
1

INTRODUCTION AND CONSERVATION EQUATIONS

SYMBOLS

Symbol	Description	Dimension
\mathbf{B}_i	Body force per unit volume in i-direction (vector)	F/L^3
C	Molar concentration	N/L^3
C_i	Molar concentration of the i^{th} species	N/L^3
d	Molecular diameter	L
D_{Ab}	Binary mass diffusivity for A-B system	L^2/t
e_{ij}	Strain rate tensor	t^{-1}
Ea_k	Activation energy for the kth reaction	Q/N
\mathbf{f}_i	External force per unit mass on species i (vector)	F/M
\mathbf{F}	Force (vector)	F
\mathbf{F}_S	Surface force (vector)	F
h	Enthalpy per unit mass	Q/M
h_t	Total enthalpy per unit mass	Q/M
\mathbf{I}	Identity matrix or vector form of Kronecker delta δ_{ij}	–
\mathbf{J}_i	Mass flux of species i relative to mass-average velocity (vector)	M/L^2t
\mathbf{J}_i^*	Molar flux of species i relative to molar-average velocity (vector)	N/L^2t
K	Boltzmann constant	$(Q/T)/\text{molecule}$

Symbol	Description	Dimension
l	Mean free path	L
$\dot{\mathbf{m}}$	Mass flux (vector)	M/L ² t
m_i	Mass of the i^{th} species in the mixture	M
m_t	Total mass of a multi component gaseous mixture	M
Mw_i	Molecular weight of i^{th} species	M/N
$\dot{\mathbf{n}}$	Molar flux (vector)	NL ² t
n_i	Number of moles of i^{th} species in the gaseous mixture	N
N_i	Number of moles of species i	—
N_A	Avogadro's number, 6.02252×10^{23} molecules/mole	—
\mathbf{q}	Heat-flux vector (vector)	Q/L ² t
T°	Fixed standard reference temperature, at 298.15 K	T
\bar{u}	Arithmetic-mean molecular speed	L/t
u_i	Velocity component in i^{th} -direction	L/t
\mathbf{v}	Mass-average velocity (vector)	L/t
V	Control volume	L ³
\mathbf{v}_i	Velocity of i^{th} species with respect to stationary coordinate axes (vector)	L/t
\mathbf{v}^*	Molar-average velocity (vector)	L/t
\mathbf{V}_i	Mass diffusion velocity of i^{th} species (vector)	L/t
\mathbf{V}_i^*	Molar diffusion velocity of i^{th} species (vector)	L/t
X_i	Mole fraction of the i^{th} species	—
y	Space coordinate in y -direction	L
Y_i	Mass fraction of the i^{th} species	—
z	Space coordination in z -direction	L
Z	Frequency of molecular collisions of gaseous species per unit surface area	L ⁻² t ⁻¹
Greek Symbols		
α	Thermal diffusivity	L ² /t
α_i	Thermal diffusion coefficient for species i	L ² /t
λ	Thermal conductivity or second viscosity	Q/tLT or Ft/L ²
μ	Dynamic viscosity or first viscosity	Ft/L ²
μ'	Bulk viscosity	Ft/L ²
μ_{ij}	Reduced mass of molecules of species i and j	M
$\sigma_{ij}, \tilde{\sigma}$	Total stress tensor	F/L ²
τ_{ij}	Viscous stress tensor	F/L ²
$\dot{\Omega}_i$	Molar rate or production of species i	N/(tL ³)
$\dot{\omega}_i$	Mass rate of production of species i	M/(tL ³)

This chapter first discusses turbulent and multiphase combustion as a major area of research for understanding and importance of solution of multiple challenging and interesting problems related to energy, environment, transportation, and chemical propulsion, among other fields. The second topic provides a summary of the major conservation equations used by researchers in the combustion community.

1.1 WHY IS TURBULENT AND MULTIPHASE COMBUSTION IMPORTANT?

Currently, a very high percentage ($\sim 80\%$) of energy is generated by combustion of liquids (such as gasoline and hydrocarbon fuels), solids (such as coal and wood), and gases (such as natural gas composed of largely methane and other hydrocarbons like ethane, propane, butanes and pentanes). For example, during the first decades of the twenty-first century more than 50% of the electricity in the United States was generated by coal-fired furnaces. This trend is expected to continue for several decades. Thus, energy generation will continue to rely heavily on combustion technology. Most practical devices involve turbulent combustion, which requires understanding of both turbulence and combustion, as well as their effects on each other. Industrial furnaces, diesel engines, liquid rocket engines, and devices using solid propellants involve multiphase and turbulent combustion. Single-phase turbulent reacting flows are complicated enough for modeling and numerical solutions, some of these flows are still unresolved problems of our time. The complexity of the problem increases even further with the presence of multiple phases.

In recent years, there has been a greater move to increase combustion efficiency while keeping the emissions level as low as possible. We live in times in which energy has become a very critical commodity. Therefore, it is important that the unresolved problems of combustion should be understood and solved. Well-trained combustion engineers and scientists are needed to engage in numerous challenging combustion problems. This chapter provides some general background about the applications of turbulent and multiphase combustion, the general concept of modeling, and basic conservation equations for gas-phase mixtures containing multiple species.

1.2 DIFFERENT APPLICATIONS FOR TURBULENT AND MULTIPHASE COMBUSTION

There are various applications of turbulent and multiphase combustion associated closely with our daily life. Some of these are:

- Power generation from combustion (one example of two-phase turbulent combustion used for energy generation from coal-fired burners can be seen in Figure 1.1)

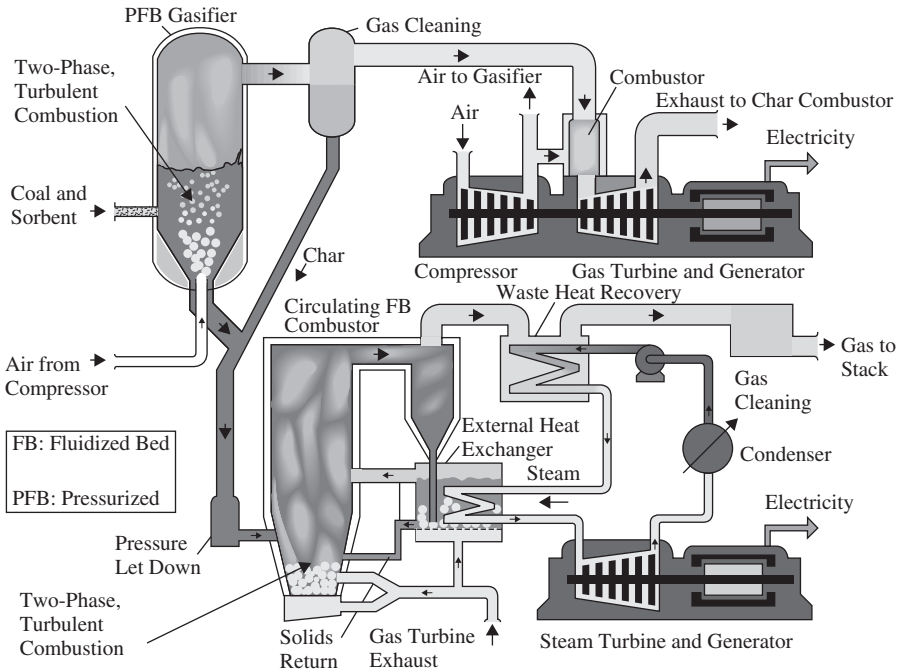


Figure 1.1 Schematic of a hybrid power generation system using coal-air combustion (modified from <http://fossil.energy.gov>).

- High rates of combustion of energetic materials for various propulsion systems
- Process industry for production of engineering materials (e.g., ceramics, H₂, nanosized particles)
- Household and industrial heating;
- Active control of combustion processes;
- Safety protections for unwanted combustion;
- Ignition of various condensed-phase combustible materials (like solid propellants airbags in automobiles) for safety enhancement under emergency situation
- Pollutant emission control of combustion products (about one-third of carbon emissions in the United States comes from coal-fired power plants, one-third from transportation, and the rest from the industrial, commercial, and residential sources)

Figure 1.2 shows the distribution of total emissions estimates in the United States by source category for specific pollutants in 2008. The major air pollutants are particulate matter, CO, CO₂, SO_x, NO_x, VOCs (volatile organic compounds), NH₃, mercury, and lead. Electric utilities contribute about 70%

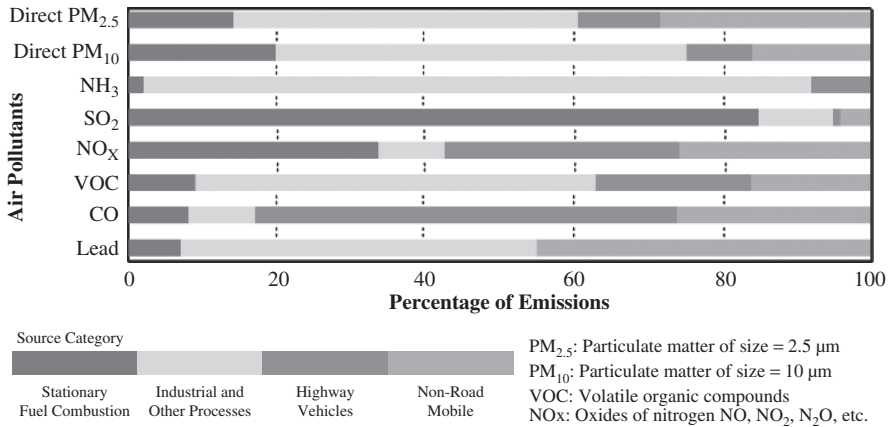


Figure 1.2 Distribution of national total emissions estimates by source category for specific pollutants in year 2008 (modified from EPA report).

of national SO₂ emissions. Agricultural operations (other processes) contribute over 80% of national NH₃ emissions. Almost 50% of the national VOC emissions originate from solvent use (other processes) and highway vehicles. Highway vehicles and nonroad mobile sources (e.g., aircrafts, agricultural vehicles, ships, etc.) together contribute approximately 80% of national CO emissions. Fossil fuel combustion is the primary source contributing to CO₂ emissions. In 2007, fossil fuel combustion contributed almost 94% of the total CO₂ emissions. Major sources of fossil fuel combustion include electricity generation, transportation (including personal and heavy-duty vehicles), industrial processes, residential, and commercial. Electricity generation contributed approximately 42% of CO₂ emissions from fossil fuel combustion while transportation contributed approximately 33%. Advance in combustion technology can lead to higher burning efficiency and less production of harmful compounds.

1.2.1 Applications in High Rates of Combustion of Materials for Propulsion Systems

Many propulsion systems employ combustion of condensed phase materials to generate thermal energy. Some of these are:

- Gas turbine engines for aircrafts;
- Liquid fuels and oxidizers for liquid rocket engines (see Figure 1.3);
- Spray of liquid fuels for diesel engines, bipropellant rockets, and ramjets, and the like
- Pre vaporized hydrocarbons for reciprocating engines
- Solid propellants in rocket motors for space and missile propulsion

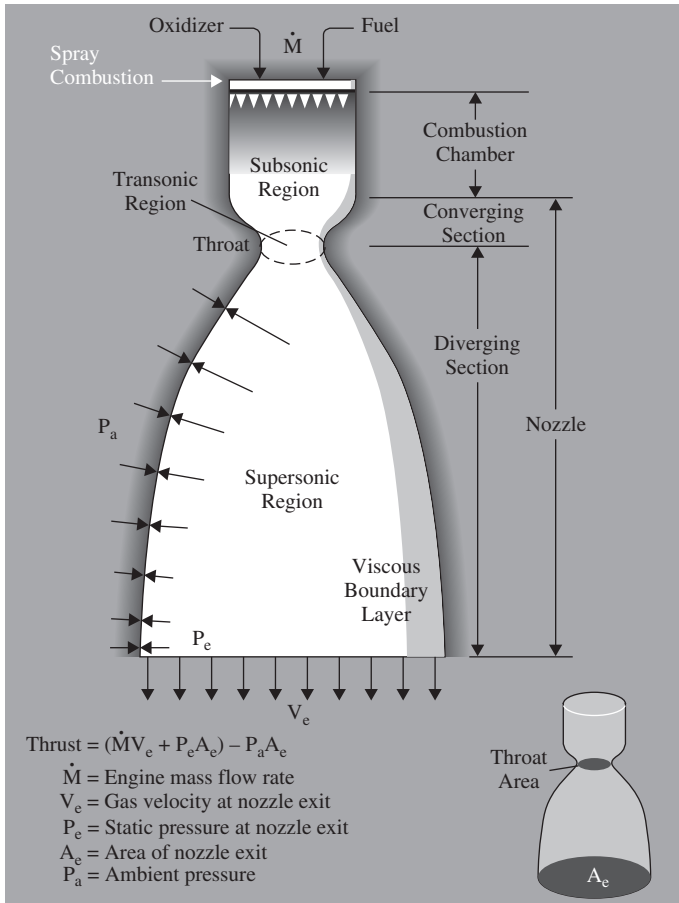


Figure 1.3 Combustion and energy conversion in a nozzle of bipropellant liquid rocket (Modified from O’ Leary and Beck, 1992).

- Solid fuels for hybrid rocket motors, ramjets, scramjets
- Monopropellants for space thrusters
- Solid propellants for gun and artillery propulsion systems

As shown in Figure 1.3, chemical energy is converted into thermal energy by combustion. The thrust of a propulsion system is proportional to the momentum of the exhaust jet. The specific impulse (I_{sp}), defined as the thrust per propellant weight flow rate, is known to be proportional to the square root of the flame temperature divided by the average molecular weight of the combustion products, as shown in Equation 1.1.

$$I_{sp} \propto \sqrt{T_f / Mw} \tag{1.1}$$

More detailed description of this relationship is given in Chapter 1 of Kuo Acharya, Applications of Turbulent and Multiphase Combustion (2012).

1.2.2 Applications in Power Generation

Condensed phase and gas-phase material are turned in various power generation systems. For example:

- *Coal particles*: Burned in furnaces of power stations to produce steam for driving turbines in order to generate electricity (see Figure 1.1)
- *Liquid fuels*: Used as the source of energy for transportation purposes with automobiles, aircrafts, and ships
- *Natural gases*: Used for gas turbines and reciprocating engines
- *Incineration of waste materials*

1.2.3 Applications in Process Industry

In the material processing industry, combustion of different types of fuels has been used for obtained elevated temperature conditions in the manufacturing process. For example:

- Production of iron, steel, glass, ceramics, cement, carbon black, and refined fuels through thermal heating processes
- Direct fabrication of ceramic materials by self-propagating high-temperature synthesis (SHS) processes
- Combustion synthesis of nanosize powders

1.2.4 Applications in Household and Industrial Heating

For various heating systems, chemical energies of fuels and oxidizers are converted to thermal energy by turbulent and multiphase combustion processes.

- *Thermal energy generated by combustion*: Used for heating of residences, factories, offices, hospitals, schools, and various types of buildings; and heating of International Space Station (ISS) and many special facilities

1.2.5 Applications in Safety Protections for Unwanted Combustion

Knowledge of turbulent and multiphase combustion is also very useful for various fire and hazard prevention systems, such as:

- Fire prevention for forest fires
- Fire prevention for building fires
- Reduction of industrial explosions
- Reduction of susceptibility for deflagration-to-detonation transitions (DDT) and shock-to-detonation transition (SDT) leading to catastrophic hazards

1.2.6 Applications in Ignition of Various Combustible Materials

Many safety protection systems depend upon the reliable ignition of various combustion materials, for example

- For safety enhancement under emergency situations
- Inflation of airbags during, collisions automobile
- Actuation of ejection pilot seats and other emergency escape systems
- Fire extinguishment by strong-flow gas generators

1.2.7 Applications in Emission Control of Combustion Products

The success of emission control of combustion products depend strongly upon the knowledge of the turbulent and multiphase combustion with application in different aspects, such as:

- For reduction of pollutants generated from combustion
- Reduction of formation of NO_x , SO_x , and CO_2
- Reduction of formation of particulates such as soot and coke
- Control of the temperature and chemical compositions of combustion products

1.2.8 Applications in Active Control of Combustion Processes

To achieve better combustion performance and to reduce combustion instabilities in various propulsion systems, certain active control systems can be employed:

- To enhance combustion efficiencies of reactors by external energy sources, such as acoustic energy emission
- To enhance combustion efficiencies of certain systems with injection of nanosize energetic particles

1.3 OBJECTIVES OF COMBUSTION MODELING

With significant advancements in computational power and numerical schemes in recent years, simulation of complicated combustion problems could be tractable. Several major objectives for combustion modeling are listed below

- To simulate certain turbulent combustion processes involving single and/or multi-phase combustible materials
- To develop predictive capability for combustion systems under various operating conditions
- To help in interpreting and understanding observed combustion phenomena
- To substitute for difficult or expensive experiments
- To guide the design of combustion experiments

- To determine the effect of individual parameters in combustion processes by parametric studies

1.4 COMBUSTION-RELATED CONSTITUENT DISCIPLINES

The science of turbulent and multiphase combustion often involves intricate inter-coupling and interactions between many constituent disciplines. Background in the following areas would be very helpful for scientists and engineers to acquire and to apply to various unresolved combustion problems

- Thermodynamics
- Chemical kinetics
- Fluid mechanics
- Heat and mass transfer
- Turbulence
- Transport phenomena
- Statistical mechanics
- Instrumentation and diagnostic techniques
- Quantum chemistry and physics
- Materials structure and behavior
- Mathematical and statistical theories
- Numerical methods
- Design of combustion test apparatus
- Data analysis and correlation methods
- Safety and hazard analysis

1.5 GENERAL APPROACH FOR SOLVING COMBUSTION PROBLEMS

For solving combustion problems, one can consider the following methods:

- Theoretical and numerical methods
- Experimental methods
- Any combination of the above methods

A theoretical model for a combustion problem consists of a set of governing equations that must be solved with multiple input parameters and initial and boundary conditions, as shown in Figure 1.4. As one can observe, there is a significant level of coupling between the intermediate solution from governing equations and the input parameters, such as reaction mechanism, turbulence closure conditions, and diffusion/transport mechanisms. The major output of the

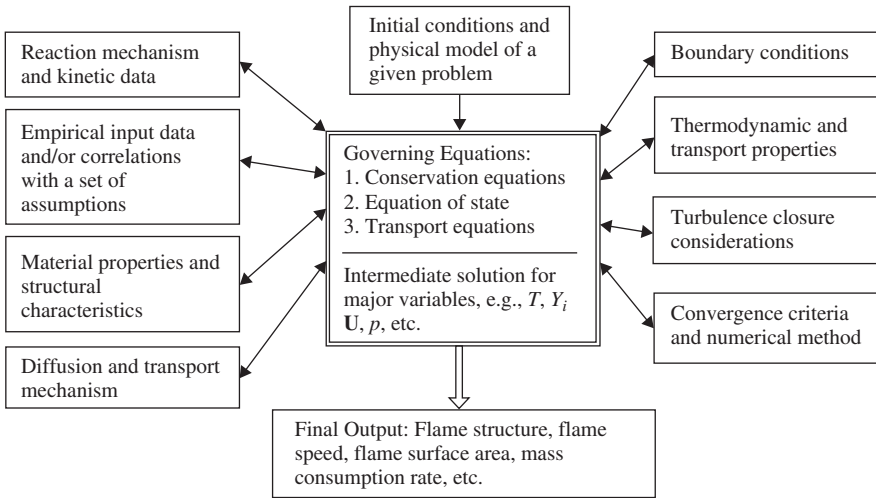


Figure 1.4 General structure of a theoretical model.

model consists of flame structure, speed, surface area, burning rate, flow field structure, and the like.

A combustion problem can be solved by using different numerical approaches. Currently there are three major categories of such approaches: Reynolds average Navies-Stokes (RANS) simulation, large-eddy simulation (LES), and direct numerical simulation (DNS). A discussion of these methods is provided in Chapter 4. The effect of these different numerical approaches on the final solution can be seen in Figure 1.5, which shows the predicted results for a diffusion flame. Currently RANS is most commonly employed in industry, but its range of validity is limited. DNS is the most detailed, but it is too

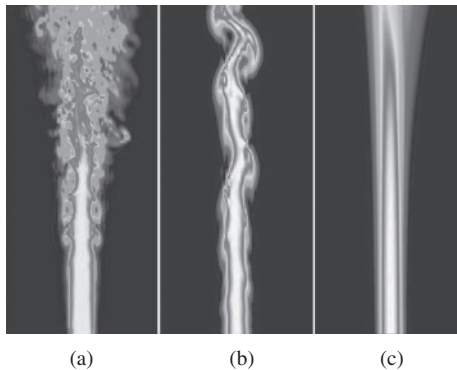


Figure 1.5 Predicted results for a diffusion flame by using (a) DNS, (b) LES, and (c) RANS (from Givi, 2009; <http://cfd.engr.pitt.edu/>).

computationally demanding for most realistic engineering problems. LES is a compromise between the two and provides excellent reliability and applicability.

1.6 GOVERNING EQUATIONS FOR COMBUSTION MODELS

1.6.1 Conservation Equations

The five groups of conservation equations consist of:

1. Conservation of mass (continuity equation)
2. Conservation of molecular species (or conservation of atomic species)
3. Conservation of momentum (for each independent spatial direction)
4. Conservation of energy
5. Conservation of angular momentum

These equations are used together with the transport equations and the equation of state to solve for flow property distributions, including temperature, density, pressure, velocity, and concentrations of chemical species. Note that the conservation equation of angular momentum is not often used unless the problems involve external torque with significant amounts of swirling or with polar fluids flowing in magnetic fields.

1.6.2 Transport Equations

Transport equations are usually required for turbulent combustion problems. They include:

1. Transport of turbulent kinetic energy
2. Transport of turbulence dissipation rate (or turbulent kinetic energy dissipation rate)
3. Transport of turbulent Reynolds stresses
4. Transport of probability density function
5. Transport of moments such as

$$\widetilde{u''Y_i''}, \widetilde{Y_i''^2}, \widetilde{T''^2}, \overline{u'Y_i'}, \overline{Y_i'^2}, \overline{T'^2}, \text{ etc.}$$

1.6.3 Common Assumptions Made in Combustion Models

Certain commonly used assumptions are listed below. Readers must recognize that some of these assumptions can be relaxed nowadays due to the advancements in numerical predictive schemes and/or the availability of thermal and transport property data.

- Reacting fluid can be treated as a continuum.
- Infinitely fast chemistry (chemical equilibrium) can be applied for high-temperature combustion problems.

- Simple, one-step, forward irreversible global reaction can sometimes be applied for less comprehensive models.
- Ideal gas law can be used for low pressure with moderately high temperature reacting flow problems
- Lewis, Schmidt, and Prandtl numbers may be assumed equal to 1, under certain combustion conditions.
- Equal mass diffusivities of all species was used by many researchers when there were no diffusivity data available.
- Fick's law of species mass diffusion can be assumed to be valid in many circumstances.
- Constant specific heats of the gas-phase species had been assumed when no thermal data were available.
- Reacting solid surfaces are sometimes assumed to be energetically homogeneous.
- Uniform pressure can be assumed for the region having low-speed combustion situations.
- Dufour and Soret effects are often assumed to be negligible
- Bulk viscosity is often assumed to be negligibly small.
- Under certain conditions, negligible combustion-generated turbulence can be assumed.

These assumptions must be examined for validity before they are adopted in modeling work.

1.6.4 Equation of State

The simplest equation of state is that for an ideal gas. The ideal gas law, which applies to both pure components and mixtures, has been established from empirical observation and is accurate for gases at low density or up to tens of atmospheric pressure for most compounds. For nondissociating molecules, this relationship holds for low to moderate pressures.

$$pV = nR_u T = m \frac{R_u}{M_w} T = mRT \quad (1.2)$$

where R_u is the universal gas constant [= 8.3144 J/(mol K)]

Other Forms of Ideal Gas Law

$$\rho = \frac{m}{V} = \frac{p}{RT} = \frac{p\overline{M_w}}{R_u T} = \frac{p}{R_u T \sum_{i=1}^N \frac{Y_i}{M_{w_i}}} \quad (1.3)$$

$$c = \frac{n}{V} = \frac{p}{R_u T} = \frac{p}{RT \overline{M_w}} \quad (1.4)$$

In terms of specific volume v , the ideal gas law can be written as:

$$pv = RT \quad \text{where } v = \frac{V}{m} \quad (1.5)$$

1.6.4.1 High-Pressure Correction

Van der Waals Equation of State The van der Waals equation of state is one of the best-known generalized equations of state. It is essentially a modified version of the ideal gas law, expressed by Equation 1.5, except that it accounts for the intermolecular forces that exist between molecules (represented by the term a/v^2) and also corrects for the covolume, b , occupied by the molecules themselves. The van der Waals equation of state is:

$$\left(p + \frac{a}{v^2}\right)(v - b) = RT \quad (1.6)$$

where a and b are evaluated from the general behavior of gases. These constants are related to the critical temperatures and pressures of pure substances by

$$a = \frac{27}{64} \frac{R^2 T_c^2}{p_c} \quad \text{and} \quad b = \frac{RT_c}{8p_c} \quad (1.7)$$

If a is equal to 0, then the van der Waals equation of state is called the Noble-Abel equation of state.

$$p = \frac{RT}{(v - b)} \quad (1.8)$$

Redlich-Kwong Equation of State The Redlich-Kwong equation of state (and many of its variants) is representative of the commonly used *empirical* cubic equations of state. It is considerably more accurate than the van der Waals equation and has been shown to be very successful not only for pure substances but also for mixture calculations and phase equilibrium correlations. The original Redlich-Kwong equation is given as

$$p = \frac{R_u T}{\bar{v} - b} - \frac{a}{\bar{v}(\bar{v} + b) T^{1/2}} \quad (1.9)$$

where

$$a = \frac{0.42748 R_u^2 T_c^{2.5}}{p_c} \quad \text{and} \quad b = \frac{0.08664 R_u T_c}{p_c} \quad (1.10)$$

The values of critical pressure (p_c) and critical temperature (T_c) for various hydrocarbon fuels are listed in Kuo (2005), Appendix C.

Soave-Redlich-Kwong and Peng-Robinson Equations of State The Soave's modified RK equation or (SRK) and the Peng-Robinson equations of state are both "cubic" equations of state developed to improve the Redlich-Kwong form. Both approaches have used the same method to set the parameters a and b . That is,

TABLE 1.1. Summary of Four Common “Cubic” Equations of State and their Constants

Equation	u	w	b	a
Van der Waals	0	0	$\frac{R_u T_c}{8P_c}$	$\frac{27 R_u^2 T_c^2}{64 P_c}$
Redlich-Kwong	1	0	$\frac{0.08664 R_u T_c}{P_c}$	$\frac{0.42748 R_u^2 T_c^{2.5}}{P_c T^{0.5}}$
Soave or Soave-Redlich-Kwong (SRK)	1	0	$\frac{0.08664 R_u T_c}{P_c}$	$\frac{0.42748 R_u^2 T_c^2}{P_c} [1 + f(\omega)(1 - T_r^{0.5})]^2$ where $f(\omega) = 0.48 + 1.574\omega - 0.176\omega^2$
Peng-Robinson	2	-1	$\frac{0.07780 R_u T_c}{P_c}$	$\frac{0.42748 R_u^2 T_c^2}{P_c} [1 + f(\omega)(1 - T_r^{0.5})]^2$ $f(\omega) = 0.37464 + 1.5423\omega - 0.26992\omega^2$

Note: Values of ω for various substances can be found in Appendix A of R.C. Reid, J. M. Prausnitz and B.E. Poling, *The Properties of Gases and Liquids*, 4th ed., McGraw Hill, 1987.

both the first and second partial derivatives of pressure with respect to specific volume are set to zero, as was done previously for the Redlich-Kwong equation of state. For brevity, the cubic form of the equations and their coefficients are provided in Table 1.1 for common cubic equations of state.

The last four equations of state discussed above can be classified as cubic equations of state; that is, if expanded, the equations would contain volume terms raised to the first, second, or third power. These equations (containing two parameters a and b) can be expressed by the following equation:

$$p = \frac{R_u T}{\bar{v} - b} - \frac{a}{\bar{v}^2 + ub\bar{v} + wb^2} \quad (1.11)$$

More detailed discussion of the equation of state and the mixing rules for multi-component mixtures are given in Appendix A of Kuo (2005).

1.7 DEFINITIONS OF CONCENTRATIONS

There are four ways to express concentration of various species in a multicomponent gas mixture:

1. Mass concentration ρ_i is the mass of the i^{th} species per unit volume of mixture or solution;
2. Molar concentration $C_i \equiv \rho_i/Mw_i$ is the number of moles of the i^{th} species per unit volume.
3. Mass fraction $Y_i \equiv \rho_i/\rho = m_i/m_t$ is the mass of the i^{th} species divided by the total mass of the mixture.

4. Mole fraction $X_i \equiv C_i/C$ is the molar concentration of the i^{th} species divided by the total molar concentration of the gaseous mixture or liquid solution.

Mole Numbers: Gaseous molecules and atoms are conveniently counted in terms of amount of substances or mole numbers. One mole (1 mol) of compound corresponds to 6.02252×10^{23} molecules (or atoms). Avogadro's number (N_A) is therefore 6.02252×10^{23} molecules/mol.

Mole Fractions:

$$X_i = \frac{n_i}{N} = \frac{n_i}{\sum_{i=1}^N n_i} \quad (1.12)$$

Mass Fractions:

$$Y_i = \frac{m_i}{N} = \frac{m_i}{\sum_{i=1}^N m_i} \quad (1.13)$$

Average Molecular Weight:

The mole fraction X_i and mass fraction Y_i are related by: $X_i = Y_i (\overline{Mw}/Mw_i)$, where \overline{Mw} is the average molecular weight of the multicomponent gas mixture in the control volume. It can be evaluated by:

$$\overline{Mw} = \sum_{i=1}^N X_i Mw_i = 1 / \sum_{i=1}^N (Y_i / Mw_i) \quad (1.14)$$

The relationship's between Y_i and X_i are given below.

$$Y_i = \frac{Mw_i n_i}{\sum_{j=1}^N Mw_j n_j} = \frac{Mw_i X_i}{\sum_{j=1}^N Mw_j X_j} = \frac{Mw_i X_i}{\overline{Mw}} \quad (1.15)$$

$$X_i = \frac{Y_i \overline{Mw}}{Mw_i} = \frac{Y_i}{Mw_i} / \sum_{j=1}^N \frac{Y_j}{Mw_j} \quad (1.16)$$

Fuel-Oxidant Ratio, F/O:

$$F/O \equiv \frac{F}{O} = \frac{\text{mass of fuel}}{\text{mass of oxidant}} \quad (1.17)$$

Equivalence Ratio:

$$\phi = \frac{(F/O)}{(F/O)_{\text{st}}} \quad \begin{cases} 0 < \phi < 1 & \text{fuel-lean} \\ \phi = 1 & \text{stoichiometric condition} \\ 1 < \phi < \infty & \text{fuel-rich} \end{cases} \quad (1.18)$$

TABLE 1.2. Definitions of Mass Fractions, Mole Fractions, Molar Concentrations, and Useful Relations

Quantity	Physical Definition	Mathematical Expression
Mass fraction, Y_i	Mass of i^{th} species/Total Mass	$Y_i = m_i/m_t$
Mole fraction, X_i	Moles of i^{th} species/Total number of moles	$X_i \equiv n_i/n_t = Y_i (\overline{Mw}/Mw_i)$
Molar concentration, C_i	Moles of i^{th} species/Total volume	$C_i \equiv n_i/V_t = \bar{\rho} (Y_i/Mw_i)$ $= \bar{\rho} (X_i/\overline{Mw})$

The next sections provide readers with basic definitions of many important parameters utilized in the conservation equations as well as various forms of these equations in different coordinate systems. The detailed derivation of these conservation equations is given in Kuo (2005), Chap. 3. The physical meaning of various terms in the conservation equations are also described in these sections.

1.8 DEFINITIONS OF ENERGY AND ENTHALPY FORMS

Several definitions of energy are useful in the conservation equations. It is very important to have a clear understanding of the physical meaning and mathematical expression of each of these energy forms as well as their relationships with each other. Sensible internal energy of i^{th} species ($e_{s,i}$) can be determined with temperature measurements; therefore, it is called *sensible*. When the heat of formation of the i^{th} species is added to the sensible internal energy, their sum is represented by e_i as shown in Table 1.3. The total internal energy of the i^{th} species ($e_{t,i}$) includes sensible, kinetic, and chemical energies. The total nonchemical energy ($e_{inc,i}$) includes sensible and kinetic energies only, as shown in Table 1.3. The same definitions are used for enthalpy terms.

TABLE 1.3. Definitions of Internal Energy and Enthalpy Forms of the i^{th} Species

Quantity	Internal Energy	Enthalpy
Sensible	$e_{s,i} = \int_{T_{ref}}^T C_{v,i} dT + \underbrace{e_{s,i}(T_{ref})}_{=-R_u T_{ref}/Mw_i}$	$h_{s,i} = \int_{T_{ref}}^T C_{p,i} dT + \underbrace{h_{s,i}(T_{ref})}_{=0}$
Sensible + chemical	$e_i = e_{s,i} + \Delta h_{f,i}^0 = \int_{T_{ref}}^T C_{v,i} dT + \Delta e_{f,i}^0$	$h_i = h_{s,i} + \Delta h_{f,i}^0$
Total	$e_{t,i} = e_i + \frac{u_j u_j}{2}$	$h_{t,i} = h_i + \frac{u_j u_j}{2}$
Total non-chemical	$e_{inc,i} = e_{s,i} + \frac{u_j u_j}{2}$	$h_{inc,i} = h_{s,i} + \frac{u_j u_j}{2}$

The enthalpy and internal energies are related by:

$$e_{s,i} = h_{s,i} - p_i/\rho_i \quad (1.19)$$

$$e_i = h_i - p_i/\rho_i \quad (1.20)$$

$$h_i = h_{s,i} + \Delta h_{f,i}^0 = \int_{T_{ref}}^T C_{p,i} dT + \underbrace{h_{s,i}(T_{ref})}_{=0} + \Delta h_{f,i}^0 \quad (1.21)$$

The sensible internal energy is defined to satisfy $h_{s,i} = e_{s,i} + p_i/\rho_i$. The sensible internal energy for the i^{th} species is defined as:

$$e_{s,i} = \int_{T_{ref}}^T C_{v,i} dT + e_{s,i}(T_{ref}) \quad (1.22)$$

Since at reference temperature of 298.15 K, the sensible enthalpy is defined to be zero, that is, $h_{s,i}(T_{ref}) = 0$, we can conclude from Equation 1.19 that $e_{s,i}(T_{ref}) = -p_i/\rho_i = -R_u T_{ref}/Mw_i$. Thus,

$$e_i = e_{s,i} + \Delta e_{f,i}^0 = h_i - \frac{p_i}{\rho_i} = h_{s,i} + \Delta h_{f,i}^0 - \frac{p_i}{\rho_i} = e_{s,i} + \Delta h_{f,i}^0 \quad (1.23)$$

Therefore,

$$\Delta e_{f,i}^0 = \Delta h_{f,i}^0 \quad (1.24)$$

The mass-based enthalpy of formation of the k^{th} species ($\Delta h_{f,i}^0$) is related to the molar enthalpy of formation ($\Delta h_{f,i}^{0,m}$) by Equation 1.25.

$$\Delta h_{f,i}^0 = \Delta h_{f,i}^{0,m}/Mw_i \quad (1.25)$$

The negative value of the enthalpy of formation indicates that when 1 mole of i^{th} species is formed from its elements at the standard state of $T_{ref} = 298.15$ K and $p = 1$ bar, there is exothermic heat release. The standard state of an element is the stable form of that element at room temperature and 1 bar pressure. For example, $\text{H}_{2(\text{g})}$, $\text{O}_{2(\text{g})}$, $\text{N}_{2(\text{g})}$, $\text{Hg}_{(\text{l})}$, $\text{C}_{(\text{s, graphite})}$ are called elements in thermochemical terms. Heats of formation of various compounds are tabulated in various sources. For example, see Kuo (2005), Chap. 1.

The mass-based constant-pressure heat capacities ($C_{p,i}$) of the i^{th} species is related to the molar heat capacities ($C_{p,i}^m$) by:

$$C_{p,i} = C_{p,i}^m/Mw_i \quad (1.26)$$

For a perfect diatomic gas:

$$C_{p,i}^m = 3.5R_u \quad \text{and} \quad C_{p,i} = 3.5R_u/Mw_i \quad (1.27)$$

In many combustion problems, the change of $C_{p,i}$ with T is quite significant in chemically reacting flows. $C_{p,i}$ values usually are tabulated as polynomial

functions of temperature (see JANAF tables compiled by Stull and Prophet, 1971). Usually the C_p increases with temperature due to an increase in the stored internal energies of different modes, including vibrational, rotational, and translational modes at higher temperatures. Near room temperature, the molar heat capacity of diatomic gases such as N_2 and H_2 are very close to $3.5R_u$; however, their heat capacities increase rapidly at high temperatures.

The mass-based and molar-based constant-volume specific heats are related to the constant-pressure specific heats by:

$$C_{v,i} = C_{p,i} - R_u/MW_i \quad \text{or} \quad C_{v,i}^m = C_{p,i}^m - R_u \quad (1.28)$$

The constant-pressure heat capacity of the mixture C_p is defined by:

$$C_p = \sum_{i=1}^N C_{p,i} Y_i = \sum_{i=1}^N C_{p,i}^m \frac{Y_i}{MW_i} \quad (1.29)$$

The constant-volume heat capacity of the mixture C_v is defined by:

$$C_v = \sum_{i=1}^N Y_i C_{v,i} = \sum_{i=1}^N Y_i \frac{C_{v,i}^m}{MW_i} \quad (1.30)$$

The specific enthalpy of the mixture is defined by:

$$h = \sum_{i=1}^N h_i Y_i = \sum_{i=1}^N Y_i \left(\int_{T_{ref}}^T C_{p,i} dT + \Delta h_{f,i}^o \right) = \int_{T_{ref}}^T C_p dT + \sum_{i=1}^N Y_i \Delta h_{f,i}^o \quad (1.31)$$

The specific internal energy of the mixture $e = h - p/\rho$ can be written as:

$$\begin{aligned} e &= \sum_{i=1}^N Y_i \left(\underbrace{\int_{T_{ref}}^T C_{p,i} dT}_{h_{s,i}} - \underbrace{R_u T / MW_i}_{p_i / \rho_i} + \Delta h_{f,i}^o \right) \\ &= \sum_{i=1}^N Y_i e_i = \sum_{i=1}^N Y_i \left(\underbrace{\int_{T_{ref}}^T C_{v,i} dT - R_u T_{ref} / MW_i}_{e_{s,i}} + \Delta h_{f,i}^o \right) \\ &= \underbrace{\int_{T_{ref}}^T C_v dT}_{e_s} - R_u T_{ref} / \bar{M}w + \sum_{i=1}^N Y_i \Delta h_{f,i}^o \end{aligned} \quad (1.32)$$

Table 1.4 summarizes the definitions of different forms of energy and enthalpy of the mixture containing multi-component chemical species.

TABLE 1.4. Definitions of Different Forms of Energy and Enthalpy

Quantity	Energy	Enthalpy
Sensible	$e_s = \int_{T_{ref}}^T C_v dT + \underbrace{e_s(T_{ref})}_{=-R_u T_{ref}/\bar{M}w}$	$h_s = \int_{T_{ref}}^T C_p dT + \underbrace{h_s(T_{ref})}_{=0}$
Sensible + chemical	$e = e_s + \sum_{i=1}^N Y_i \Delta h_{f,i}^o$	$h = h_s + \sum_{i=1}^N Y_i \Delta h_{f,i}^o$
Total	$e_t = e + \frac{u_j u_j}{2}; \quad j = 1, 2, 3$	$h_t = h + \frac{u_j u_j}{2}; \quad j = 1, 2, 3$
Total nonchemical	$e_{inc} = e_s + \frac{u_j u_j}{2}; \quad j = 1, 2, 3$	$h_{inc} = h_s + \frac{u_j u_j}{2}; \quad j = 1, 2, 3$

1.9 VELOCITIES OF CHEMICAL SPECIES

In a multicomponent system, various chemical species move at different average velocities. For a mixture of N species with respect to the stationary coordinate axis, the local mass-average velocity \mathbf{v} can be defined as:

$$\mathbf{v} = \frac{\sum_{i=1}^N \rho_i \mathbf{v}_i}{\sum_{i=1}^N \rho_i} = \frac{\sum_{i=1}^N \rho_i \mathbf{v}_i}{\rho} = \sum_{i=1}^N Y_i \mathbf{v}_i \quad (1.33)$$

The local molar-average velocity \mathbf{v}^* can be defined as

$$\mathbf{v}^* = \frac{\sum_{i=1}^N C_i \mathbf{v}_i}{\sum_{i=1}^N C_i} = \frac{\sum_{i=1}^N C_i \mathbf{v}_i}{C} = \sum_{i=1}^N X_i \mathbf{v}_i \quad (1.34)$$

The molar-averaged velocity \mathbf{v}^* differs from the mass-averaged velocity \mathbf{v} in both magnitude and direction. Often we are interested in velocity of a given species with respect to the bulk mass-averaged or molar-averaged velocity rather than with respect to stationary coordinates. Therefore, two *diffusion velocities* are introduced.

- Mass diffusion velocity of the i^{th} species is defined as:

$$\mathbf{V}_i \equiv \mathbf{v}_i - \mathbf{v} \quad (1.35)$$

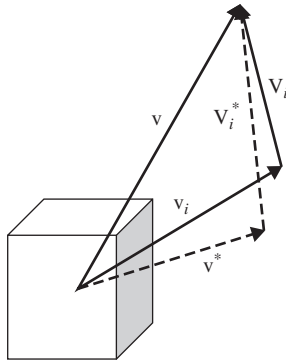


Figure 1.6 Vector description of various local velocities in a multispecies system.

TABLE 1.5. Definitions of diffusion velocities

Quantity	Physical Definition	Mathematical Expression
Mass diffusion velocity of i^{th} species	$\mathbf{V}_i \equiv \mathbf{v}_i - \mathbf{v}$, where \mathbf{v} is local mass-average velocity	$\mathbf{v} = \frac{\sum_{i=1}^N \rho_i \mathbf{v}_i}{\sum_{i=1}^N \rho_i} = \frac{\sum_{i=1}^N \rho_i \mathbf{v}_i}{\rho} = \sum_{i=1}^N Y_i \mathbf{v}_i$
Molar diffusion velocity of i^{th} species	$\mathbf{V}_i^* \equiv \mathbf{v}_i - \mathbf{v}^*$, where \mathbf{v}^* is local molar-average velocity	$\mathbf{v}^* = \frac{\sum_{i=1}^N C_i \mathbf{v}_i}{\sum_{i=1}^N C_i} = \frac{\sum_{i=1}^N C_i \mathbf{v}_i}{C} = \sum_{i=1}^N X_i \mathbf{v}_i$

- Molar diffusion velocity of the i^{th} species is defined as:

$$\mathbf{V}_i^* \equiv \mathbf{v}_i - \mathbf{v}^* \tag{1.36}$$

These diffusion velocities indicate average motion of component i relative to the local motion of the mixture in the control volume. These velocity components are shown in Fig. 1.6 and also summarized in Table 1.5.

1.9.1 Definitions of Absolute and Relative Mass and Molar Fluxes

Absolute mass or molar flux of species i is a vector quantity denoting the mass or number of moles of species i that passes through a unit area per unit time. They are defined as:

$$\dot{\mathbf{m}}_i \equiv \rho_i \mathbf{v}_i \text{ (mass flux)} \tag{1.37}$$

$$\dot{\mathbf{n}}_i \equiv C_i \mathbf{v}_i \text{ (molar flux)} \tag{1.38}$$

Relative mass and molar fluxes are defined as:

$$\mathbf{J}_i \equiv \rho_i (\mathbf{v}_i - \mathbf{v}) = \rho_i \mathbf{V}_i \quad (1.39)$$

$$\mathbf{J}_i^* \equiv C_i (\mathbf{v}_i - \mathbf{v}^*) = C_i \mathbf{V}_i^* \quad (1.40)$$

In a multicomponent system, the relative molar flux \mathbf{J}_i^* and absolute molar flux $\dot{\mathbf{n}}_i$ are related to each other. From the definitions of \mathbf{v}^* and \mathbf{J}_i^*

$$\mathbf{J}_i^* \equiv C_i (\mathbf{v}_i - \mathbf{v}^*) = C_i \mathbf{v}_i - \frac{C_i}{C} \sum_{j=1}^N C_j \mathbf{v}_j \quad (1.41)$$

From the definitions of $\dot{\mathbf{n}}_i$ and X_i

$$\mathbf{J}_i^* = \dot{\mathbf{n}}_i - X_i \sum_{j=1}^N \dot{\mathbf{n}}_j \quad (1.42)$$

Summation of Equation 1.42 from $i = 1$ to $i = N$ gives

$$\sum_{i=1}^N \mathbf{J}_i^* = 0 \quad (1.43)$$

Fick's Law of Diffusion In a binary system with two chemical species, species A always diffuses in the direction from high concentration of A to low concentration of A, and species B always diffuses from high concentration of B to low concentration of B. The binary mass diffusivity can be expressed by D_{BA} or D_{AB} with dimensions of (L^2/t), usually given in (m^2/s). Fick's first law of diffusion in terms of molar diffusion flux \mathbf{J}_A^* for the binary system is:

$$\mathbf{J}_A^* = -C D_{AB} \nabla X_A \quad (1.44)$$

Equation 1.44 states that species A diffuses in the direction of decreasing mole fraction of A. This is similar to heat transfer by conduction in the direction of decreasing temperature. Molar flux relative to stationary coordinates can now be given as the sum of two molar fluxes

$$\dot{\mathbf{n}}_A = C_A \mathbf{v}^* - C D_{AB} \nabla X_A \quad (1.45)$$

The first term represents the molar flux of A from the bulk motion of the fluid, while the second term with the minus sign represents the relative molar flux of A resulting from the diffusion of species A. In terms of mass flux relative to stationary coordinates, Fick's law also can be written as the sum of two mass fluxes:

$$\dot{\mathbf{m}}_A = \rho_A \mathbf{v} - \rho D_{AB} \nabla Y_A \quad (1.46)$$

where $\mathbf{J}_A = -\rho D_{AB} \nabla Y_A$

Note that the mathematical form of Fick’s law of mass transport for a constant density situation in the transverse direction (y -direction) of a binary system is similar to Newton’s law of momentum transport and Fourier’s law of energy transport in the transverse direction.

$$q_y = -\alpha \frac{\partial}{\partial y} (\rho C_p T) \quad (\text{Fourier's law for constant } \rho C_p) \quad (1.47)$$

$$\tau_{yx} = -v \frac{\partial}{\partial y} (\rho v_x) \quad (\text{Newton's law for constant } \rho) \quad (1.48)$$

$$\mathbf{J}_{Ay} = -D_{AB} \frac{\partial}{\partial y} (\rho_A) \quad (\text{Fick's law for constant } \rho) \quad (1.49)$$

Mass diffusivity D_{AB} for binary mixtures of nonpolar gases (without any dipole moments) is predictable within about 5% by kinetic theory. For a nonpolar gas containing two molecular species A and A* with the same mass m_A and the same size and shape, with constant temperature T and molar concentration C , the random motion molecular velocity relative to fluid velocity \mathbf{v} has an average magnitude:

$$\bar{u} = \sqrt{\frac{8 k_B T}{\pi m_A}} \quad (1.50)$$

where

$$k_B = \text{Boltzmann constant} = R_u / N_A$$

with the Avogadro’s number, $N_A = 6.02252 \times 10^{23}$ molecules/mol, and universal gas constant, $R_u = 8.3144$ J/(mol · K). A schematic representation of the bulk and random velocities is shown in Fig. 1.7.

The frequency of molecular collisions per unit area (Z) on a stationary surface exposed to the gas is

$$Z = \frac{1}{4} \tilde{n} \bar{u} \quad (1.51)$$

where \tilde{n} represents molecules per unit volume, which is constant since the molar concentration C is constant and $\tilde{n} = C \times N_A$. The mean free path l from kinetic theory is

$$l = \frac{1}{\sqrt{2} \pi d_A^2 \tilde{n}} \quad (1.52)$$

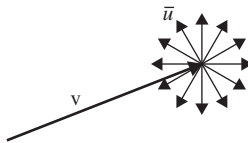


Figure 1.7 Schematic representation of bulk and random velocities.

where d_A is the diameter of the molecule A. The new molar flux equation corresponds to Fick's law of diffusion in the y -direction, with D_{AA^*} approximately given by

$$D_{AA^*} = \frac{1}{3} \bar{u} l \quad (1.53)$$

Substituting for \bar{u} and l into Equation 1.53, we have

$$D_{AA^*} = \frac{1}{3} \sqrt{\frac{8 k_B T}{\pi m_A}} \frac{1}{\sqrt{2\pi} d_A^2 \tilde{n}} = \frac{2}{3} \sqrt{\frac{k_B^3 T^{3/2}}{\pi^3 m_A d_A^2}} \frac{1}{\tilde{n} k_B T} \quad (1.54)$$

Further substitution using the perfect gas law $p = C R_u T = \tilde{n} k_B T$ allows calculation of an approximate value for D_{AA^*} from

$$D_{AA^*} = \frac{2}{3} \sqrt{\frac{k_B^3 T^{3/2}}{\pi^3 m_A p d_A^2}} \propto \frac{T^{3/2}}{p} \quad (1.55)$$

D_{AA^*} represents the mass diffusivity of a mixture of two species of rigid spheres of identical mass and diameter. Calculation of D_{AB} for rigid spheres of unequal mass and diameter results in

$$D_{AB} = \frac{2}{3} \left(\frac{k_B^3}{\pi^3} \right)^{1/2} \left(\frac{1}{2m_A} + \frac{1}{2m_B} \right)^{1/2} \frac{T^{3/2}}{p \left(\frac{d_A + d_B}{2} \right)^2} \quad (1.56)$$

1.10 DIMENSIONLESS NUMBERS

Mass diffusivity (D), momentum diffusivity (ν), and thermal diffusivity (α) all have the same dimensions. Schmidt number, Prandtl number, and Lewis number can then be defined as the ratios between these quantities (see Table 1.6).

$$\text{Sc} \equiv \nu/D \quad (1.57)$$

$$\text{Pr} \equiv \nu/\alpha \quad (1.58)$$

$$\text{Le} \equiv \alpha/D \quad (1.59)$$

1.11 DERIVATION OF SPECIES MASS CONSERVATION EQUATION AND CONTINUITY EQUATION FOR MULTICOMPONENT MIXTURES

We start with a mass balance over an infinitesimal differential fluid element in a binary mixture to derive the mass conservation equation of each species in a multicomponent mixture. We then apply the law of conservation of mass of species A to a volume element $\Delta x \Delta y \Delta z$ fixed in space through which a binary mixture of A and B is flowing (see Fig. 1.8).

TABLE 1.6. Definitions of Three Important Dimensional Numbers

Quantity	Physical Meaning	Mathematical Definition
Schmidt number	Ratio of momentum transport to mass transport	$Sc \equiv \nu/D$
Prandtl number	Ratio of momentum transport to thermal transport	$Pr \equiv \nu/\alpha$
Lewis number	Ratio of thermal transport to mass transport	$Le \equiv \alpha/D$

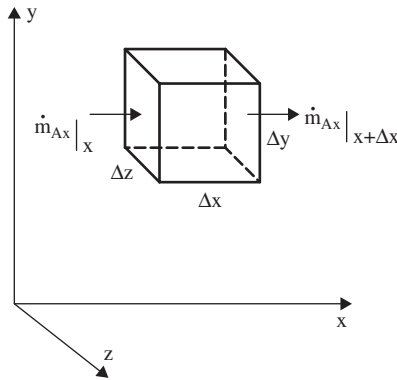


Figure 1.8 Fixed infinitesimal control volume $\Delta x \Delta y \Delta z$ through which a fluid is flowing.

The rate of accumulation of mass of species A is:

$$\frac{\partial \rho_A}{\partial t} \Delta x \Delta y \Delta z$$

The rate of mass of species A flowing into the control volume due to the x -direction mass flux at the x station is:

$$\dot{m}_{Ax}|_x \Delta y \Delta z$$

The rate of mass of species A flowing out of the control volume due to the x -direction mass flux at the $x + \Delta x$ station is:

$$\dot{m}_{Ax}|_{x+\Delta x} \Delta y \Delta z = \dot{m}_{Ax}|_x \Delta y \Delta z + \frac{\partial \dot{m}_{Ax}}{\partial x} \Delta x \Delta y \Delta z$$

Within this infinitesimal control volume, species A can be produced by chemical reactions at a net rate of $\dot{\omega}_A$ ($\text{kg m}^{-3}\text{s}^{-1}$). The net rate of production of species A by chemical reactions is:

$$\dot{\omega}_A \Delta x \Delta y \Delta z$$

Adding the input and output terms in the y and z directions and dividing the entire mass balance by $\Delta x \Delta y \Delta z$, it yields:

$$\frac{\partial \rho_A}{\partial t} + \left(\frac{\partial \dot{m}_{Ax}}{\partial x} + \frac{\partial \dot{m}_{Ay}}{\partial y} + \frac{\partial \dot{m}_{Az}}{\partial z} \right) = \dot{\omega}_A \quad (1.60)$$

which is the *mass conservation equation of species A* in a binary mixture. Equation 1.60 can be rewritten in a vector form as:

$$\frac{\partial \rho_A}{\partial t} + (\nabla \cdot \dot{\mathbf{m}}_A) = \dot{\omega}_A \quad (1.61)$$

where $\dot{\mathbf{m}}_A = (\dot{m}_{Ax}, \dot{m}_{Ay}, \dot{m}_{Az})$ is the mass flux vector with $\dot{m}_{Ax}, \dot{m}_{Ay}, \dot{m}_{Az}$ components in rectangular coordinates.

Similarly, the mass conservation equation of species B is

$$\frac{\partial \rho_B}{\partial t} + (\nabla \cdot \dot{\mathbf{m}}_B) = \dot{\omega}_B \quad (1.62)$$

When the equations of continuity for components A and B are added together, the result is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (1.63)$$

which is the *equation of continuity for the mixture*. This equation makes use of the relation $\dot{\mathbf{m}}_A + \dot{\mathbf{m}}_B = \rho \mathbf{v}$ and the law of conservation of mass in the form $\dot{\omega}_A + \dot{\omega}_B = 0$, since the combustion process does not produce or destroy mass. The combustion process converts one group of species (reactants) into another group of species (products).

Substituting the mass flux term ($\dot{\mathbf{m}}_A$) in Equation 1.61 by using Fick's law shown in Equation 1.46, we have:

$$\frac{\partial \rho_A}{\partial t} + \nabla \cdot \rho_A \mathbf{v} = \nabla \cdot \rho D_{AB} \nabla Y_A + \dot{\omega}_A \quad (1.64)$$

Using the relationships that $\rho_i = Y_i \rho$ and $\mathbf{v}_i = \mathbf{v} + \mathbf{V}_i$ for a multicomponent system, Equation 1.61 can be generalized into this form:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot [\rho Y_i (\mathbf{v} + \mathbf{V}_i)] = \dot{\omega}_i \quad (1.65)$$

The divergence form in Equation 1.65 can be reduced to the Euler form by first expanding parts of the terms on the left-hand side

$$\rho \frac{\partial Y_i}{\partial t} + Y_i \frac{\partial \rho}{\partial t} + Y_i \nabla \cdot (\rho \mathbf{v}) + \rho \mathbf{v} \cdot \nabla Y_i + \nabla \cdot (\rho Y_i \mathbf{V}_i) = \dot{\omega}_i \quad (1.66)$$

Then, using the overall continuity equation, the Euler form is obtained

$$\rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{v} \cdot \nabla Y_i + \nabla \cdot (\rho Y_i \mathbf{V}_i) = \dot{\omega}_i \quad i = 1, 2, \dots, N \quad (1.67)$$

In a general multicomponent system, there are N equations of the Euler form. All values of Y_i are considered as unknown in the numerical solution. It is not necessary to solve all N partial differential equations for Y_i , since

$$\sum_{i=1}^N Y_i = 1 \quad (1.68)$$

This allows one of the N species conservation equations to be replaced by the above algebraic Equation 1.68.

Usually $N - 1$ independent equations for Y_i are solved with other conservation equations for the chemically reacting mixture.

Using C_A for molar concentration and $\dot{\Omega}_A$ for the molar rate of production per unit volume, the continuity (or mass conservation) equation for species A can be written as:

$$\frac{\partial C_A}{\partial t} + \nabla \cdot \mathbf{n}_A = \dot{\Omega}_A \quad (1.69)$$

Substituting the molar flux equation yields

$$\frac{\partial C_A}{\partial t} + \nabla \cdot C_A \mathbf{v}^* = \nabla \cdot CD_{AB} \nabla X_A + \dot{\Omega}_A \quad (1.70)$$

In a generalized form, the species conservation equation for the i^{th} species in terms of molar concentration can be written as:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{n}_i = \dot{\Omega}_i \quad (1.71)$$

Substituting the molar flux equation yields

$$\frac{\partial C_i}{\partial t} + \nabla \cdot C_i \mathbf{v}^* = \nabla \cdot CD_{im} \nabla X_i + \dot{\Omega}_i \quad (1.72)$$

In the Equation 1.72, D_{im} is the mass diffusivity of the i^{th} species with respect to the rest of the mixture.

A detailed treatment of diffusion velocity representations and mass diffusivities is given in Chapter 2, where the equations for D_{im} are also shown. It is also shown that a correction velocity \mathbf{V}_c is required in order to satisfy the overall mass conservation. By summing over all the species from 1 to N , the summed species conservation equation is:

$$\sum_{i=1}^N \frac{\partial (\rho Y_i)}{\partial t} + \sum_{i=1}^N \nabla \cdot [\rho Y_i (\mathbf{v} + \mathbf{V}_i)] = \sum_{i=1}^N \dot{\omega}_i \quad (1.73)$$

Taking the summation inside, we get:

$$\frac{\partial}{\partial t} \left(\rho \sum_{i=1}^N Y_i \right) + \nabla \cdot \left[\rho \left(\mathbf{v} \sum_{i=1}^N Y_i + \sum_{i=1}^N Y_i \mathbf{V}_i \right) \right] = \sum_{i=1}^N \dot{\omega}_i$$

or

$$\underbrace{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v})}_{=0} + \nabla \cdot \left[\rho \left(\sum_{i=1}^N Y_i \mathbf{V}_i \right) \right] = 0$$

This equation implies that the next relationship must be satisfied by the diffusion velocity definition to achieve overall mass conservation:

$$\sum_{i=1}^N Y_i \mathbf{V}_i = 0 \quad (1.74)$$

Readers should refer to Section 2.1 of Chapter 2 to understand the requirement for a correction velocity and the derivation of the expression for a correction velocity. For convenience, the correction velocity expression is given next:

$$\mathbf{V}_c = - \sum_{i=1}^N Y_i \mathbf{V}_i \quad (1.75)$$

With this correction velocity, the species conservation equation then becomes:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot [\rho Y_i (\mathbf{v} + \mathbf{V}_i + \mathbf{V}_c)] = \dot{\omega}_i \quad (1.76)$$

Different models for \mathbf{V}_i by using multicomponent species diffusion, the Hirschfelder-Curtiss approximation, Fick's law, the constant Lewis number for the i^{th} species, or unity Lewis number approaches are shown in Table 2.1 of Chapter 2.

A summary of overall mass conservation equation (or continuity equation) in different coordinate systems is given in Table 1.7.

TABLE 1.7. Equation of Continuity in Several Coordinate Systems

Rectangular coordinates (x, y, z) :

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) + \frac{\partial}{\partial y} (\rho u_y) + \frac{\partial}{\partial z} (\rho u_z) = 0 \quad (1.77)$$

Cylindrical coordinates (r, θ, z) :^a

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho r u_r) + \frac{1}{r} \frac{\partial}{\partial \theta} (\rho u_\theta) + \frac{\partial}{\partial z} (\rho u_z) = 0 \quad (1.78)$$

Spherical coordinates (r, θ, ϕ) :^b

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\rho u_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\rho u_\phi) = 0 \quad (1.79)$$

^a $r \geq 0, 2\pi \geq \theta \geq 0.$

^b $r \geq 0, 2\pi \geq \phi \geq 0, \pi \geq \theta \geq 0.$

A summary of species mass conservation equation in different coordinate systems is given in Table 1.8.

In the model of Hirschfelder, Curtiss, and Bird (1954), an approximate diffusion coefficient for i^{th} species against the rest of the mixture is calculated by the following equation:

$$D_{im}^* = (1 - Y_i) \left(\frac{1}{Mw} \sum_{j=1, j \neq i}^N \frac{Y_j}{Mw_j D_{ij}} \right)^{-1} = \frac{(1 - Y_i)}{\sum_{j=1, j \neq i}^N X_j / D_{ij}} \quad (1.80)$$

TABLE 1.8. Mass Conservation Equation for i^{th} Species in Several Coordinate Systems

Rectangular coordinates (x, y, z) :

$$\begin{aligned} & \rho \left(\frac{\partial Y_i}{\partial t} + u_x \frac{\partial Y_i}{\partial x} + u_y \frac{\partial Y_i}{\partial y} + u_z \frac{\partial Y_i}{\partial z} \right) \\ & + \frac{\partial}{\partial x} (\rho Y_i V_{ix}) + \frac{\partial}{\partial y} (\rho Y_i V_{iy}) + \frac{\partial}{\partial z} (\rho Y_i V_{iz}) \\ & + \frac{\partial}{\partial x} (\rho Y_i V_{c,x}) + \frac{\partial}{\partial y} (\rho Y_i V_{c,y}) + \frac{\partial}{\partial z} (\rho Y_i V_{c,z}) = \dot{\omega}_i \end{aligned} \quad (1.81)$$

Mass diffusion velocities by Hirschfelder-Curtiss approximation:

$$V_{ix} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial x}, \quad V_{iy} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial y}, \quad V_{iz} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial z}$$

Cylindrical coordinates (r, θ, z) :

$$\begin{aligned} & \rho \left(\frac{\partial Y_i}{\partial t} + u_r \frac{\partial Y_i}{\partial r} + \frac{u_\theta}{r} \frac{\partial Y_i}{\partial \theta} + u_z \frac{\partial Y_i}{\partial z} \right) \\ & + \frac{1}{r} \frac{\partial}{\partial r} (r \rho Y_i V_{ir}) + \frac{1}{r} \frac{\partial}{\partial \theta} (r \rho Y_i V_{i\theta}) + \frac{\partial}{\partial z} (\rho Y_i V_{iz}) \\ & + \frac{1}{r} \frac{\partial}{\partial r} (r \rho Y_i V_{c,r}) + \frac{1}{r} \frac{\partial}{\partial \theta} (r \rho Y_i V_{c,\theta}) + \frac{\partial}{\partial z} (\rho Y_i V_{c,z}) = \dot{\omega}_i \end{aligned} \quad (1.82)$$

Mass diffusion velocities by Hirschfelder-Curtiss approximation:

$$V_{ir} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial r}, \quad V_{i\theta} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{r \partial \theta}, \quad V_{iz} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial z}$$

TABLE 1.8. (continued)

 Spherical coordinates (r, θ, ϕ) :

$$\begin{aligned}
 & \rho \left(\frac{\partial Y_i}{\partial t} + u_r \frac{\partial Y_i}{\partial r} + \frac{u_\theta}{r} \frac{\partial Y_i}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial Y_i}{\partial \phi} \right) \\
 & + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho Y_i V_{ir}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho Y_i V_{i\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\rho Y_i V_{i\phi}) \\
 & + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho Y_i V_{c,r}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \rho Y_i V_{c,\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\rho Y_i V_{c,\phi}) = \dot{\omega}_i
 \end{aligned} \tag{1.83}$$

Mass diffusion velocities by Hirschfelder-Curtiss approximation:

$$V_{ir} = -\frac{D_{im}^*}{Y_i} \frac{\partial Y_i}{\partial r}, \quad V_{i\theta} = -\frac{D_{im}^*}{Y_i r} \frac{\partial Y_i}{\partial \theta}, \quad V_{i\phi} = -\frac{D_{im}^*}{Y_i r \sin \theta} \frac{\partial Y_i}{\partial \phi}$$

1.12 MOMENTUM CONSERVATION EQUATION FOR MIXTURE

In this section we present the momentum equations in the form of partial differential equations. The basic assumption is that we are dealing with continuous, isotropic, homogeneous, and Newtonian fluids. For Newtonian fluids, there is a linear relationship between shear stress and rate of deformation. Readers interested in the derivation of the momentum equation by various approaches are referred to Kuo (2005), Chap. 3.

For a Newtonian fluid, the stress tensor can be written as:

$$\sigma_{ij} = -p\delta_{ij} + \tau_{ij} = -p\delta_{ij} + \left[\left(\mu' - \frac{2}{3}\mu \right) \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \tag{1.84}$$

In this constitutive relationship between stress and strain rate, the coefficient μ is usually called the dynamic viscosity or the first viscosity and μ' is called the bulk viscosity. For monatomic gas mixtures, kinetic theory shows that $\mu' = 0$. For most practical purposes, μ' can be treated as zero. In Equation 1.84, the Kronecker delta function, δ_{ij} , is defined in such way that

$$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \tag{1.85}$$

In Equation 1.84, the total stress tensor is expressed as a sum of the hydrostatic pressure component and the viscous stress component, which is further expressed in terms of the volume dilatation contribution due to $(\partial u_k / \partial x_k)$ and strain-rate tensor e_{ij} contribution, where

$$e_{ij} \equiv (\partial u_i / \partial x_j + \partial u_j / \partial x_i) / 2 \tag{1.86}$$

The i^{th} direction momentum equation can be written in the Euler form as:

$$\underbrace{\rho \left[\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right]}_{\text{Inertial force}} = \frac{\partial \sigma_{ji}}{\partial x_j} + B_i = \underbrace{-\frac{\partial p}{\partial x_i}}_{\text{Pressure gradient force}} + \underbrace{\frac{\partial \tau_{ji}}{\partial x_j}}_{\text{Viscous stress force}} + \underbrace{\rho \sum_{k=1}^N (Y_k f_k)_i}_{\text{Body forces}} \quad (1.87)$$

This equation represents the balance of four different forces: inertial force, pressure gradient force, viscous stress force, and body forces. The body forces act on the control volume due to gravity or the Lorenz force acting in distance. If the fluid mixture in the control volume consists of N species, the body forces acting on different chemical species may differ. For example, some species could be ionized. If the reacting mixture flows through a magnetic field, these ionized species will experience Lorenz forces depending the degree of ionization and the mass of each species. Thus, for a multicomponent system, we have

$$B_i = \rho \sum_{k=1}^N (Y_k f_k)_i \quad (1.88)$$

where $f_{k,i}$ is the force per unit mass of k^{th} species in i^{th} direction,

A summary of momentum conservation equation in rectangular, cylindrical, and spherical coordinate systems are given in Table 1.9, Table 1.10, and

TABLE 1.9. Momentum Conservation Equation in Rectangular Coordinate Systems (Modified* from Bird, Stewart, and Lightfoot, 1960)

In terms of viscous stress, τ:	
x:	$\rho \left(\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right) = -\frac{\partial p}{\partial x} + \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) + B_x$ (1.89)
y:	$\rho \left(\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right) = -\frac{\partial p}{\partial y} + \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + B_y$ (1.90)
z:	$\rho \left(\frac{\partial u_z}{\partial t} + u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) + B_z$ (1.91)
In terms of velocity gradients for Newtonian fluid with constant ρ and μ:	
x:	$\rho \left(\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right) = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) + B_x$ (1.92)
y:	$\rho \left(\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right) = -\frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right) + B_y$ (1.93)
z:	$\rho \left(\frac{\partial u_z}{\partial t} + u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) + B_z$ (1.94)

*These equation numbers are continuous with these in the main text

TABLE 1.10. Momentum Conservation Equation in Cylindrical Coordinate Systems (Modified from Bird, Stewart, and Lightfoot, 1960)

In terms of viscous stress, τ :	
r:	$\rho \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta^2}{r} + u_z \frac{\partial u_r}{\partial z} \right)$ $= -\frac{\partial p}{\partial r} + \left(\frac{1}{r} \frac{\partial}{\partial r} (r \tau_{rr}) + \frac{1}{r} \frac{\partial \tau_{r\theta}}{\partial \theta} - \frac{\tau_{\theta\theta}}{r} + \frac{\partial \tau_{rz}}{\partial z} \right) + B_r$ (1.95)
θ :	$\rho \left(\frac{\partial u_\theta}{\partial t} + u_r \frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\theta}{\partial \theta} - \frac{u_r u_\theta}{r} + u_z \frac{\partial u_\theta}{\partial z} \right)$ $= -\frac{1}{r} \frac{\partial p}{\partial \theta} + \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\theta}) + \frac{1}{r} \frac{\partial \tau_{\theta\theta}}{\partial \theta} + \frac{\partial \tau_{\theta z}}{\partial z} \right) + B_\theta$ (1.96)
z:	$\rho \left(\frac{\partial u_z}{\partial t} + u_r \frac{\partial u_z}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_z}{\partial \theta} + u_z \frac{\partial u_z}{\partial z} \right)$ $= -\frac{\partial p}{\partial z} + \left(\frac{1}{r} \frac{\partial}{\partial r} (r \tau_{rz}) + \frac{1}{r} \frac{\partial \tau_{\theta z}}{\partial \theta} + \frac{\partial \tau_{zz}}{\partial z} \right) + B_z$ (1.97)
In terms of velocity gradients of Newtonian fluids with constant ρ & μ :	
r:	$\rho \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta^2}{r} + u_z \frac{\partial u_r}{\partial z} \right)$ $= -\frac{\partial p}{\partial r} + \mu \left[\frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} (r u_r) \right) + \frac{1}{r^2} \frac{\partial^2 u_r}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial u_\theta}{\partial \theta} + \frac{\partial^2 u_r}{\partial z^2} \right] + B_r$ (1.98)
θ :	$\rho \left(\frac{\partial u_\theta}{\partial t} + u_r \frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r u_\theta}{r} + u_z \frac{\partial u_\theta}{\partial z} \right)$ $= -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left[\frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} (r u_\theta) \right) + \frac{1}{r^2} \frac{\partial^2 u_\theta}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u_r}{\partial \theta} + \frac{\partial^2 u_\theta}{\partial z^2} \right] + B_\theta$ (1.99)
z:	$\rho \left(\frac{\partial u_z}{\partial t} + u_r \frac{\partial u_z}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_z}{\partial \theta} + u_z \frac{\partial u_z}{\partial z} \right)$ $= -\frac{\partial p}{\partial z} + \mu \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u_z}{\partial \theta^2} + \frac{\partial^2 u_z}{\partial z^2} \right] + B_z$ (1.100)

Table 1.11, respectively. In each of these tables, there are two sets of momentum equations; the first set is written in terms of the viscous stress components, and the second set is written in terms of velocity components with the constant density and constant viscosity assumptions. Readers interested in compressible fluids and/or variable viscosity cases can substitute the constitutive relationship given by Equation 1.84. The stress tensor components in different coordinate systems are given in Bird, Stewart, and Lightfoot (1960), Chap. 3 and Kuo (2005), Chap. 3.

The term $\rho u_\theta^2/r$ in the r -direction momentum equation [Equation's 1.95 and 1.98] is the *centrifugal force*. It gives the effective force in the r -direction resulting from fluid motion in the θ -direction. This term arises automatically on transformation from rectangular to cylindrical coordinates. The term $\rho u_r u_\theta/r$

TABLE 1.11. Momentum Conservation Equation in Spherical Coordinate Systems (Modified from Bird, Stewart, and Lightfoot, 1960)

In terms of viscous stress, τ:	
$R:$	$\rho \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_r}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_r}{\partial \phi} - \frac{u_\theta^2 + u_\phi^2}{r} \right)$ $= -\frac{\partial p}{\partial r} + \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{r\theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \tau_{r\phi}}{\partial \phi} \right. \\ \left. - \frac{\tau_{\theta\theta} + \tau_{\phi\phi}}{r} \right) + B_r \quad (1.101)$
$\theta:$	$\rho \left(\frac{\partial u_\theta}{\partial t} + u_r \frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_\theta}{\partial \phi} + \frac{u_r u_\theta}{r} - \frac{u_\phi^2 \cot \theta}{r} \right)$ $= -\frac{1}{r} \frac{\partial p}{\partial \theta} + \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{\theta\theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \tau_{\theta\phi}}{\partial \phi} + \frac{\tau_{r\theta}}{r} \right. \\ \left. - \frac{\cot \theta}{r} \tau_{\phi\phi} \right) + B_\theta \quad (1.102)$
$\phi:$	$\rho \left(\frac{\partial u_\phi}{\partial t} + u_r \frac{\partial u_\phi}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\phi}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + \frac{u_\phi u_r}{r} + \frac{u_\theta u_\phi}{r} \cot \theta \right)$ $= -\frac{1}{r \sin \theta} \frac{\partial p}{\partial \phi} + \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\phi}) + \frac{1}{r} \frac{\partial \tau_{\phi\theta}}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \tau_{\phi\phi}}{\partial \phi} + \frac{\tau_{r\phi}}{r} \right. \\ \left. - \frac{2 \cot \theta}{r} \tau_{\theta\phi} \right) + B_\phi \quad (1.103)$
In terms of velocity gradients of Newtonian fluids with constant ρ and μ:	
$R:$	$\rho \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_r}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_r}{\partial \phi} - \frac{u_\theta^2 + u_\phi^2}{r} \right)$ $= -\frac{\partial p}{\partial r} + \mu \left(\nabla^2 u_r - \frac{2}{r^2} u_r - \frac{2}{r^2} \frac{\partial u_\theta}{\partial \theta} - \frac{2}{r^2} u_\theta \cot \theta - \frac{2}{r^2 \sin \theta} \frac{\partial u_\phi}{\partial \phi} \right) + B_r \quad (1.104)$
$\theta:$	$\rho \left(\frac{\partial u_\theta}{\partial t} + u_r \frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_\theta}{\partial \phi} + \frac{u_r u_\theta}{r} - \frac{u_\phi^2 \cot \theta}{r} \right)$ $= -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left(\nabla^2 u_\theta + \frac{2}{r^2} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r^2 \sin^2 \theta} - \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial u_\phi}{\partial \phi} \right) + B_\theta \quad (1.105)$
$\phi:$	$\rho \left(\frac{\partial u_\phi}{\partial t} + u_r \frac{\partial u_\phi}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\phi}{\partial \theta} + \frac{u_\phi}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + \frac{u_\phi u_r}{r} + \frac{u_\theta u_\phi}{r} \cot \theta \right)$ $= -\frac{1}{r \sin \theta} \frac{\partial p}{\partial \phi} + \mu \left(\nabla^2 u_\phi - \frac{u_\phi}{r^2 \sin^2 \theta} + \frac{2}{r^2 \sin \theta} \frac{\partial u_r}{\partial \phi} \right. \\ \left. + \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial u_\theta}{\partial \phi} \right) + B_\phi \quad (1.106)$

in the θ -direction momentum equation Equations.1.96 and 1.99 is the *Coriolis force*. It is an effective force in the θ -direction when there is flow in both the r and θ directions. This term also arises automatically in the coordinate transformation. The Coriolis force arises in the problem of flow near a rotating disk. (See, e.q., Schlichting, 1968), Chap. 5.

In Table 1.10, the Laplacian operator (∇^2) is given as:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right) \quad (1.107)$$

1.13 ENERGY CONSERVATION EQUATION FOR MULTICOMPONENT MIXTURE

The energy conservation equation requires the greatest attention because multiple forms exist. Note first that because of continuity, the relation shown in Equation 1.108 (which may be used in all left-hand sides of enthalpy, energy, or temperature equations) holds for any quantity f :

$$\rho \frac{Df}{Dt} = \rho \left(\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} \right) = \frac{\partial \rho f}{\partial t} + \frac{\partial \rho u_i f}{\partial x_i} \quad (1.108)$$

In this equation, D/Dt is called the *material derivative* or *substantial derivative*. In the Lagrangian point of view, this time derivative is taken while following the motion of the fluid particle with a fixed mass. In the Eulerian frame of reference, the D/Dt operator can be expressed by the sum of four terms on the right-hand side of Equation 1.109, since there are four independent variables in the Eulerian coordinates. Thus,

$$\frac{d}{dt} \equiv \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u_1 \frac{\partial}{\partial x_1} + u_2 \frac{\partial}{\partial x_2} + u_3 \frac{\partial}{\partial x_3} \quad (1.109)$$

As shown in Table 1.4, there are eight different forms of energy for the gaseous mixture. The energy conservation equation can be written in terms of any of these eight forms. In addition, the energy conservation equation also can be given in terms of temperature. Although there are many different choices for writing the energy conservation equation, only one energy equation for the gaseous mixture can be used since all forms of energy are interrelated. Readers can find the detailed derivation of energy equation in Kuo (2005), Chap. 3. Next we present different forms of energy equations.

In terms of total energy (internal with chemical and kinetic) e_t , the energy conservation equation can be written as:

$$\underbrace{\rho \frac{\partial e_t}{\partial t}}_{\text{Rate of accumulation of internal and kinetic energy per unit volume stored in control volume}} + \underbrace{\rho u_i \frac{\partial e_t}{\partial x_i}}_{\text{Net rate of energy transported out of control volume by advection}} = \underbrace{-\frac{\partial q_i}{\partial x_i}}_{\text{Net rate of heat addition to control volume by conduction, interdiffusion, & Dufour flux}} + \underbrace{\dot{Q}}_{\text{Net rate of external energy input per unit volume to control volume}} + \underbrace{\frac{\partial \sigma_{ji} u_i}{\partial x_j}}_{\text{Work done by surface stress induced forces on control volume}} + \underbrace{\rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i})}_{\text{Body force work}} \quad (1.110)$$

where q_i is the i^{th} component of the flux vector \mathbf{q} , which contains conduction heat flux, interdiffusion heat flux, and the Dufour heat flux; that is

$$\begin{aligned}\mathbf{q} &= \mathbf{q}_{\text{conduction}} + \mathbf{q}_{\text{interdiffusion}} + \mathbf{q}_{\text{Dufour}} \\ &= -\lambda \nabla T + \rho \sum_{k=1}^N h_k Y_k \mathbf{V}_k + R_u T \sum_{k=1}^N \sum_{j=1}^N \left(\frac{X_j D_{T_k}}{M W_k D_{kj}} \right) (\mathbf{V}_k - \mathbf{V}_j)\end{aligned}\quad (1.111)$$

By neglecting the Dufour effect, q_i can be written as:

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^N h_k Y_k V_{k,i}\quad (1.112)$$

The kinetic energy equation can be written as shown in Equation 1.113, by using the product of u_i with the momentum conservation equation:

$$\rho \frac{\partial (\frac{1}{2} u_i u_i)}{\partial t} + \rho u_j \frac{\partial (\frac{1}{2} u_i u_i)}{\partial x_j} = u_i \frac{\partial \sigma_{ji}}{\partial x_j} + \rho \sum_{k=1}^N Y_k f_{k,i} u_i\quad (1.113)$$

Substituting Equation 1.113 in Equation 1.110, we obtain a conservation equation for sensible and chemical energy, e :

$$\rho \frac{De}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}\quad (1.114)$$

The equation for sensible internal energy e_s is:

$$\begin{aligned}\rho \frac{De_s}{Dt} &= -\underbrace{\sum_{k=1}^N \dot{\omega}_k \Delta h_{f,k}^o}_{\dot{\omega}_T} - \frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} - \sum_{k=1}^N \Delta h_{f,k}^o \frac{\partial}{\partial x_i} \left(\rho \underbrace{D_k \frac{\partial Y_k}{\partial x_i}}_{=-Y_k V_{k,i}} \right) \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}\end{aligned}\quad (1.115)$$

$$\begin{aligned}&= \dot{\omega}_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}\end{aligned}$$

In Equation 1.115, the source term due to heat released by chemical reactions is $\dot{\omega}_T$, and it is defined as:

$$\dot{\omega}_T \equiv -\sum_{k=1}^N \dot{\omega}_k \Delta h_{f,k}^o\quad (1.116)$$

The equation for total nonchemical energy (sensible + kinetic) energy e_{tnc} is:

$$\begin{aligned} \rho \frac{De_{tnc}}{Dt} &= \dot{\omega}_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial \sigma_{ij} u_i}{\partial x_j} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \end{aligned} \quad (1.117)$$

The conservation equation for (sensible + chemical) enthalpy is:

$$\begin{aligned} \rho \frac{Dh}{Dt} &= \frac{Dp}{Dt} - \frac{\partial q_i}{\partial x_i} + \underbrace{\tau_{ji} \frac{\partial u_i}{\partial x_j}}_{\Phi = \text{Viscous dissipation}} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \\ &= \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \end{aligned} \quad (1.118)$$

The conservation equation for total enthalpy (sensible + chemical + kinetic energy) is:

$$\begin{aligned} \rho \frac{Dh_t}{Dt} &= \frac{\partial p}{\partial t} + \frac{\partial (\tau_{ji} u_i)}{\partial x_j} + \dot{Q} - \frac{\partial q_i}{\partial x_i} + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \\ &= \frac{\partial p}{\partial t} + \frac{\partial (\tau_{ji} u_i)}{\partial x_j} + \dot{Q} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \end{aligned} \quad (1.119)$$

The conservation equation for sensible enthalpy is:

$$\begin{aligned} \rho \frac{Dh_s}{Dt} &= \dot{\omega}_T + \frac{Dp}{Dt} - \frac{\partial q_i}{\partial x_i} + \underbrace{\tau_{ji} \frac{\partial u_i}{\partial x_j}}_{\Phi = \text{Viscous dissipation}} + \dot{Q} - \sum_{k=1}^N \Delta h_{f,k}^o \frac{\partial}{\partial x_i} \left(\rho \underbrace{D_k \frac{\partial Y_k}{\partial x_i}}_{=-Y_k V_{k,i}} \right) \\ &\quad + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \\ &= \dot{\omega}_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} \\ &\quad + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \end{aligned} \quad (1.120)$$

The conservation equation for total nonchemical (sensible + kinetic energy) enthalpy is:

$$\rho \frac{Dh_{inc}}{Dt} = \dot{\omega}_T + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial \tau_{ij} u_i}{\partial x_j} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \quad (1.121)$$

The energy conservation equation in terms of temperature can be very useful. The enthalpy (sensible + chemical) can be written as:

$$h = \int_{T_{ref}}^T C_p dT + \sum_{i=1}^N Y_i \Delta h_{f,i}^0 = \int_{T_{ref}}^T \left(\sum_{i=1}^N C_{p,i} Y_i \right) dT + \sum_{i=1}^N Y_i \Delta h_{f,i}^0 = \sum_{i=1}^N h_i Y_i \quad (1.122)$$

Since the mass fraction of the i^{th} species is an independent variable, the fractional change in enthalpy (sensible + chemical) can be written as:

$$dh = C_p dT = \left(\sum_{i=1}^N C_{p,i} Y_i \right) dT \quad (1.123)$$

$$dh_k = C_{p,k} dT \quad \text{or} \quad \frac{\partial h_k}{\partial x_i} = C_{p,k} \frac{\partial T}{\partial x_i} \quad (1.124)$$

The constant-pressure specific heat of the i^{th} species is a function of temperature; therefore,

$$C_p = C_p(Y_i, T) \quad \text{and} \quad h = h(Y_i, T) \quad (1.125)$$

By applying the chain rule, the time derivative and spatial gradients of the enthalpy (sensible + chemical) can be written as:

$$\frac{\partial h}{\partial t} = \frac{\partial h}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial h}{\partial Y_i} \frac{\partial Y_i}{\partial t} \quad (1.126)$$

$$\frac{\partial h}{\partial x_i} = \frac{\partial h}{\partial T} \frac{\partial T}{\partial x_i} + \frac{\partial h}{\partial Y_k} \frac{\partial Y_k}{\partial x_i} \quad (1.127)$$

From Equation 1.123,

$$\frac{\partial h}{\partial T} = C_p(Y_k, T) \quad (1.128)$$

$$\frac{\partial h}{\partial Y_k} = \frac{\partial}{\partial Y_k} \left(\sum_{k=1}^N h_k(T) Y_k \right) = \sum_{k=1}^N \left(Y_k \frac{\partial h_k(T)}{\partial Y_k} + h_k(T) \frac{\partial Y_k}{\partial Y_k} \right) = \sum_{k=1}^N h_k(T) \quad (1.129)$$

Therefore,

$$\frac{\partial h}{\partial t} = C_p(Y_k, T) \frac{\partial T}{\partial t} + \sum_{k=1}^N h_k(T) \frac{\partial Y_k}{\partial t} \quad (1.130)$$

$$\frac{\partial h}{\partial x_i} = C_p(Y_k, T) \frac{\partial T}{\partial x_i} + \sum_{k=1}^N h_k(T) \frac{\partial Y_k}{\partial x_i} \quad (1.131)$$

The material derivative of enthalpy (sensible + chemical) can be written as:

$$\frac{Dh}{Dt} = \frac{\partial h}{\partial t} + u_i \frac{\partial h}{\partial x_i} \quad (1.132)$$

Substituting Equations 1.130 and 1.131 into Equation 1.132, we have:

$$\begin{aligned} \frac{Dh}{Dt} &= C_p(Y_k, T) \frac{\partial T}{\partial t} + \sum_{k=1}^N h_k(T) \frac{\partial Y_k}{\partial t} + u_i \left(C_p(Y_k, T) \frac{\partial T}{\partial x_i} + \sum_{k=1}^N h_k(T) \frac{\partial Y_k}{\partial x_i} \right) \\ &= C_p(Y_k, T) \frac{DT}{Dt} + \sum_{k=1}^N h_k(T) \frac{DY_k}{Dt} \end{aligned} \quad (1.133)$$

Therefore,

$$\rho C_p(Y_k, T) \frac{DT}{Dt} = \rho \frac{Dh}{Dt} - \rho \sum_{k=1}^N h_k(T) \frac{DY_k}{Dt} \quad (1.134)$$

By substituting the species conservation equation, we have:

$$\rho C_p(Y_k, T) \frac{DT}{Dt} = \rho \frac{Dh}{Dt} - \sum_{k=1}^N h_k(T) [\dot{\omega}_k - \nabla \cdot (\rho Y_k \mathbf{V}_k)] \quad (1.135)$$

Next, substituting the energy conservation equation Equation 1.118 into Equation 1.135, we get:

$$\begin{aligned} \rho C_p(Y_k, T) \frac{DT}{Dt} &= \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} \\ &\quad + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} - \sum_{k=1}^N h_k(T) \left[\dot{\omega}_k - \frac{\partial}{\partial x_i} (\rho Y_k V_{k,i}) \right] \end{aligned} \quad (1.136)$$

Equation 1.136 can be simplified by the following step:

$$\begin{aligned} \rho C_p(Y_k, T) \frac{DT}{Dt} &= \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) \\ &\quad + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} - \underbrace{\sum_{k=1}^N h_k(T) \dot{\omega}_k}_{=\dot{\omega}'_T} \\ &\quad + \sum_{k=1}^N h_k(T) \frac{\partial}{\partial x_i} (\rho Y_k V_{k,i}) \end{aligned} \quad (1.137)$$

The last term on the RHS of Equation 1.137 can be written as:

$$\begin{aligned} \sum_{k=1}^N h_k(T) \frac{\partial}{\partial x_i} (\rho Y_k V_{k,i}) &= \sum_{k=1}^N \frac{\partial}{\partial x_i} (\rho Y_k V_{k,i} h_k(T)) - \sum_{k=1}^N \rho Y_k V_{k,i} \frac{\partial h_k(T)}{\partial x_i} \\ &= \frac{\partial}{\partial x_i} \sum_{k=1}^N (\rho Y_k V_{k,i} h_k(T)) - \sum_{k=1}^N \rho Y_k V_{k,i} \frac{\partial h_k(T)}{\partial x_i} \end{aligned} \quad (1.138)$$

Substituting Equation 1.138 into Equation 1.137, we get:

$$\begin{aligned} \rho C_p \frac{DT}{Dt} &= \dot{\omega}'_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \\ &\quad - \sum_{k=1}^N \rho Y_k V_{k,i} \frac{\partial h_k}{\partial x_i} \end{aligned} \quad (1.139)$$

where

$$\dot{\omega}'_T \equiv - \sum_{k=1}^N h_k(T) \dot{\omega}_k = - \sum_{k=1}^N h_{s,k}(T) \dot{\omega}_k - \sum_{k=1}^N \Delta h_{f,k}^0(T) \dot{\omega}_k \quad (1.140)$$

By using Equation 1.124 and substituting it in Equation 1.139, we have:

$$\begin{aligned} \rho C_p \frac{DT}{Dt} &= \dot{\omega}'_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \\ &\quad - \left(\rho \sum_{k=1}^N Y_k V_{k,i} C_{p,k} \right) \frac{\partial T}{\partial x_i} \end{aligned} \quad (1.141)$$

Similarly, we can show that Equation 1.141 can be written by using constant-volume specific heat:

$$\begin{aligned} \rho C_v \frac{DT}{Dt} &= \dot{\omega}''_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \\ &\quad - \left(\rho \sum_{k=1}^N Y_k V_{k,i} C_{p,k} \right) \frac{\partial T}{\partial x_i} - R_u T \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N \frac{Y_k V_{k,i}}{M w_k} \right) \end{aligned} \quad (1.142)$$

where

$$\dot{\omega}''_T \equiv - \sum_{k=1}^N e_k(T) \dot{\omega}_k = - \sum_{k=1}^N e_{s,k}(T) \dot{\omega}_k - \sum_{k=1}^N \Delta h_{f,k}^0(T) \dot{\omega}_k \quad (1.143)$$

All 10 forms of the energy conservation equation are summarized in Table 1.12. These are most general forms of the energy conservation equations, for which the specific heats are considered temperature dependent quantities. Also, the fluid is considered compressible.

TABLE 1.12. Energy Conservation Equation in Various Forms

In terms of energy:	
e_t	$\rho \frac{\partial e_t}{\partial t} + \rho u_i \frac{\partial e_i}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \dot{Q} + \frac{\partial \sigma_{ji} u_i}{\partial x_j} + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \quad (1.144)$
e	$\rho \frac{De}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \quad (1.145)$
e_s	$\rho \frac{De_s}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \quad (1.146)$
e_{inc}	$\rho \frac{De_{inc}}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial \sigma_{ij} u_i}{\partial x_j} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \quad (1.147)$
In terms of enthalpy:	
h_t	$\rho \frac{Dh_i}{Dt} = \frac{\partial p}{\partial t} + \frac{\partial (\tau_{ji} u_i)}{\partial x_j} + \dot{Q} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \quad (1.148)$
h	$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_k Y_k V_{k,i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \quad (1.149)$
h_s	$\rho \frac{Dh_s}{Dt} = \dot{\omega}_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i} \quad (1.150)$
h_{inc}	$\rho \frac{Dh_{inc}}{Dt} = \dot{\omega}_T + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial \tau_{ij} u_i}{\partial x_i} + \dot{Q} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \rho \sum_{k=1}^N Y_k f_{k,i} (u_i + V_{k,i}) \quad (1.151)$

(continued overleaf)

TABLE 1.12. (continued)

Temperature	
T, C _p	$\rho C_p \frac{DT}{Dt} = \dot{\omega}'_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \tau_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}$ $- \left(\rho \sum_{k=1}^N Y_k V_{k,i} C_{p,k} \right) \frac{\partial T}{\partial x_i} \tag{1.152}$
T, C _v	$\rho C_v \frac{DT}{Dt} = \dot{\omega}''_T + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}$ $- \left(\rho \sum_{k=1}^N Y_k V_{k,i} C_{p,k} \right) \frac{\partial T}{\partial x_i} - R_u T \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N \frac{Y_k V_{k,i}}{M w_k} \right) \tag{1.153}$

In addition to the conservation equations shown in Table 1.12, there is a set of independent equations for conservation of angular momentum. In the absence of external torques, the angular momentum is automatically conserved since it can be obtained by taking the moment of the linear momentum conservation equation. If an external torque is present, the angular momentum conservation equation cannot be obtained directly just by taking the moment of the linear momentum conservation equation. Major applications of angular momentum conservation equations include polar fluids in magnetic fields and combustion systems with externally applied torque. Readers interested in the derivation of the angular momentum conservation equation are referred to Yamaguchi (2008), Chap. 2.

1.14 TOTAL UNKNOWNNS VERSUS GOVERNING EQUATIONS

Depending on the treatment of the diffusion velocity, the total number of unknowns and required governing equations for combustion problems in laminar flows are listed in Table 1.13 and Table 1.14.

TABLE 1.13. Unknowns versus Available Equations when the Fick’s Law Is Used for Diffusion Velocity

Unknowns	Equations
$\rho, p, T,$ $u_i = (u_1, u_2, u_3),$ $Y_k = (Y_1, Y_2, \dots, Y_N)$	1 continuity, 1 energy, 1 equation of state, 3 linear momentum, $N - 1$ species conservation equation, and $\sum_{k=1}^N Y_k = 1$
Number of unknowns = $N+6$	Number of equations = $N+6$

TABLE 1.14. Unknowns versus Available Equations when the Hirschfelder-Curtiss Approximation Is Used for Diffusion Velocity

Unknowns	Equations
$\rho, p, T,$ $u_i = (u_1, u_2, u_3),$ $Y_k = (Y_1, Y_2, \dots, Y_N)$ $V_{k,i} = \begin{pmatrix} V_{1,1}, V_{2,1}, \dots, V_{N,1} \\ V_{1,2}, V_{2,2}, \dots, V_{N,2} \\ V_{1,3}, V_{2,3}, \dots, V_{N,3} \end{pmatrix}$ $X_k = (X_1, X_2, \dots, X_N)$	1 continuity, 1 energy, 1 equation of state 3 linear momentum, $N - 1$ species conservation equation, $\sum_{k=1}^N Y_k = 1$ $3N$ diffusion equations for all chemical species, and N relationships between X_k and Y_k
Number of unknowns = $5N + 6$	Number of equations = $5N + 6$

For turbulent reacting flows, the turbulent transport equations and closure problems must be considered.

HOMEWORK PROBLEMS

1. Show that the expression for the j^{th} component of the correction velocity \mathbf{V}_c in the species conservation equation $\frac{\partial(\rho Y_k)}{\partial t} + \nabla \cdot [\rho Y_k (\mathbf{v} + \mathbf{V}_k + \mathbf{V}_c)] = \dot{\omega}_k$ can be written as:

$$V_{c,j} = \sum_{k=1}^N D_k \frac{MW_k}{M_w} \frac{\partial X_k}{\partial x_j}$$

where D_k can be written in the following form, based upon the Hirschfelder and Curtiss approximation for the diffusion velocity.

$$D_k = \frac{1 - Y_k}{\sum_{l \neq k}^N X_l / D_{lk}}$$

Start the problem by adopting the above equation for D_k and then substitute the diffusion velocity into the following species conservation equation:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} [\rho (u_i + V_{ki}) Y_k] = \dot{\omega}_k \quad \text{for } k = 1, 2, \dots, N$$

2. Make sure that you understand the equivalence of these two forms of the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \text{and} \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0.$$

Also, express $\nabla \cdot \mathbf{v}$ in terms of the density variations with respect to time in order to understand the meaning of volume dilatation.

3. Show that the momentum equation given in vector form can be written as:

$$\begin{aligned} \rho \frac{D\mathbf{v}}{Dt} &= \rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = \rho \left[\frac{\partial \mathbf{v}}{\partial t} + \nabla \left(\frac{\mathbf{v} \cdot \mathbf{v}}{2} \right) - \mathbf{v} \times (\nabla \times \mathbf{v}) \right] \\ &= \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} = \mathbf{f} - \nabla p + \nabla \cdot \boldsymbol{\tau} \end{aligned}$$

where $\boldsymbol{\sigma}$ is the total stress tensor, $\boldsymbol{\tau}$ is the viscous stress tensor, and \mathbf{f} is the body force.

In the Cartesian coordinate,

$$\begin{aligned} \nabla \cdot \boldsymbol{\tau} &= \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) \mathbf{e}_x + \left(\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right) \mathbf{e}_y \\ &\quad + \left(\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) \mathbf{e}_z \end{aligned}$$

4. Familiarize yourself with the following vector algebra and a set of vector identities involving del operators (∇). At the end of this list given in section A.14 of Appendix A, there are several equations associated with the Gauss divergence theorem. Make sure that you can to utilize them.