015,2199
15.1
        105(2),248(2),453(2),540(2),677,1240,1694,1999,2245
        284i,278,361,362,419(2),1310,1356,1510(2),1850(2)
16.0
        272(2),317,364,365,687,1015(2),1189,1229,1527(2)
14.0
        80(2),212(2),357(2),594,602(2),670(2),1135,1631,1939,2193,2202
19.3
        217,221,232,263,351,356(2),387,424(2),963,1187(2),1450,1984,2113(2),2259
23.6
        62,64,161,162,276,277,429(2),518,533(2),557(2),984,1410,1715,2005,2128,2233
21.5
        49(2),132(2),248(2),350(2),467,543(2),628(2),657(2),905,1312,1676,1938,2042,2196,2266
25.7
30.6
         190,193,230(2),397,398,403,428(2),443(2),471,484(2),787,1064(2),1499(2),1819,2030(2),2185(2)
```

Note: The number in parenthesis represents the degeneracy of the mode

d) Electronic

The most stable configuration of electrons orbiting an atom or molecule is called the ground electronic state. At very high temperature, both atoms or molecules can be moved into other electron configurations representing an additional source of internal energy. Such effects can usually be ignored in hypersonic flows (sub-orbital speed).

Remark

Since e, c_v and c_p are all specific quantities (per unit mass), overall values in a gas mixture require summation over all species weighted by their mass fraction.

3.2.2 Chemistry

a) Dissociation

As air temperature is increased, the vibrational energy mode becomes activated. However, well before full activation occurs, the molecules begin to react chemically, primarily through dissociation

$$A_2 \stackrel{diss.}{\rightleftharpoons} A + A$$
 (3.21)

From statistical mechanics, at equilibrium, the atomic mass fraction $\alpha \equiv \frac{m_A n_A}{m_A n_A + m_{A_2} n_{A_2}}$ follows the law of mass action

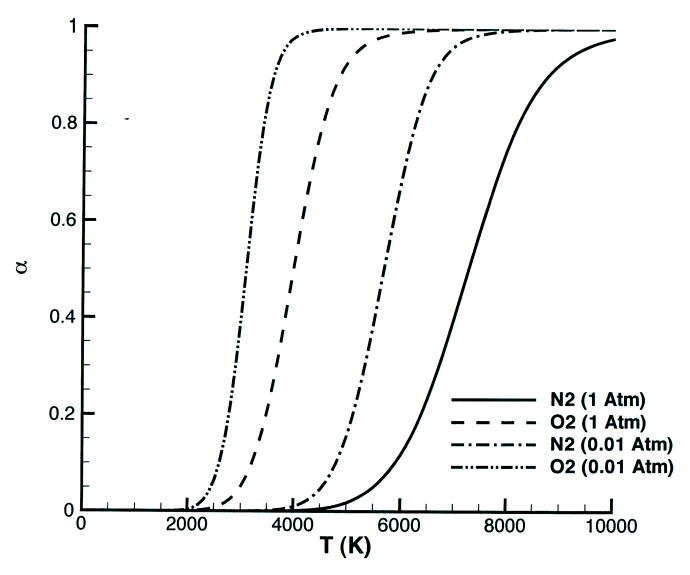
$$\frac{\alpha^2}{1-\alpha} = \frac{\rho_d}{\rho} \exp\left(\frac{-\theta_d}{T}\right) \tag{3.22}$$

where θ_d is the characteristic temperature of dissociation and ρ_d is a function of temperature, although almost constant

For air

	$ heta_d$	$ ho_d$	
N ₂	113 000 K	130 000 kg/m ³	
O ₂	59 500 K	150 000 kg/m ³	

Thus, chemical composition depends on two state variables, e.g. $\alpha = \alpha(T, P)$, and is itself a state variable.



Behavior of N_2 and O_2 at two different densities, function of temperature

Comments:

- $lackbox{O}_2$ dissociates at lower T than N_2 due to smaller θ_d (weaker chemical bond)
- Dissociation of both O_2 and N_2 is reduced at higher ρ (or p) due to increased recombination

The chemical composition of air at these temperatures involve 5 species (N_2 , O_2 , NO, N and O)

The chemical composition of Mars' atmosphere involve 8 species $(N_2, O_2, NO, N, O, CO_2, CO \text{ and } C)$

Carbon ablation in air, without the long carbon chains, (C_4 , C_5 and C_7) involves 11 species

b) Ionization

At very high temperature, air molecules are all converted into atoms which may then become ionized

$$A \rightleftharpoons A^+ + e^-$$

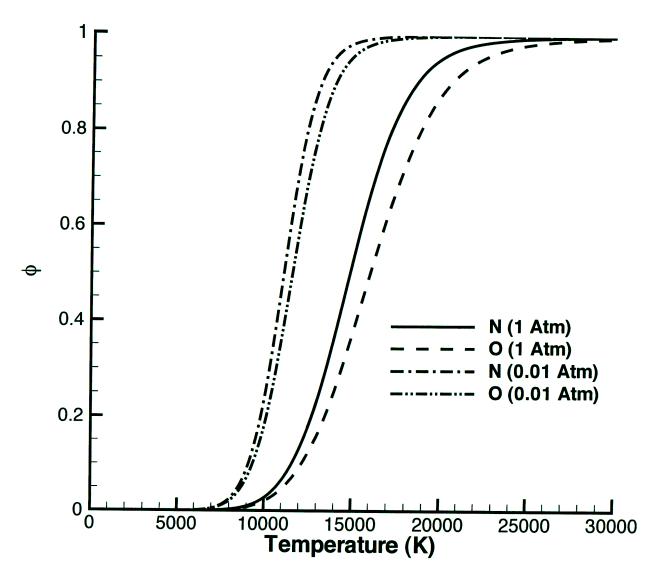
At equilibrium, the ionization fraction $\phi \equiv n_{A^+}/n_{A^0}$ (where n_{A^0} is the number of initial number density of atoms) is given by the Saha equation:

$$\frac{\phi^2}{1 - \phi^2} = 0.066C \frac{T^{5/2}}{p} \exp\left(\frac{-\theta_i}{T}\right) \quad \text{(3.23)}$$

where θ_i is the characteristic temperature of ionization and C is the ion-to-atom ratio of partition functions

For air

	$ heta_i$	C	
N	168 000 K	9/4	
0	158 000 K	4/9	



Behavior of N and O at two different pressure, function of temperature

Comments:

- No significant ionization below 10 000K
- N ionizes a little more easily that O
- Increased pressure reduces ionization

Carbon ablation in air, with ionization but without long carbon chains, (C_4 , C_5 and C_7) involves 20 species

Determination of the chemical composition of air at high temperature is complex and may involve I I species (N_2 , O_2 , N_2 , N_3 , N_4 , N_5 , N_5 , N_5 , N_6 , N_7 , N_8

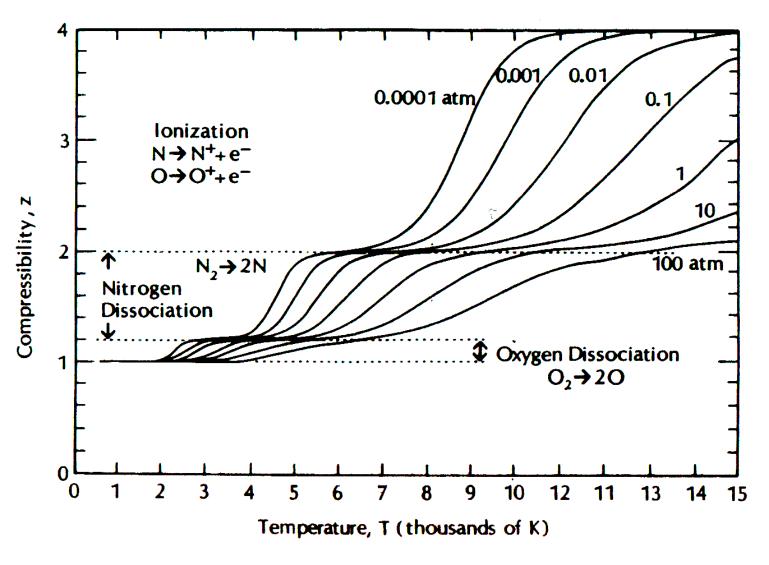
The change in molecular weight due to air chemistry is described by a compressibility factor

$$z \equiv rac{W_0}{W(T)}$$
 (3.24)

where W_0 is the value STP, \approx 28.8 kg/kg-mol

Changes in z are introduced into the equation of state of a volumetrically perfect gas:

$$p = \rho \frac{\hat{R}}{W}T = \rho \frac{\hat{R}}{W_0} \frac{W_0}{W}T = \rho RzT \qquad \boxed{\textbf{(3.25)}}$$



Comments:

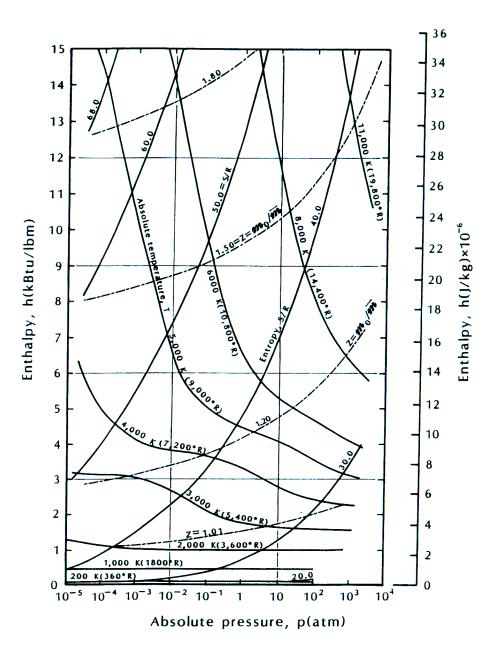
The variation of z with T is shown, indicating

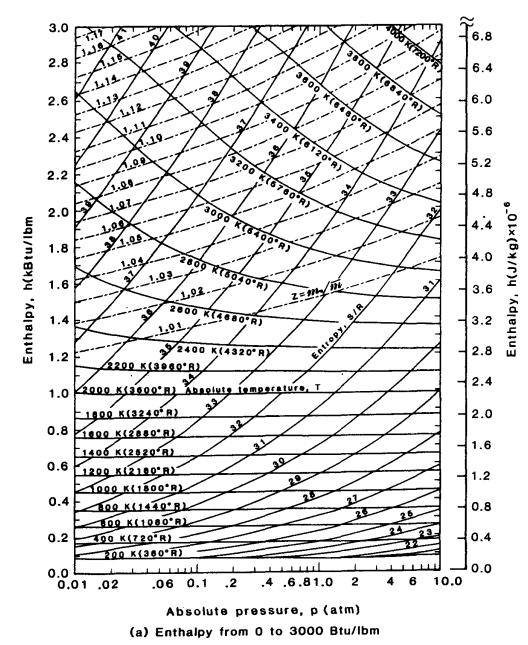
- ightharpoonup z ightharpoonup 1.2 as a result of O_2 dissociation
- ightharpoonup z
 ightharpoonup 2.0 as a result of O_2 and N_2 dissociation
- ightharpoonup z ightharpoonup 4.0 as a result of complete single ionization

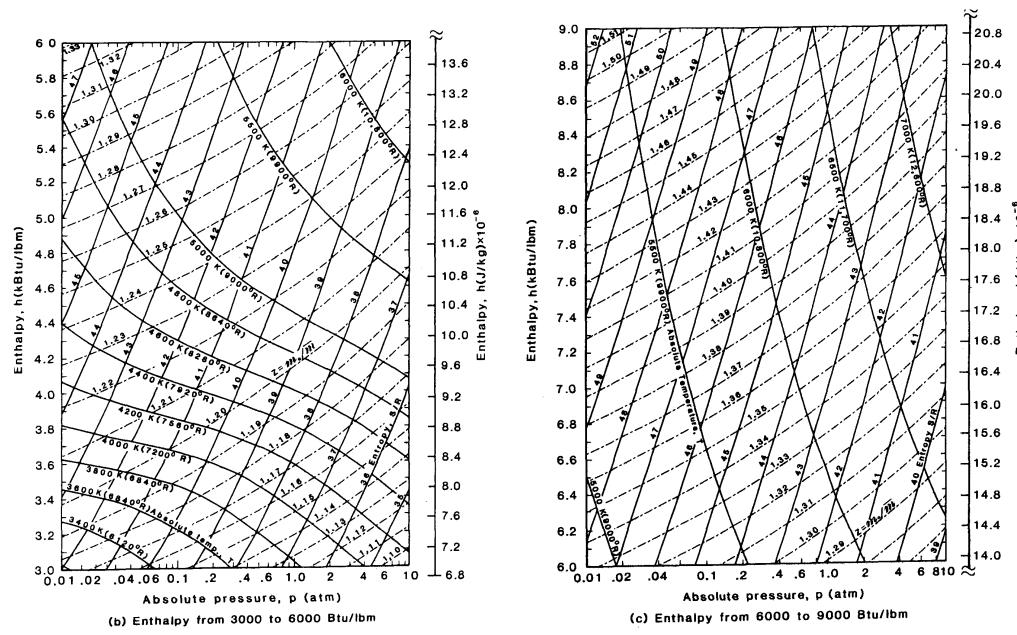
Evaluation of other thermodynamic properties of reacting air can be conveniently performed using the following figures. These are graphical representations of equations of state for air, including real gas effects:

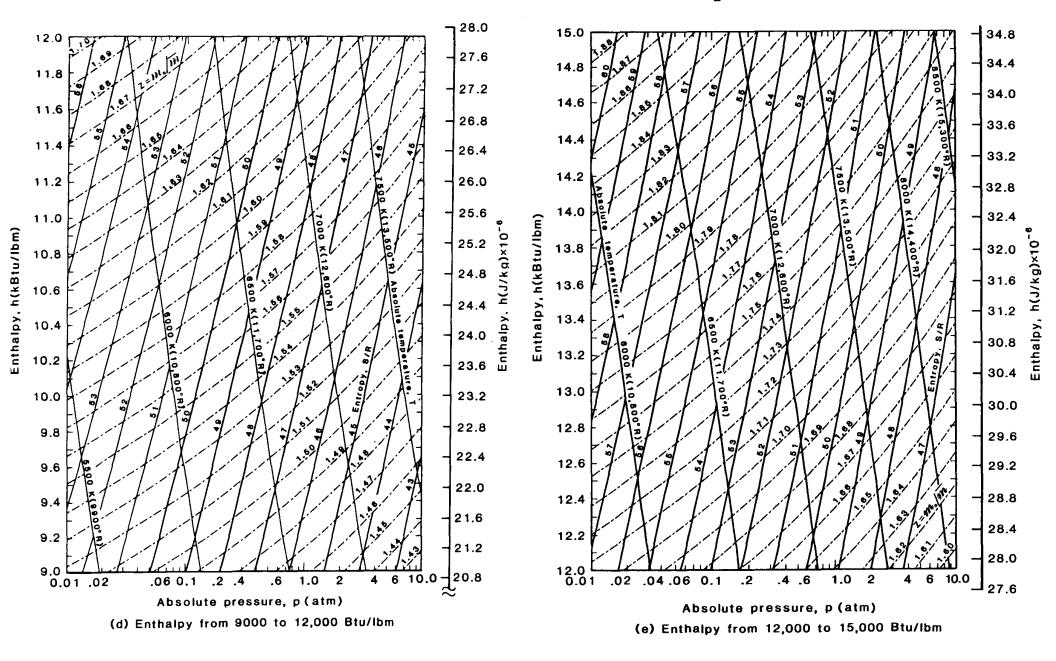
$$z(p,h)$$
, $s(p,h)$, $T(p,h)$

that must be used to accurately predict the high-T, high-P conditions behind hypersonic shock waves









Example 3.1

Determine the flow properties behind a normal shock wave formed by the blunt nose of the Space Shuttle flying at 70 km, at 7 km/s.

Example 3.1

Table 1.1a (continued)

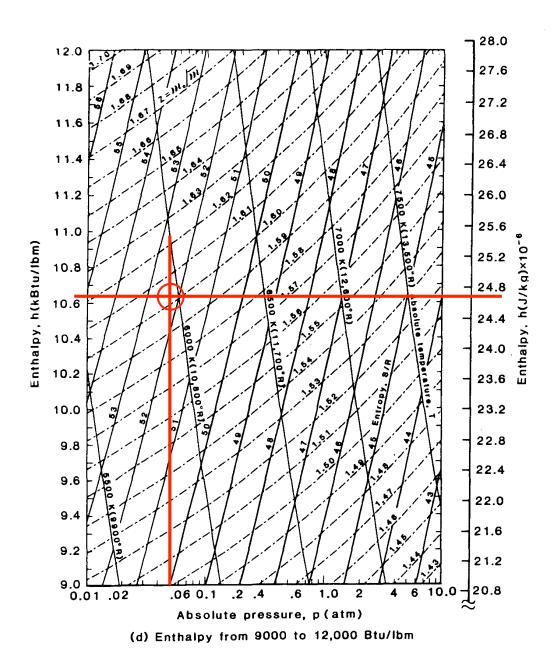
Geometric Altitude (km)	Pressure (p/p_{SL})	Temperature (K)	Density (ρ/ρ_{SL})	Viscosity (μ/μ_{SL})	Speed of Sound (m/s)
41	2.4784 E-03	253.114	2.8216 E-03	0.90262	318.94
42	2.1709 E-03	255.878	2.4447 E-03	0.91052	320.67
43	1.9042 E-03	258.641	2.1216 E-03	0.91838	322.40
44	1.6728 E-03	261.403	1.8440 E-03	0.92620	324.12
45	1.4715 E-03	264.164	1.6051 E-03	0.93398	325.82
46	1.2962 E-03	266.925	1.3993 E-03	0.94172	327.52
47	1.1433 E-03	269.684	1.2217 E-03	0.94941	329.21
48	1.0095 E-03	270.650	1.0749 E-03	0.95210	329.80
49	8.9155 E-04	270.650	9.4920 E-04	0.95210	329.80
- 50	7.8735 E-04	270.650	8.3827 E-04	0.95210	329.80
55	4.1969 E-04	260.771	4.6376 E-04	0.92442	323.72
60	2.1671 E-04	247.021	2.5280 E-04	0.88506	315.07
- <u>65</u>	1.0786 E-04	233.292	1.3323 E-04	0.84476	306.19
70	5.1526 E-05	219.585	6.7616 E-05	0.80346	297.06
75	2.3569 E-05	208.399	3.2589 E-05	0.76892	289.40
80	1.0387 E-05	198.639	1.5068 E-05	0.73813	282.54
85	4.3985 E-06	188.893	6.7099 E-06	0.70677	275.52

Reference values: $p_{SL} = 1.01325 \times 10^5 \text{ N/m}^2$; $T_{SL} = 288.150 \text{ K}$ $\rho_{SL} = 1.2250 \text{ kg/m}^3$; $\mu_{SL} = 1.7894 \times 10^{-5} \text{ kg/s·m}$

At 70 km, we obtain:

$$\rho_1 = 8.28296 \times 10^{-5} \text{ kg/m}^3$$
 $p_1 = 5.22 \text{ N/m}^2$
 $T_1 = 219.585 \text{ K}$
 $M_1 = 23.5$

Example 3.1



For

$$p_2 = 0.04 \text{ Atm}$$

$$h_0 = 24.7 \times 10^6 \text{ J/kg}$$

We obtain:

$$z_2 \approx 1.60$$

$$T_2 \approx 6000 \text{ K}$$