1

Foundations of Pyrodynamics

Pyrodynamics describes the process of energy conversion from chemical energy to mechanical energy through combustion phenomena, including thermodynamic and fluid dynamic changes. Propellants and explosives are energetic condensed materials composed of oxidizer-fuel components that produce high-temperature molecules. Propellants are used to generate high-temperature and low-molecular combustion products that are converted into propulsive forces. Explosives are used to generate high-pressure combustion products accompanied by a shock wave that yields destructive forces. This chapter presents the fundamentals of the thermodynamics and fluid dynamics needed to understand the pyrodynamics of propellants and explosives.

1.1
Heat and Pressure

1.1.1
First Law of Thermodynamics

The first law of thermodynamics relates the energy conversion produced by chemical reaction of an energetic material to the work acting on a propulsive or explosive system. The heat produced by chemical reaction (q) is converted into the internal energy of the reaction product (e) and the work done to the system (w) according to

$$dq = de + dw \tag{1.1}$$

The work is done by the expansion of the reaction product, as given by

$$dw = pdv \quad \text{or} \quad dw = pd\left(\frac{1}{\rho}\right) \tag{1.2}$$

where p is the pressure, v is the specific volume (volume per unit mass) of the reaction product, and ρ is the density defined as $v = 1/\rho$. Enthalpy h is defined by

$$dh = de + d\,(pv) \tag{1.3}$$

Substituting Eqs. (1.1) and (1.2) into Eq. (1.3), one gets

$$dh = dq + vdp \tag{1.4}$$

The equation of state for one mole of a perfect gas is represented by

$$pv = R_g T \quad \text{or} \quad p = \rho R_g T \tag{1.5a}$$

where T is the absolute temperature and R_g is the gas constant. The gas constant is given by

$$R_g = \frac{R}{M_g} \tag{1.5b}$$

where M_g is the molecular mass and R is the universal gas constant, $R = 8.314472\ \text{J mol}^{-1}\ \text{K}^{-1}$. In the case of n moles of a perfect gas, the equation of state is represented by

$$pv = nR_g T \quad \text{or} \quad p = n\rho R_g T \tag{1.6}$$

1.1.2
Specific Heat

Specific heat is defined as

$$c_v = \left(\frac{de}{dT} \right)_v \quad c_p = \left(\frac{dh}{dT} \right)_p \tag{1.7}$$

where c_v is the specific heat at constant volume and c_p is the specific heat at constant pressure. Both specific heats represent conversion parameters between energy and temperature. Using Eqs. (1.3) and (1.5a), one obtains the relationship

$$c_p - c_v = R_g \tag{1.8}$$

The specific heat ratio γ is defined by

$$\gamma = \frac{c_p}{c_v} \tag{1.9}$$

Using Eq. (1.9), one obtains the relationships

$$c_v = \frac{R_g}{\gamma - 1} \quad c_p = \frac{\gamma R_g}{\gamma - 1} \tag{1.10}$$

Specific heat is an important parameter for energy conversion from heat energy to mechanical energy through temperature, as defined in Eqs. (1.7) and (1.4). Hence, the specific heat of gases is discussed to understand the fundamental physics of the energy of molecules based on kinetic theory [1, 2]. The energy of a single molecule, ε_m, is given by the sum of the internal energies, which comprise the translational energy ε_t, rotational energy ε_r, vibrational energy ε_v, electronic energy ε_e, and their interaction energy ε_i:

$$\varepsilon_m = \varepsilon_t + \varepsilon_r + \varepsilon_v + \varepsilon_e + \varepsilon_i$$

A molecule containing n atoms has $3n$ degrees of freedom of motion in space:

Molecular structure	Degrees of freedom	Translational	Rotational	Vibrational
Monatomic	3	$= 3$		
Diatomic	6	$= 3$	$+ 2$	$+ 1$
Polyatomic linear	$3n$	$= 3$	$+ 2$	$+ (3n-5)$
Polyatomic nonlinear	$3n$	$= 3$	$+ 3$	$+ (3n-6)$

A statistical theorem on the equipartition of energy shows that an energy amounting to $kT/2$ is given to each degree of freedom of the translational and rotational modes, and that an energy kT is given to each degree of freedom of the vibrational modes. The Boltzmann constant k is 1.38065×10^{-23} J K^{-1}. The universal gas constant R defined in Eq. (1.5b) is given by $R = k\zeta$, where ζ is Avogadro's number, $\zeta = 6.02214 \times 10^{23}$ mol^{-1}.

When the temperature of a molecule is increased, rotational and vibrational modes are excited and the internal energy is increased. The excitation of each degree of freedom as a function of temperature can be calculated through statistical mechanics. Though the translational and rotational modes of a molecule are fully excited at low temperatures, the vibrational modes become excited only above room temperature. The excitation of electrons and interaction modes usually occurs only well above combustion temperatures. Nevertheless, dissociation and ionization of molecules can occur when the combustion temperature is very high.

When the translational, rotational, and vibrational modes of monatomic, diatomic, and polyatomic molecules are fully excited, the energies of the molecules are given by

$$\varepsilon_m = \varepsilon_t + \varepsilon_r + \varepsilon_v$$

$$\varepsilon_m = 3 \times kT/2 = 3 \ kT/2 \ \text{ for monatomic molecules;}$$

$$\varepsilon_m = 3 \times kT/2 + 2 \times kT/2 + 1 \times kT = 7 \ kT/2 \ \text{for diatomic molecules;}$$

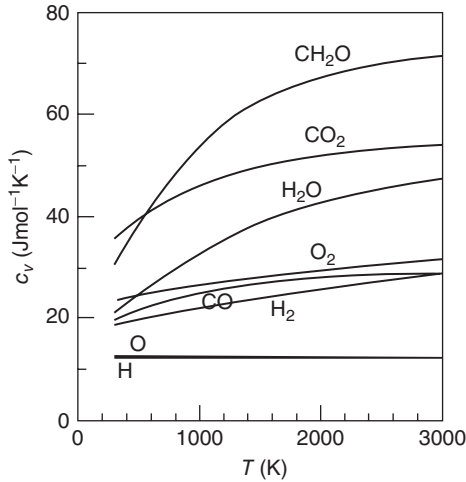$$\varepsilon_m = 3 \times kT/2 + 2 \times kT/2 + (3n - 5) \times kT = (6n - 5) \ kT/2$$
$$\text{for linear molecules;}$$

$$\varepsilon_m = 3 \times kT/2 + 3 \times kT/2 + (3n - 6) \times kT = 3(n - 1) \ kT$$
$$\text{for nonlinear molecules.}$$

Since the specific heat at constant volume is given by the temperature derivative of the internal energy as defined in Eq. (1.7), the specific heat of a molecule, $c_{v,m}$, is represented by

$$c_{v,m} = \frac{d_{\varepsilon m}}{dT} = \frac{d\varepsilon_t}{dT} + \frac{d\varepsilon_r}{dT} + \frac{d\varepsilon_v}{dT} + \frac{d\varepsilon_e}{dT} + \frac{d\varepsilon_i}{dT} \ \text{ J molecule}^{-1} \ \text{K}^{-1}$$

Figure 1.1 Specific heats of gases at constant volume as a function of temperature.

Thus, one obtains the specific heats of gases composed of monatomic, diatomic, and polyatomic molecules as follows:

$c_v = 3R/2 = 12.47$ J mol^{-1} K^{-1} for monatomic molecules;

$c_v = 7R/2 = 29.10$ J mol^{-1} K^{-1} for diatomic molecules;

$c_v = (6n - 5)R/2$ J mol^{-1} K^{-1} for linear molecules;

$c_v = 3(n - 1)R$ J mol^{-1} K^{-1} for nonlinear molecules.

The specific heat ratio defined by Eq. (1.9) is 5/3 for monatomic molecules and 9/7 for diatomic molecules. Since the excitations of rotational and vibrational modes occur only at certain temperatures, the specific heats determined by kinetic theory are different from those determined experimentally. Nevertheless, the theoretical results are valuable for understanding the behavior of molecules and the process of energy conversion in the thermochemistry of combustion. Figure 1.1 shows the specific heats of real gases encountered in combustion as a function of temperature [3]. The specific heats of monatomic gases remain constant with increasing temperature, as determined by kinetic theory. However, the specific heats of diatomic and polyatomic gases increase with increasing temperature as the rotational and vibrational modes are excited.

1.1.3
Entropy Change

Entropy *s* is defined according to

$$ds \equiv \frac{dq}{T} \tag{1.11}$$

Substituting Eqs. (1.4), (1.5a), and (1.7) into Eq. (1.11), one gets

$$ds = c_p \frac{dT}{T} - R_g \frac{dp}{p} \tag{1.12}$$

In the case of isentropic change, $ds = 0$, and Eq. (1.12) is integrated as

$$\frac{p}{p_1} = \left(\frac{T}{T_1} \right)^{c_p/R_g} \tag{1.13}$$

 where the subscript 1 indicates the initial state 1. Using Eqs. (1.10), (1.5a), and (1.13), one gets

$$\frac{p}{p_1} = \left(\frac{T}{T_1} \right)^{\frac{\gamma}{\gamma-1}} \quad \text{and} \quad p \left(\frac{1}{\rho} \right)^{\gamma} = p_1 \left(\frac{1}{\rho_1} \right)^{\gamma} \tag{1.14}$$

When a system involves dissipative effects, such as friction caused by molecular collisions or turbulence caused by a nonuniform molecular distribution, even under adiabatic conditions, ds becomes a positive value, and then Eqs. (1.13) and (1.14) are no longer valid. However, when these physical effects are very small and heat loss from the system or heat gain by the system is also small, the system is considered to undergo an isentropic change.

1.2
Thermodynamics in a Flow Field

1.2.1
One-Dimensional Steady-State Flow

1.2.1.1   Sonic Velocity and Mach Number
The sonic velocity propagating in a perfect gas, a, is given by

$$a = \left(\frac{\partial p}{\partial \rho} \right)_s^{1/2} \tag{1.15}$$

Using the equation of state, Eq. (1.8), and the expression for adiabatic change (Eq. (1.14)), one gets

$$a = \sqrt{\gamma R_g \cdot T} \tag{1.16}$$

The Mach number M is defined as

$$M = \frac{u}{a} \tag{1.17}$$

where u is the local flow velocity in a flow field. Mach number is an important parameter in characterizing a flow field.

1.2.1.2 Conservation Equations in a Flow Field

Let us consider a simplified flow, that is, a one-dimensional steady-state flow without viscous stress or a gravitational force. The conservation equations of continuity, momentum, and energy are represented by

rate of mass in − rate of mass out = 0, that is

$$d(\rho u) = 0 \tag{1.18}$$

rate of momentum gain by convection + pressure difference acting on flow = 0, that is,

$$\rho u du + dp = 0 \tag{1.19}$$

rate of energy input by conduction + rate of energy input by convection = 0, that is

$$d\left(h + \frac{u^2}{2}\right) = 0 \tag{1.20}$$

Combining Eqs. (1.20) and (1.4), one obtains the relationship for the enthalpy change due to a change of flow velocity as

$$dh = dq - u\,du \tag{1.21}$$

1.2.1.3 Stagnation Point

If one can assume that the process in the flow field is adiabatic and that dissipative effects are negligibly small, the flow in the system is isentropic ($ds = 0$), and then Eq. (1.21) becomes

$$dh = -u\,du \tag{1.22}$$

Integration of Eq. (1.22) gives

$$h_0 = h + \frac{u^2}{2} \tag{1.23}$$

where h_0 is the stagnation enthalpy at $u = 0$ of a stagnation flow point. Substituting Eq. (1.7) into Eq. (1.23), one gets

$$c_p T_0 = c_p T + \frac{u^2}{2} \tag{1.24}$$

where T_0 is the stagnation temperature at $u = 0$.

The changes in temperature, pressure, and density in a flow field are expressed as a function of Mach number as follows:

$$\frac{T_0}{T} = 1 + \frac{\gamma - 1}{2} M^2 \tag{1.25}$$

$$\frac{p_0}{p} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma}{\gamma - 1}} \tag{1.26}$$

$$\frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma}{\gamma - 1}} \tag{1.27}$$
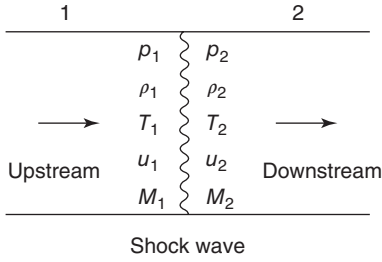
Figure 1.2 Shock wave propagation.

1.2.2
Formation of Shock Waves

One assumes that a discontinuous flow occurs between regions 1 and 2, as shown in Figure 1.2. The flow is also assumed to be one dimensional and in a steady state, and not subject to a viscous force, an external force, or a chemical reaction. The mass continuity equation is given by

$$\rho_1 u_1 = \rho_2 u_2 = m \tag{1.28}$$

The momentum equation is represented by

$$p_1 + m u_1{}^2 = p_2 + m u_2{}^2 \tag{1.29}$$

The energy equation is represented by the use of Eq. (1.20) as

$$c_p T_1 + \frac{u_1{}^2}{2} = c_p T_2 + \frac{u_2{}^2}{2} \tag{1.30}$$

where m is the mass flux in a duct of constant area, and the subscripts 1 and 2 indicate the upstream and the downstream of the discontinuity, respectively. Substituting Eq. (1.29) into Eq. (1.30), one gets

$$p_1 + \rho_1 u_1{}^2 = p_2 + \rho_2 u_2{}^2 \tag{1.31}$$

Using Eq. (1.25), the temperature ratio in regions 2 and 1 is represented by the Mach number in 2 and 1 according to

$$\frac{T_2}{T_1} = \frac{1 + \dfrac{\gamma - 1}{2} M_1^2}{1 + \dfrac{\gamma - 1}{2} M_2^2} \tag{1.32}$$

Using Eqs. (1.5a), (1.17), and (1.28), one gets

$$\frac{T_2}{T_1} = \left(\frac{M_2}{M_1} \right)^2 \left(\frac{p_2}{p_1} \right)^2 \tag{1.33}$$

Combining Eqs. (1.31) and (1.32), the pressure ratio is obtained as a function of M_1 and M_2:

$$\frac{p_2}{p_1} = \frac{M_1}{M_2} \frac{\sqrt{1 + \dfrac{\gamma - 1}{2} M_1^2}}{\sqrt{1 + \dfrac{\gamma - 1}{2} M_2^2}} \tag{1.34}$$

Combining Eqs. (1.33) and (1.34), the Mach number relationship in the upstream 1 and downstream 2 is obtained as

$$
\frac{M_1\sqrt{1 + \dfrac{\gamma - 1}{2}M_1^2}}{1 + \gamma M_1^2} = \frac{M_2\sqrt{1 + \dfrac{\gamma - 1}{2}M_2^2}}{1 + \gamma M_2^2}
\tag{1.35}
$$

One obtains two solutions from Eq. (1.35):

$$
M_2 = M_1
\tag{1.36}
$$

$$
M_2 = \left[\frac{\dfrac{2}{\gamma - 1} + M_1^2}{\dfrac{2\gamma}{\gamma - 1}M_1^2 - 1} \right]^{1/2}
\tag{1.37}
$$

The solution expressed by Eq. (1.36) indicates that there is no discontinuous flow between the upstream 1 and the downstream 2. However, the solution given by Eq. (1.37) indicates the existence of a discontinuity of pressure, density, and temperature between 1 and 2. This discontinuity is called a "*normal shock wave,*" which is set up in a flow field perpendicular to the flow direction. Discussions on the structures of normal shock waves and supersonic flow fields can be found in the relevant monographs [4, 5].

Substituting Eq. (1.37) into Eq. (1.34), one obtains the pressure ratio as

$$
\frac{p_2}{p_1} = \frac{2\gamma}{\gamma + 1}M_1^2 - \frac{\gamma - 1}{\gamma + 1}
\tag{1.38}
$$

Substituting Eq. (1.37) into Eq. (1.33), one also obtains the temperature ratio as

$$
\frac{T_2}{T_1} = \frac{1}{M_1^2}\frac{2(\gamma - 1)}{(\gamma + 1)^2}\left(1 + \frac{\gamma - 1}{2}M_1^2\right)\left(\frac{2\gamma}{\gamma - 1}M_1^2 - 1\right)
\tag{1.39}
$$

The density ratio is obtained by the use of Eqs. (1.38), (1.39), and (1.8) as

$$
\frac{\rho_2}{\rho_1} = \frac{p_2}{p_1}\frac{T_2}{T_1}
\tag{1.40}
$$

Using Eq. (1.24) for upstream and downstream and Eq. (1.38), one obtains the ratio of the stagnation pressures as

$$
\frac{p_{02}}{p_{01}} = \left(\frac{\gamma + 1}{2}M_1^2\right)^{\frac{\gamma}{\gamma - 1}}\left(1 + \frac{\gamma - 1}{2}M_1^2\right)^{\frac{\gamma}{1 - \gamma}}\left(\frac{2\gamma}{\gamma + 1}M_1^2 - \frac{\gamma - 1}{\gamma + 1}\right)^{\frac{1}{1 - \gamma}}
\tag{1.41}
$$

The ratios of temperature, pressure, and density downstream and upstream are expressed by the following relationships:

$$
\frac{T_2}{T_1} = \frac{p_2}{p_1}\frac{\left(1 + \dfrac{1}{\xi}\dfrac{p_2}{p_1}\right)}{\left(\dfrac{1}{\xi} + \dfrac{p_2}{p_1}\right)}
\tag{1.42}
$$

$$\frac{p_2}{p_1} = \frac{\left(\xi \dfrac{\rho_2}{\rho_1} - 1\right)}{\left(\xi - \dfrac{\rho}{\rho_1}\right)} \tag{1.43}$$

$$\frac{\rho_2}{\rho_1} = \frac{\left(\xi \dfrac{p_2}{p_1} + 1\right)}{\left(\xi + \dfrac{p_2}{p_1}\right)} \tag{1.44}$$

where $\zeta = (\gamma + 1)/(\gamma - 1)$. The set of Eqs. (1.42), (1.43), and (1.44) is known as the *Rankine–Hugoniot* equation for a shock wave without any chemical reactions. The relationship of p_2/p_1 and ρ_2/ρ_1 at $\gamma = 1.4$ (for example, in the case of air) shows that the pressure of the downstream increases infinitely when the density of the downstream is increased approximately 6 times. This is evident from Eq. (1.43), as when $\rho_2/\rho_1 \to \zeta$, then $p_2/p_1 \to \infty$.

Though the form of the Rankine–Hugoniot equation, Eqs. (1.42)–(1.44), is obtained when a stationary shock wave is created in a moving coordinate system, the same relationship is obtained for a moving shock wave in a stationary coordinate system. In a stationary coordinate system, the velocity of the moving shock wave is u_1, and the particle velocity u_p is given by $u_p = u_1 - u_2$. The ratios of temperature, pressure, and density are the same for both moving and stationary coordinates.

A shock wave is characterized by the entropy change across it. Using the equation of state for a perfect gas shown in Eq. (1.5a), the entropy change is represented by

$$s_2 - s_1 = c_p \ln\left(\frac{T_2}{T_1}\right) - R_g \ln\left(\frac{p_2}{p_1}\right) \tag{1.45}$$

Substituting Eqs. (1.38) and (1.39) into Eq. (1.45), one gets

$$s_2 - s_1 = c_p \ln\left[\frac{2}{(\gamma + 1)M_1^2} + \frac{1}{\xi}\right] + \frac{c_p}{\gamma} \ln\left[\frac{2\gamma}{\gamma + 1}M_1^2 - \frac{1}{\xi}\right] \tag{1.46}$$

It is obvious that the entropy change will be positive in the region $M_1 > 1$ and negative in the region $M_1 < 1$ for gases with $1 < \gamma < 1.67$. Thus, Eq. (1.46) is valid only when M_1 is greater than unity. In other words, a discontinuous flow is formed only when $M_1 > 1$. This discontinuous surface perpendicular to the flow direction is the normal shock wave. The downstream Mach number M_1 is always < 1, that is, subsonic flow, and the stagnation pressure ratio is obtained as a function of M_1 by Eqs. (1.37) and (1.41). The ratios of temperature, pressure, and density across the shock wave are obtained as a function of M_1 by the use of Eqs. (1.38)–(1.40) and

Eqs. (1.25)–(1.27). The characteristics of a normal shock wave are summarized as follows:

	Front	← Shock wave←	Behind
Velocity	u_1	>	u_2
Pressure	p_1	<	p_2
Density	ρ_1	<	ρ_2
Temperature	T_1	<	T_2
Mach number	M_1	>	M_2
Stagnation pressure	p_{01}	>	p_{02}
Stagnation density	ρ_{01}	>	ρ_{02}
Stagnation temperature	T_{01}	=	T_{02}
Entropy	s_1	<	s_2

1.2.3
Supersonic Nozzle Flow

When gas flows from stagnation conditions through a nozzle, thereby undergoing an isoentropic change, the enthalpy change is represented by Eq. (1.23). The flow velocity is obtained by substitution of Eq. (1.14) into Eq. (1.24) as

$$u^2 = 2c_p T_0 \left\{ 1 - \left(\frac{p}{p_0} \right)^{\frac{Rg}{cp}} \right\} \tag{1.47}$$

Substitution of Eqs. (1.10) and (1.47) gives the following relationship:

$$u = \left[\frac{2\gamma}{\gamma - 1} R_g T_0 \left\{ 1 - \left(\frac{p}{p_0} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \tag{1.48a}$$

The flow velocity at the nozzle exit is represented by

$$u_e = \left[\frac{2\gamma}{\gamma - 1} R_g T_0 \left\{ 1 - \left(\frac{p_e}{p_0} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \tag{1.48b}$$

where the subscript e denotes the exit of the nozzle. The mass flow rate is given by the law of mass conservation for a steady-state, one-dimensional flow as

$$\dot{m} = \rho u A \tag{1.49}$$

where $\dot{m}$ is the mass flow rate in the nozzle, ρ is the gas density, and A is the cross-sectional area of the nozzle. Substituting Eqs. (1.48a), (1.5), and (1.14) into Eq. (1.49), one obtains

$$\dot{m} = p_0 A \left[\frac{2\gamma}{\gamma - 1} \frac{1}{R_g T_0} \left(\frac{p}{p_0} \right)^{2/\gamma} \left\{ 1 - \left(\frac{p}{p_0} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \tag{1.50}$$

Thus, the mass flux defined in $\dot{m}/A$ is given by

$$\frac{\dot{m}}{A} = p_0 \left[\frac{2\gamma}{\gamma-1} \frac{1}{R_g T_0} \left(\frac{p}{p_0}\right)^{2/\gamma} \left\{ 1 - \left(\frac{p}{p_0}\right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \tag{1.51a}$$

The mass flux can also be expressed as a function of Mach number using Eqs. (1.25) and (1.26) as follows:

$$\frac{\dot{m}}{A} = pu = \frac{pu}{R_g T}$$

$$= \sqrt{\frac{\gamma}{R_g T_0}} \, pM \left(1 + \frac{\gamma-1}{2} M^2 \right)^{1/2}$$

$$= \sqrt{\frac{\gamma}{R_g T_0}} \, p_0 M \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\zeta/2} \tag{1.51b}$$

Differentiation of Eq. (1.50) yields

$$\frac{d}{dM}\left(\frac{\dot{m}}{A}\right) = \sqrt{\frac{\gamma}{R_g T_0}} \, p_0 (1 - M^2) \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1-3\gamma}{2(\gamma-1)}} \tag{1.51c}$$

It is evident that $\dot{m}$ is maximum at $M = 1$. The maximum mass flux, $(\dot{m}/A)_{max}$, is obtained when the cross-sectional area is A^*, given by

$$\left(\frac{\dot{m}}{A^*}\right)_{max} = \sqrt{\frac{\gamma}{R_g T_0}} \, p_0 \left(\frac{2}{\gamma+1} \right)^{\zeta/2} \tag{1.52}$$

Thus, the area ratio A/A^* is obtained as

$$\frac{A}{A^*} = \frac{1}{M} \left\{ \frac{2}{\gamma+1} \left(1 + \frac{\gamma-1}{2} M^2 \right) \right\}^{\zeta/2} \tag{1.53}$$

The flow Mach number at A is obtained by the use of Eq. (1.53) when $\dot{m}$, T_0, p_0, R_g, and γ are given. In addition, T, p, and ρ are obtained by the use of Eqs. (1.25), (1.26), and (1.27). Differentiation of Eq. (1.53) with respect to the Mach number yields Eq. (1.54):

$$\frac{d}{dM}\left(\frac{A}{A^*}\right) = \frac{M^2-1}{M^2} \frac{2}{\gamma+1} \left\{ \frac{2}{\gamma+1} \left(1 + \frac{\gamma-1}{2} M^2 \right) \right\}^{\frac{2}{\gamma-1} - \frac{\zeta}{2}} \tag{1.54}$$

Equation (1.54) indicates that A/A^* becomes a minimum at $M = 1$. The flow Mach number increases as A/A^* decreases when $M < 1$, and also increases as A/A^* increases when $M > 1$. When $M = 1$, the relationship $A = A^*$ is obtained and is independent of γ. It is evident that A^* is the minimum cross-sectional area of the nozzle flow, the so-called nozzle throat, in which the flow velocity becomes the sonic velocity. Furthermore, it is evident that the velocity increases in the subsonic flow of a convergent part and also in the supersonic flow of a divergent part.

The velocity u^*, temperature T^*, pressure p^*, and density ρ^* in the nozzle throat are obtained by the use of Eqs. (1.16), (1.18), (1.19), and (1.20), respectively:

$$u^* = \sqrt{\gamma RT^*} \tag{1.55}$$

$$\frac{T^*}{T_0} = \frac{2}{\gamma + 1} \tag{1.56}$$

$$\frac{p^*}{p_0} = \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma - 1}} \tag{1.57}$$

$$\frac{\rho^*}{\rho_0} = \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma - 1}} \tag{1.58}$$

For example, $T^*/T_0 = 0.833$, $p^*/p_0 = 0.528$, and $\rho^*/\rho_0 = 0.664$ are obtained when $\gamma = 1.4$. The temperature T_0 at the stagnation condition decreases by 17% and the pressure p_0 decreases by 50% in the nozzle throat. The pressure decrease is more rapid than the temperature decrease when the flow expands through a convergent nozzle. The maximum flow velocity is obtained at the exit of the divergent part of the nozzle. When the pressure at the nozzle exit corresponds to a vacuum, the maximum velocity is obtained by the use of Eqs. (1.48) and (1.5b) as

$$u_{e,\max} = \sqrt{\frac{2\gamma}{\gamma - 1} \frac{R}{M_g} T_0} \tag{1.59}$$

This maximum velocity depends on the molecular mass M_g, the specific heat γ, and the stagnation temperature T_0. The velocity increases as γ and M_g decrease, and as T_0 increases. Based on Eq. (1.52), a simplified expression for mass flow rate in terms of the nozzle throat area $A_t (= A^*)$ and the chamber pressure $p_c (= p_0)$ is given by

$$\dot{m} = c_D A_t p_c \tag{1.60}$$

where c_D is the nozzle discharge coefficient given by

$$c_D = \sqrt{\frac{M_g}{T_0}} \sqrt{\frac{\gamma}{R}\left(\frac{2}{\gamma + 1}\right)^{\zeta}} \tag{1.61}$$

1.3
Formation of Propulsive Forces

1.3.1
Momentum Change and Thrust

Let us assume a propulsion engine operated in the atmosphere, as shown in Figure 1.3. Air enters in the front end i, passes through the combustion chamber c, and is expelled from the exit e. The heat generated by the combustion of an
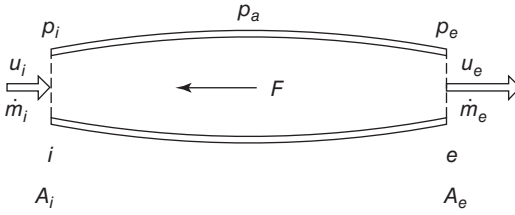
Figure 1.3 Momentum change for propulsion.

energetic material is transferred to the combustion chamber. The momentum balance to generate thrust F is represented by the following terms:

$$F + p_a(A_e - A_i) = (\dot{m}_e\,u_e - p_e\,A_e) - (\dot{m}_i\,u_i + p_i\,A_i) \tag{1.62}$$

where $\dot{m}_i\,u_i = $ incoming momentum at i,
$\dot{m}_e\,u_e = $ outgoing momentum at e,
$p_i\,A_i = $ pressure force acting at i,
$p_e\,A_e = $ pressure force acting at e,
$F + p_a(A_e - A_i) = $ force acting on the outer surface of engine

where u is the flow velocity, $\dot{m}$ is the mass flow rate, A is the area, and the subscripts i, e, and a denote the inlet, exit, and ambient atmosphere, respectively. The mass flow rate of the energetic material supplied to the combustion chamber, $\dot{m}_p$, is given by the difference in the mass flow rates at the exit and the inlet, $\dot{m}_e - \dot{m}_i$. In the case of rocket propulsion, the front end is closed ($A_i = 0$) and there is no influx of mass to the combustion chamber ($\dot{m}_i = 0$). Thus, the thrust for rocket propulsion is represented by

$$F = \dot{m}_e\,u_e + A_e\,(p_e - p_a) \tag{1.63}$$

where $\dot{m}_p = \dot{m}_g$. Thus, the thrust is determined by the flow velocity and pressure at the exit when $\dot{m}_e$, A_e, and p_a are given.

Differentiation of Eq. (1.63) with respect to A_e gives

$$\frac{dF}{dA_e} = u_e\frac{d\dot{m}_g}{dA_e} + \dot{m}_g\frac{du_e}{dA_e} + A_e\frac{dp_e}{dA_e} + p_e - p_a \tag{1.64}$$

The momentum equation at the nozzle exit is represented by $\dot{m}_g du_e = -A_e dp_e$, and $d\dot{m}_g = 0$ for a steady-state flow at the nozzle. Thus, from Eq. (1.64), one obtains the relationship

$$\frac{dF}{dA_e} = p_e - p_a \tag{1.65}$$

The maximum thrust is obtained at $p_e = p_a$, that is, when the pressure at the nozzle exit is equal to the ambient pressure.

However, it must be noted that Eq. (1.62) is applicable for ramjet propulsion, as in ducted rockets and solid-fuel ramjets, because in these cases air enters through the inlet and a pressure difference between the inlet and the exit is set up. The mass
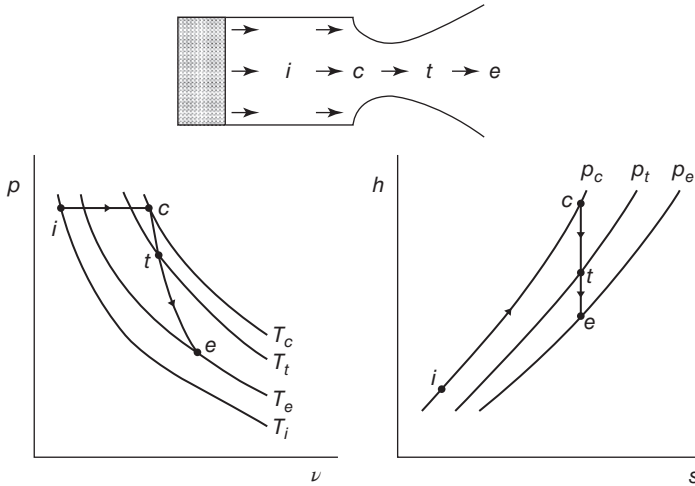
Figure 1.4 Pressure–volume and enthalpy–entropy diagrams for rocket propulsion.

flow rate from the inlet, $\dot{m}_i$, plays a significant role in the generation of thrust in the case of ramjet propulsion.

1.3.2
Rocket Propulsion

Figure 1.4 shows a schematic drawing of a rocket motor composed of the propellant, the combustion chamber, and the nozzle. The nozzle is a convergent–divergent nozzle designed to accelerate the combustion gas from subsonic to supersonic flow through the nozzle throat. The thermodynamic process in a rocket motor is shown in Figure 1.4 by a pressure–volume diagram and an enthalpy–entropy diagram [6]. The propellant contained in the chamber burns and generates combustion products, and this increases the temperature from T_i to T_c at a constant pressure p_c. The combustion products expand through the convergent nozzle to give pressure p_t and temperature T_t at the nozzle throat. The combustion products continue to expand through a divergent nozzle to give pressure p_e and temperature T_e at the nozzle exit.

If one can assume that (i) the flow is one dimensional and in a steadystate, (ii) the flow is an isentropic process, and (iii) the combustion gas is an ideal gas and the specific heat ratio is constant, the plots of p versus v and of h versus s are uniquely determined [6–9]. The enthalpy change due to the combustion of the propellant is given by

$$\Delta h = c_p (T_c - T_i) \tag{1.66}$$

where Δh is the heat of reaction of propellant per unit mass. The expansion process $c \rightarrow t \rightarrow e$ shown in Figure 1.4 follows the thermodynamic process described in Section 1.2.3.

1.3.2.1   Thrust Coefficient

The thrust generated by a rocket motor is represented by Eq. (1.63). Substituting Eqs. (1.48b) and (1.52) into Eq. (1.63), one gets

$$F = A_t p_c \left[\frac{2\gamma^2}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \left\{ 1 - \left(\frac{p_e}{p_c} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} + (p_e - p_a) A_e \qquad (1.67)$$

As shown by Eq. (1.65), the maximum thrust F_{max} is obtained when $p_e = p_a$ at a given specific heat ratio of the combustion gas:

$$F_{max} = A_t p_c \left[\frac{2\gamma^2}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \left\{ 1 - \left(\frac{p_e}{p_c} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \qquad (1.68)$$

Equation (1.68) can be represented by a simplified expression for thrust in terms of the nozzle throat area and chamber pressure:

$$F = c_F A_t p_c \qquad (1.69)$$

where c_F is the thrust coefficient and is given by

$$c_F = \left[\frac{2\gamma^2}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \left\{ 1 - \left(\frac{p_e}{p_c} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} + \frac{p_e - p_a}{p_c} \frac{A_e}{A_t} \qquad (1.70)$$

The maximum thrust coefficient $c_{F,max}$ is then given by

$$c_{F,max} = \left[\frac{2\gamma^2}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \left\{ 1 - \left(\frac{p_e}{p_c} \right)^{\frac{\gamma-1}{\gamma}} \right\} \right]^{1/2} \qquad (1.71)$$

When the nozzle expansion ratio becomes infinity, the pressure ratio p_c/p_a also becomes infinity. The maximum thrust coefficient $c_{F,max}$ then becomes

$$c_{F,max} = \left[\frac{2\gamma^2}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \right]^{1/2} \qquad (1.72)$$

For example, $c_{F,max}$ is 2.246 for $\gamma = 1.20$, and 1.812 for $\gamma = 1.40$.

1.3.2.2   Characteristic Velocity

The characteristic velocity c^* is defined according to

$$c^* = \frac{A_t p_c}{\dot{m}_g} \qquad (1.73)$$

Substituting Eq. (1.52) into Eq. (1.73), one gets

$$c^* = \sqrt{\frac{RT_c}{\gamma M_g}} \left(\frac{2}{\gamma+1}\right)^{-\frac{\zeta}{2}} \tag{1.74}$$

It can be shown that c^* is dependent only on T_g, M_g, and γ and that it is independent of the pressure and the physical dimensions of the combustion chamber and exhaust nozzle; c^*, as defined in Eq. (1.74), is a parameter used to describe the energetics of combustion.

1.3.2.3 Specific Impulse

Specific impulse I_{sp} is a parameter used to describe the energy efficiency of propellant combustion, which is represented by

$$I_{sp} = \frac{F}{\dot{m}_g g} \tag{1.75}$$

where g is the gravitational acceleration (9.80665 m s^{-2}); hence specific impulse is expressed in terms of seconds. Thermodynamically, specific impulse is the effective time required to generate a thrust that can sustain the propellant mass against the gravitational force through energy conversion. Since the mass flow rate $\dot{m}_g$ is given by Eq. (1.50) and F is given by Eq. (1.67), I_{sp} is represented by

$$I_{sp} = \frac{1}{g}\left[\frac{2\gamma}{\gamma-1}\frac{R}{M_g}T_c\left\{1-\left(\frac{p_e}{p_c}\right)^{\frac{\gamma-1}{\gamma}}\right\}\right]^{1/2} + \frac{1}{g}\left(\frac{\gamma+1}{2}\right)^{\zeta/2}\sqrt{\frac{RT_c}{\gamma M_g}}\left(\frac{p_e-p_a}{p_c}\right)\frac{A_e}{A_t} \tag{1.76}$$

$$\sim \left(\frac{T_g}{M_g}\right)^{1/2} \tag{1.77}$$

where T_g is the combustion temperature and M_g is the molecular mass of the combustion products. Though $I_{sp,max}$ is also a function of the specific heat ratio γ of the combustion products, γ varies very little among propellants. It is evident from Eq. (1.77) that an energetic material that produces high-T_g and high-M_g combustion products is not always a useful propellant. A propellant that generates low-T_g combustion can also be useful if M_g is sufficiently low. Similar to F_{max} and $c_{F,max}$, the maximum specific impulse $I_{sp,max}$ is obtained when $p_e = p_a$:

$$I_{sp,max} = \frac{1}{g}\left[\frac{2\gamma}{\gamma-1}\frac{R}{M_g}T_g\left\{1-\left(\frac{p_a}{p_c}\right)^{\frac{\gamma-1}{\gamma}}\right\}\right]^{1/2} \tag{1.78}$$

In addition, the specific impulse is given by the thrust coefficient and the characteristic velocity according to

$$I_{\text{sp}} = c_F \, \frac{c^*}{g} \tag{1.79}$$

Since c_F indicates the efficiency of the expansion process in the nozzle flow, and c^* indicates the efficiency of the combustion process in the chamber, I_{sp} gives an indication of the overall efficiency of a rocket motor.

1.3.3
Gun Propulsion

1.3.3.1 Thermochemical Process of Gun Propulsion
Gun propellants burn under conditions of nonconstant volume and nonconstant pressure. The rate of gas generation changes rapidly with time, and the temperature changes simultaneously because of the displacement of the projectile in the combustion chamber of the gun barrel [10–12]. Though the pressure change is rapid, the linear burning rate is assumed to be expressed by a pressure exponent law, the so-called Vieille's law: that is

$$r = ap^n \tag{1.80}$$

where r is the burning rate (mm s^{-1}), p is the pressure (MPa), n is a constant dependent on the composition of the propellant, and a is a constant dependent on the initial chemical composition and temperature of the propellant.

The fundamental difference between gun propellants and rocket propellants lies in the magnitude of the burning pressure. Since the burning pressure in guns is extremely high, more than 100 MPa, the parameters of the above equation are empirically determined. Though rocket propellant burns at below 20 MPa, in general, the burning rate expression of gun propellants appears to be similar to that of rocket propellants. The mass burning rate of the propellant is also dependent on the burning surface area of the propellant, which increases or decreases as the burning proceeds. The change in the burning surface area is determined by the shape and dimensions of the propellant grains used.

The effective work done by a gun propellant is the pressure force that acts on the base of the projectile. Thus, the work done by propellant combustion is expressed in terms of the thermodynamic energy f, which is represented by

$$f = pv = \frac{RT_g}{M_g} = p_0 v_0 \frac{T_g}{T_0} \tag{1.81}$$

where p_0, v_0, and T_0 are the pressure, volume, and temperature, respectively, generated by the combustion of unit mass of the propellant in the standard state. The thermodynamic energy f is expressed in units of MJ kg^{-1}. It is evident that a higher f value is favorable for a gun propellant, similar to I_{sp} used to evaluate the thermodynamic energy of rocket propellants.

The thermal energy generated by propellant combustion is distributed to various noneffective energies [10]. The energy losses of a caliber gun are approximately as follows:

Sensible heat of combustion gas	42%
Kinetic energy of combustion gas	3%
Heat loss to gun barrel and projectile	20%
Mechanical losses	3%

The remaining part of the energy, 32%, is used to accelerate the projectile. It is obvious that the major energy loss is the heat released from the gun barrel. This is an unavoidable heat loss based on the laws of thermodynamics: the pressure in the gun barrel can be expended only by the cooling of the combustion gas to the atmospheric temperature.

1.3.3.2 Internal Ballistics

The one-dimensional momentum equation for the internal ballistics of a gun is represented by [10−12]

$$M_w \frac{du}{dt} = M_w u \frac{du}{dx} = pA_{bi} \tag{1.82}$$

where M_w is the mass of the projectile, u is its velocity, x is the distance traveled, t is time, p is pressure, and A_{bi} is the cross-sectional area of the gun barrel. Integration of Eq. (1.82) from 0 to L_b gives

$$u_{be} = \sqrt{\frac{2[p]L_b A_{bi}}{M_w}} \tag{1.83}$$

where u_{be} is the velocity at the barrel exit and L_b is the effective length of the barrel used to accelerate the projectile. If one assumes an averaged pressure in the barrel, $[p]$, given by

$$f = pv = R\frac{T_g}{M_g} \tag{1.84}$$

the velocity of the projectile is given by

$$u_{be} = \left(2\,[p]\,A_{bi}\frac{L_b}{M_w} \right)^{1/2} \tag{1.85}$$

With fixed physical dimensions of a gun barrel, the thermodynamic efficiency of a gun propellant is expressed by its ability to produce as high a pressure in the barrel as possible from a given propellant mass within a limited time.

In general, the internal pressure in a gun barrel exceeds 200 MPa, and the pressure exponent n of the propellant burning rate, given by Eq. (1.80), is 1. When $n = 1$, the burning rate of a gun propellant is represented by

$$r = ap \tag{1.86}$$

where r is the burning rate, p is the pressure, and a is a constant dependent on the chemical ingredients and the initial temperature of the propellant grain. The volumetric burning rate of a propellant grain is represented by $S(t)r$, where $S(t)$ is the surface area of the propellant grain at time t. The volumetric burning change of the propellant grain is defined by

$$\frac{dz}{dt} = \frac{V(t)}{V_0}$$

$$= \frac{S_0}{V_0}\frac{S(t)}{S_0}r(t) = \sigma\frac{S(t)}{S_0}r(t) \tag{1.87}$$

where V_0 is the initial volume of the propellant grain, $\sigma = S_0/V_0$, $V(t)$ is the volume of the propellant grain at time t, and z is a geometric function of the grain. The surface area ratio change, termed the "*form function*," φ, is defined according to

$$\varphi(z) = \frac{S(t)}{S_0} \tag{1.88}$$

Table 1.1 shows the form functions for several types of propellant grains. Substituting Eqs. (1.80), (1.86), and (1.88) into Eq. (1.87), one obtains a simplified expression for the volumetric burning rate change:

$$\frac{dz}{dt} = a\sigma\varphi(z)p \tag{1.89}$$

Substituting Eq. (1.89) into Eq. (1.82), the velocity change of the projectile is determined by

$$du = \left(\frac{A_{bi}}{M_w}\right)\left(\frac{1}{a\sigma}\right)\frac{dz}{\varphi(z)} \tag{1.90}$$

The velocity of the projectile is obtained by integration of Eq. (1.90) from the initial stage to the stage z_1:

$$u = \left(\frac{A_{bi}}{M_w}\right)\left(\frac{1}{a\sigma}\right)\int_0^{z_1}\frac{dz}{\phi(z)} \tag{1.91}$$

Table 1.1 Form functions for various types of propellant grain.

Grain shape	$\varphi(z)$
Spherical, cubic grain	$(1-z)^{2/3}$
Disk, square, strand	$(1-z)^{1/2}$
Short column	$(1-z)^{3/5}$
Short tubular	$(1-0.57z)^{1/2}$
Center perforated disk	$(1-0.33z)^{1/2}$
Long tubular	1
Seven-holes short tubular	$(1+z)^{1/2}$

where u is the velocity when $z = z_1$. In general, the projectile starts to move when the pressure in the barrel reaches a certain initial pressure p_c due to the action of the shot resistance between the projectile and the barrel. The velocity of the projectile is then represented by

$$u = \left(\frac{A_{bi}}{M_w} \right) \left(\frac{1}{a\sigma} \right) \left\{ \int_0^{z_1} \frac{dz}{\phi(z)} - \int_0^{z_0} \frac{dz}{\phi(z)} \right\} \qquad (1.92)$$

where z_0 is the volumetric burning change at p_c. After the propellant grain is completely consumed, the pressure in the barrel changes isentropically according to

$$p = \frac{\rho_g p^*}{\rho_g *} \qquad (1.93)$$

where p^* and $\rho_g *$ denote the pressure and density, respectively, when burning is complete.

1.4
Formation of Destructive Forces

1.4.1
Pressure and Shock Wave

When a propellant grain burns in a closed chamber, a large number of gaseous molecules are produced. The pressure generated by these molecules acts on the inner surface the chamber. The pressure increases slowly as a result of the continuous burning of the propellant. When the pressure exceeds the mechanical strength of the chamber wall, mechanical breakage occurs at the weakest portion of the chamber wall. The force acting on the chamber wall is caused by the static pressure of the combustion gas.

When an explosive detonates in a closed container, a shock wave is formed. The shock wave travels toward the inner surface of the chamber and acts on the chamber wall. The pressure wave is caused by this shock wave, rather than by the pressure created by the detonated burned gases. The shock wave travels first through the air in the chamber, and the burned gas follows somewhat later. When the shock wave reaches the inner surface of the chamber wall, the chamber will be damaged if the mechanical strength of the chamber wall is lower than the mechanical force created by the shock wave. Though the time for which the shock wave acts on the wall is very short, in contrast to the static pressure built up by combustion gases, the impulsive force caused at the wall leads to destructive damage. Though no pressure is formed when a propellant grain burns outside of the chamber, a shock wave is still formed when an explosive detonates externally. When this shock wave reaches the outer surface of the chamber, the chamber wall may well be damaged.

1.4.2
Shock Wave Propagation and Reflection in Solid Materials

When a shock wave travels in a solid wall from one end to the other, a compressive force is created at the front end of the shock wave. When the shock wave reaches the other end, a reflection wave is formed, which travels back in the reverse direction. This reflection wave forms an expansion force that acts on the wall.

There are two general modes for the destruction of solid materials, namely ductile fracture and brittle fracture. These modes are dependent on the type of material and on the type of forces acting on the material. The mechanical force created by a shock wave is similar to the force created by an impact stress. The breakage mechanism of materials is dependent on the action of the mechanical force. When a shock wave travels in a concrete wall from one end to the other, it generates a compressive stress, and no damage is observed. However, when the shock wave is reflected at the other end of the wall, a reflection wave is formed, accompanied by an expansion stress. Since the compression strength of the concrete is sufficient to endure the compressive stress created by the shock wave, no mechanical damage results from the shock wave itself. However, when the concrete wall is subjected to the tensile stress created by the expansion wave, the expansion force exceeds the tensile strength of the wall, thus leading to its breakage.

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