1 Overview and Basic Equations

1.1. Thermodynamic Relations in a Multicomponent Perfect Gas

This chapter presents the key equations for a multicomponent, chemically reacting perfect gas that will be used in this text [1–5]. These equations describe the thermodynamic relationships among state variables in a perfect gas, such as the interrelationship among pressure, density, and entropy. They also describe the physical laws of conservation of mass, which relate the density and velocity; the momentum equation, which relates the velocity and pressure; and the energy equation, which relates internal and kinetic energy of the flow to work and heat transfer to the fluid.

This chapter's primary purpose is to compile the key equations to be used throughout the text in one place, and assumes that the reader has some prior familiarity with them. A number of references are provided to readers for further details and derivations of these equations. It is not necessary to follow the derivations to understand the subsequent chapters, although an understanding of the physics embodied in each equation is critical. For these reasons, discussions of various terms in these expressions are included in this chapter.

We will use the following perfect gas equations of state:

$$p = \frac{\rho \mathscr{R}_u T}{\overline{MW}} \tag{1.1}$$

and

$$de = T d\mathscr{s} + p\frac{d\rho}{\rho^2} + \sum_{i=1}^{N} \frac{\mu_i}{MW_i} dY_i, \tag{1.2}$$

where $e = \sum_{i=1}^{N} Y_i e_i$, $\mathscr{s} = \sum_{i=1}^{N} Y_i \mathscr{s}_i$ and $\mu_i = \frac{\partial E}{\partial n_i}\big|_{\mathscr{s},\rho,n_{j\neq i}}$ is the chemical potential of species i. All variables are defined in the nomenclature in Section 1.7. The mixture averaged molecular weight is given by:

$$\overline{MW} = \sum_{i=1}^{N} X_i \cdot MW_i, \tag{1.3}$$

where the mole fractions, X_i are related to the mass fractions, Y_i, by:

$$X_i = \frac{Y_i \overline{MW}}{MW_i}. \tag{1.4}$$

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The enthalpy is written as:

$$h = \sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N} Y_i \int_{T_{ref}}^{T} c_{p,i}(T^*)\,dT^* + \sum_{i=1}^{N} h_{f,i}^0 Y_i$$
$$= \underbrace{\int_{T_{ref}}^{T} c_p(T^*)\,dT^*}_{h_{sens}} + \underbrace{\sum_{i=1}^{N} h_{f,i}^0 Y_i}_{h_{chem}}. \tag{1.5}$$

The first and second terms on the right-hand side of Eq. (1.5) are the sensible enthalpy, h_{sens}, and chemical enthalpy, h_{chem}, of the system, respectively. The internal energy and enthalpy are related as follows:

$$e = h - \frac{p}{\rho} = \int_{T_{ref}}^{T} c_p(T^*)\,dT^* - \frac{\mathscr{R}_u T}{MW} + \sum_{i=1}^{N} h_{f,i}^0 Y_i = \sum_{i=1}^{N} Y_i e_i. \tag{1.6}$$

Additionally, the "stagnation" or "total" enthalpy and internal energy, defined as the enthalpy or internal energy of the flow when adiabatically brought to rest, are given by:

$$h_T = h + |\vec{u}|^2/2; \quad e_T = e + |\vec{u}|^2/2. \tag{1.7}$$

The rest of the chapter overviews the conservation of mass, fluid momentum, and energy equations, while also providing evolution equations for certain other important quantities such as fluid dilatation, entropy, vorticity, and kinetic energy.

1.2. Continuity Equation

The continuity equation is given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0. \tag{1.8}$$

Rewriting this equation in terms of the substantial derivative,

$$\frac{D}{Dt}(\ ) = \frac{\partial(\ )}{\partial t} + \vec{u} \cdot \nabla(\ ). \tag{1.9}$$

It can be cast in the alternative form:

$$\frac{1}{\rho}\frac{D\rho}{Dt} + \nabla \cdot \vec{u} = 0. \tag{1.10}$$

Physically, this equation states that if one follows a given (i.e., fixed mass) packet of fluid, the normalized time rate of change of its density is equal to the negative of the local divergence of the velocity. The local velocity divergence is, itself, directly proportional to the rate of change of volume of a fluid element; that is, its "dilatation rate," given by the symbol $\Lambda = \nabla \cdot \vec{u}$. Moreover, the dilatation rate is also equal to the instantaneous flux of fluid out of a differential volume element of space.

This can be seen by integrating the dilatation rate over a volume and, utilizing Gauss's divergence theorem:

$$\iiint \Lambda dV = \iint \vec{u} \cdot \vec{n} dA. \tag{1.11}$$

The resulting surface integral is simply the instantaneous volume flux of fluid through the control surface.

1.3. Momentum Equation

The momentum equation is given by:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{\nabla p}{\rho} + \frac{\nabla \cdot \underline{\underline{\tau}}}{\rho} + \sum_{i=1}^{N} Y_i \vec{F}_i, \tag{1.12}$$

where the viscous stress tensor is given by:

$$\underline{\underline{\tau}} = \mu_\lambda (\nabla \cdot \vec{u}) \underline{\underline{\delta}} + 2\mu \underline{\underline{S}} \tag{1.13}$$

and μ, μ_λ are the first and second coefficients of viscosity, $\underline{\underline{\delta}}$ is the Kronecker delta unit tensor, and $\underline{\underline{S}}$ is the symmetric "strain rate tensor," given by:

$$\underline{\underline{S}} = \frac{1}{2}\left[\nabla \vec{u} + (\nabla \vec{u})^T\right]. \tag{1.14}$$

The momentum equation is an expression of Newton's second law, stating that the net acceleration of a fixed fluid element $(D\bar{u}/Dt)$ equals the force per unit mass exerted on it. The force terms on the right side denote surface forces due to pressure and viscous stress, and body forces. We will write three useful rearrangements of the momentum equation next.

First, we can write a vector equation for the flow vorticity, $\vec{\Omega} = \nabla \times \vec{u}$, by taking the curl of Eq. (1.12):

$$\nabla \times \left(\frac{\partial \vec{u}}{\partial t}\right) + \nabla \times (\vec{u} \cdot \nabla \vec{u}) = -\nabla \times \left(\frac{\nabla p}{\rho}\right) + \nabla \times \left(\frac{\nabla \cdot \underline{\underline{\tau}}}{\rho}\right) + \nabla \times \left(\sum_{i=1}^{N} Y_i \vec{F}_i\right). \tag{1.15}$$

Expanding further,

$$\begin{aligned} &\frac{\partial}{\partial t}(\nabla \times \vec{u}) + \nabla \times \left(\nabla\left(\frac{1}{2}|\vec{u}|^2\right) + (\vec{\Omega} \times \vec{u})\right) \\ &\quad = -\left(\frac{1}{\rho}\nabla \times \nabla p - \frac{\nabla \rho \times \nabla p}{\rho^2}\right) + \nabla \times \left(\frac{\nabla \cdot \underline{\underline{\tau}}}{\rho}\right) + \nabla \times \left(\sum_{i=1}^{N} Y_i \vec{F}_i\right). \end{aligned} \tag{1.16}$$

Noting that $\nabla \cdot \vec{\Omega} = 0$ and expanding $\nabla \times (\vec{\Omega} \times \vec{u}) = (\nabla \cdot \vec{u} + \vec{u} \cdot \nabla)\vec{\Omega} - (\vec{\Omega} \cdot \nabla)\vec{u}$, the vorticity equation can be written as follows:

$$\frac{D\vec{\Omega}}{Dt} = -(\nabla \cdot \vec{u})\vec{\Omega} + (\vec{\Omega} \cdot \nabla)\vec{u} + \frac{\nabla \rho \times \nabla p}{\rho^2} + \nabla \times \left(\frac{\nabla \cdot \underline{\underline{\tau}}}{\rho}\right) + \nabla \times \left(\sum_{i=1}^{N} Y_i \vec{F}_i\right). \tag{1.17}$$

Aside 1.1 discusses the terms in this equation.

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Aside 1.1. Discussion of the Vorticity Equation

This section discusses the various terms in the vorticity equation:

$$\frac{D\vec{\Omega}}{Dt} = (\vec{\Omega}\cdot\nabla)\vec{u} - \vec{\Omega}(\nabla\cdot\vec{u}) - \frac{\nabla p \times \nabla\rho}{\rho^2} + \nabla\times\left(\frac{\nabla\cdot\underline{\underline{\tau}}}{\rho}\right) + \sum_{i=1}^{N}\nabla\times(Y_i\vec{F}_i). \tag{A–1.1}$$

The left-hand side of this equation physically describes the time rate of change of vorticity of a fixed fluid element. The right side describes vorticity source or sink terms. The first term, $(\vec{\Omega}\cdot\nabla)\vec{u}$, is the vortex stretching and bending term. This term is intrinsically three-dimensional and, therefore, is identically zero in a two-dimensional flow. Two processes are described in this term, as illustrated in Figure A–1.1. The first process is the increase or decrease of vorticity by vortex stretching or contraction, respectively. For example, consider a vortex tube oriented in the axial direction, Ω_x. If this axial flow is accelerating, $\partial u_x/\partial x > 0$, then the tube is stretched, causing an increase in axial vorticity – that is, $D\Omega_x/Dt = \Omega_x\,\partial u_x/\partial x > 0$.

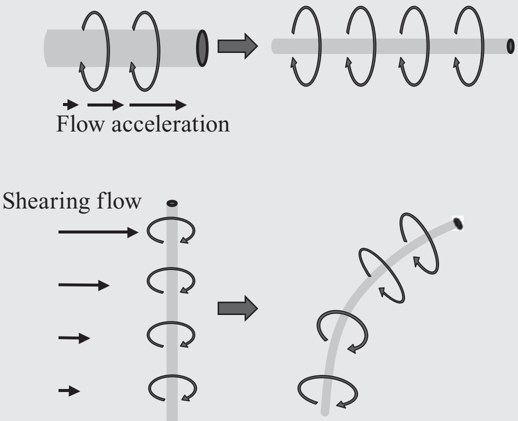

Figure A–1.1. Illustration of stretching (top) and bending (bottom) effects on a vortex tube.

The second phenomenon is the bending of a vortex tube originally inclined in another dimension by the local flow. For example, a vortex tube that is initially oriented vertically – that is, Ω_y – is rotated toward the x-axis in an axially shearing flow, $\partial u_x/\partial y > 0$. This rotation of the vortex tube causes it to be partially oriented in the axial direction, inducing a Ω_x component; that is, $D\Omega_x/Dt = \Omega_y\,\partial u_x/\partial y > 0$.

Returning to the full vorticity equation, the second term, $(\nabla\cdot\vec{u})\vec{\Omega}$, describes flow dilatation impacts on vorticity. It is only nonzero in compressible flows. Positive dilatation – expansion in cross sectional area of a vortex tube – leads to a reduction in vorticity. This effect is analogous to a spinning skater who extends the arms outward, leading to a slowing in angular velocity, or vice versa. This term has important damping influences on vorticity as it propagates through the flame.

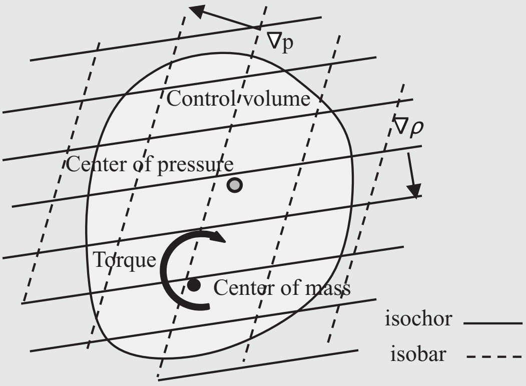

Figure A–1.2. Illustration of processes by which a misaligned pressure and density gradient lead to torque on a fluid element and, thus, vorticity production.

The third term, $\frac{\nabla p \times \nabla \rho}{\rho^2}$, describes vorticity production via the baroclinic mechanism, which occurs when the density and pressure gradients are misaligned. This term is identically zero in flows where $\rho = \rho(p)$, such as in isentropic flows of a perfect gas. The torque induced on the flow by a misaligned pressure and density gradient can be understood from Figure A–1.2. Consider the shaded control volume in a field with a spatially varying pressure and density. The pressure gradient induces a net force on the control volume, which acts through the center of pressure, shown in the figure. Because of the density gradient, the center of mass is displaced from the center of pressure. If the pressure and density gradients are not aligned (i.e., $\nabla \rho \times \nabla p \neq 0$), then the force acting at the center of pressure induces a torque on the fluid element about this center of mass, creating vorticity.

Pressure enters the vorticity equation only through this baroclinic term. This reflects the fact that only under certain conditions can the normal pressure forces exert a torque on the flow.

It is also important to note that vorticity can be generated only at no-slip boundaries, by baroclinic torque, or through body forces. All the other terms in Eq. (A–1.1) describe the amplification, stretching, bending, or diffusion of vorticity that already exists in the flow. Thus, large-scale vortical structures that play such a key role in Chapters 3 and 4 arise not “from nothing,” but from the complex reorganization of vorticity that enters the flow from boundary layers (e.g., in jets or wakes). An enormous range of possible flow structures can arise from this vorticity, depending on the characteristics of the specific flow in which it arises.

We next write a scalar equation for the evolution of the fluid dilatation, Λ, by taking the divergence of Eq. (1.12):

$$\rho \frac{D\Lambda}{Dt} = -\rho \nabla \vec{u} : \nabla \vec{u} - \nabla^2 p + \frac{\nabla \rho \cdot \nabla p}{\rho} + \nabla \cdot (\nabla \cdot \underline{\underline{\tau}}) - \frac{\nabla \rho \cdot (\nabla \cdot \underline{\underline{\tau}})}{\rho} + \rho \sum_{i=1}^{N} \nabla \cdot (Y_i \vec{F}_i). \tag{1.18}$$

The double dot product appearing in the first term on the right-hand side is expressed in tensor notation as:

$$\rho\nabla\vec{u}:\nabla\vec{u}=\rho\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}. \tag{1.19}$$

The last equation to be developed from the momentum equation relates to the evolution of kinetic energy per unit mass, $|\vec{u}|^2/2$. This is obtained by taking the dot product of the velocity vector, $\vec{u}$, with Eq. (1.12). This leads to the scalar equation:

$$\rho\frac{D}{Dt}\left(\frac{\vec{u}\cdot\vec{u}}{2}\right)=-\left(\vec{u}\cdot\nabla\right)p+\vec{u}\cdot\left(\nabla\cdot\underline{\underline{\tau}}\right)+\rho\left(\sum_{i=1}^{N}Y_i\vec{u}\cdot\vec{F}_i\right). \tag{1.20}$$

We will use all these momentum equation variants in the following sections and subsequent chapters.

1.4. Species Conservation Equation

The species conservation equation is given by:

$$\frac{\partial(\rho Y_i)}{\partial t}+\nabla\cdot(\rho Y_i\vec{u}_i)=\dot{w}_i. \tag{1.21}$$

Note the distinction between the mass averaged fluid velocity, $\vec{u}$, and the velocity of a given species, $\vec{u}_i$. Their difference is the diffusion velocity, $\vec{u}_i-\vec{u}=\vec{u}_{D,i}$. This species conservation equation simply states that the time rate of change of a fixed mass of a given element of species, i, equals the rate of production or consumption by chemical reaction, w_i.

It is typically more useful to replace the species velocities, $\vec{u}_i$, in this expression with the bulk gas velocity, $\vec{u}$, and diffusion velocity, $\vec{u}_{D,i}$. This leads to:

$$\rho\frac{DY_i}{Dt}=\dot{w}_i-\nabla\cdot\left(\rho Y_i\vec{u}_{D,i}\right). \tag{1.22}$$

These diffusion velocities are described implicitly by the following equation:

$$\nabla X_i=\left\{\begin{array}{l}\displaystyle\sum_{j=1}^{N}\left(\frac{X_iX_j}{\mathscr{D}_{ij}}\right)\left(\vec{u}_{D,j}-\vec{u}_{D,i}\right)+\left(Y_i-X_i\right)\left(\frac{\nabla p}{p}\right)\\ \displaystyle+\sum_{j=1}^{N}\left[\left(\frac{X_iX_j}{\rho\mathscr{D}_{ij}}\right)\left(\frac{\mathscr{D}_{T,j}}{Y_j}-\frac{\mathscr{D}_{T,i}}{Y_i}\right)\right]\left(\frac{\nabla T}{T}\right)+\frac{\rho}{p}\sum_{j=1}^{N}Y_iY_j(\vec{F}_i-\vec{F}_j)\end{array}\right. . \tag{1.23}$$

The reader is referred to Refs. [1, 4] for discussion of the terms in this expression, which describe the diffusion of mass by gradients in concentration, pressure, and temperature, as well as a species-dependent body force term. Equation (1.23) leads to the familiar Fickian diffusion expression for a binary mixture when Soret, pressure, and body force terms are neglected:

$$\vec{u}_{D,i}=-\mathscr{D}_i\nabla\ln Y_i. \tag{1.24}$$

This expression can be used to recast the species conservation equation as the following unsteady convection–diffusion-reaction equation:

$$\rho \frac{DY_i}{Dt} = \dot{w}_i + \nabla \cdot (\rho \mathscr{D}_i \nabla Y_i). \tag{1.25}$$

The species equations can also be recast into "conserved scalar" equations that are source free. The key idea is that although atoms may move from one compound to another during chemical reactions, they themselves are "conserved" and not created or destroyed. For example, one can define conserved scalars based on each particular atom, such as the hydrogen atom, H, and combine the different H-containing species equations (e.g., H_2, H_2O) to arrive at a source- and chemistry-free equation [4, 5]. This approach is particularly useful in a system with a single fuel and single oxidizer stream with the same mass diffusivities, where the mixture fraction, $\mathscr{Z}$, is commonly defined as the mass fraction of material originating from the fuel jet. Assuming that all constituent species have equal diffusivities, the governing equation for the mixture fraction is given by (see Exercise 1.7):

$$\rho \frac{\partial \mathscr{Z}}{\partial t} + \rho \vec{u} \cdot \nabla \mathscr{Z} - \nabla \cdot (\rho \mathscr{D} \nabla \mathscr{Z}) = 0. \tag{1.26}$$

We will return to this equation in the treatment of nonpremixed flames, starting in Chapter 9. This equation is generally valid for premixed systems as well, but is less useful as $\mathscr{Z}$ is constant everywhere in a perfectly premixed system.

1.5. Energy Equation

The energy equation is given by:

$$\rho \frac{De_T}{Dt} = -\nabla \cdot \vec{q} - \nabla \cdot (p\vec{u}) + \nabla \cdot (\vec{u} \cdot \underline{\underline{\tau}}) + \rho \sum_{i=1}^{N} Y_i \left(\vec{u} + \vec{u}_{D,i}\right) \cdot \vec{F}_i . \tag{1.27}$$

This is a statement of the first law of thermodynamics – the time rate of change of internal and kinetic energy per unit mass of a given fluid element (the left side) equals the rate of heat addition,$\nabla \cdot \vec{q}$, minus the rate of work out (the latter three terms on the right side of this equation). There are three work terms, relating to work on the fluid at the surfaces by pressure forces, $\nabla \cdot (p\vec{u})$, viscous forces,$\nabla \cdot (\vec{u} \cdot \underline{\underline{\tau}})$, and body forces, $\sum_{i=1}^{N} (\vec{u} + \vec{u}_{D,i}) \cdot (\rho_i \vec{F}_i)$. The heat flux vector, $\vec{q}$, is given by:

$$\vec{q} = -k_T \nabla T + \rho \sum_{i=1}^{N} h_i Y_i \vec{u}_{D,i} + \mathscr{R}_u T \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\frac{X_j \mathscr{D}_{T,i}}{W_i \mathscr{D}_{ij}} \right) (\vec{u}_{D,i} - \vec{u}_{D,j}) + \vec{q}_{Rad} \tag{1.28}$$

See Ref. [1] for a discussion of these terms, which describe heat transfer by conduction, mass diffusion, multicomponent mass diffusion due to concentration gradients, and radiation, respectively.

Alternatively, the energy equation can be written in terms of total enthalpy, $h_T = e_T + (p/\rho)$, by moving the pressure work term from the right side of Eq. (1.27) to the left, as follows:

$$\rho \frac{Dh_T}{Dt} = -\nabla \cdot \vec{q} + \frac{\partial p}{\partial t} + \nabla \cdot (\vec{u} \cdot \underline{\underline{\tau}}) + \rho \sum_{i=1}^{N} Y_i \left(\vec{u} + \vec{u}_{D,i}\right) \cdot \vec{F}_i . \tag{1.29}$$

Equations for the internal energy and enthalpy can be obtained by subtracting the kinetic energy equation, Eq. (1.20), leading to:

$$\rho\frac{De}{Dt} = -\nabla\cdot\vec{\mathscr{q}} - p\,(\nabla\cdot\vec{u}) + \underline{\underline{\tau}} : (\nabla\vec{u}) + \rho\sum_{i=1}^{N} Y_i\vec{u}_{D,i}\cdot\vec{F}_i \tag{1.30}$$

and

$$\rho\frac{Dh}{Dt} = -\nabla\cdot\vec{\mathscr{q}} + \frac{Dp}{Dt} + \underline{\underline{\tau}} : (\nabla\vec{u}) + \rho\sum_{i=1}^{N} Y_i\vec{u}_{D,i}\cdot\vec{F}_i. \tag{1.31}$$

It is useful to explicitly bring out the chemical component of the enthalpy. This is done by first writing an evolution equation for the chemical enthalpy of the system using the species conservation equation, Eq. (1.22) as follows:

$$\frac{Dh_{chem}}{Dt} = \sum_{i=1}^{N} h^0_{f,i}\frac{DY_i}{Dt} = \frac{1}{\rho}\sum_{i=1}^{N} h^0_{f,i}\dot{w}_i - \frac{1}{\rho}\nabla\cdot\left(\rho\sum_{i=1}^{N} h^0_{f,i}Y_i\vec{u}_{D,i}\right). \tag{1.32}$$

This can be further simplified to yield:

$$\rho\frac{Dh_{chem}}{Dt} = -\dot{q} - \nabla\cdot\left(\rho\sum_{i=1}^{N} h^0_{f,i}Y_i\vec{u}_{D,i}\right), \tag{1.33}$$

where the chemical source term $\dot{q}$ is the volumetric heat release rate due to combustion, given by:

$$\dot{q} = -\sum_{i=1}^{N} h^0_{f,i}\dot{w}_i. \tag{1.34}$$

This chemical enthalpy equation, Eq. (1.33), is then subtracted from Eq. (1.31) to yield the following equation for sensible enthalpy:

$$\rho\frac{Dh_{sens}}{Dt} = \dot{q} - \nabla\cdot\vec{\mathscr{q}} + \frac{Dp}{Dt} + \underline{\underline{\tau}} : (\nabla\vec{u}) + \nabla\cdot\left(\rho\sum_{i=1}^{N} h^0_{f,i}Y_i\vec{u}_{D,i}\right) + \rho\sum_{i=1}^{N} Y_i\vec{u}_{D,i}\cdot\vec{F}_i. \tag{1.35}$$

The energy equation can also be written in terms of entropy, s. From Eq. (1.2),

$$T\frac{D\mathscr{s}}{Dt} = \frac{De}{Dt} - \frac{p}{\rho^2}\frac{D\rho}{Dt} - \sum_{i=1}^{N}\frac{\mu_i}{MW_i}\frac{DY_i}{Dt}. \tag{1.36}$$

Substituting Eqs. (1.30) and (1.25) into this expression yields:

$$\rho T\frac{D\mathscr{s}}{Dt} = -\nabla\cdot\vec{\mathscr{q}} + \underline{\underline{\tau}} : (\nabla\vec{u}) - \rho\sum_{i=1}^{N}\mathscr{D}_i\,\nabla Y_i\cdot\vec{F}_i - \sum_{i=1}^{N}\frac{\mu_i}{MW_i}\left(\dot{w}_i + \nabla\cdot(\rho\mathscr{D}_i\,\nabla Y_i)\right). \tag{1.37}$$

This equation shows how entropy of a given mass of fluid is altered by mass, momentum, and energy diffusion, as well as body forces, and chemical reaction.

Finally, the energy equation is written in terms of temperature and pressure. This can be done by starting from the equation for sensible enthalpy, Eq. (1.35), and noting that $dh_{sens} = c_p dT$. Equation (1.35) can be rewritten as:

$$\rho \frac{Dh_{sens}}{Dt} - \frac{Dp}{Dt} = \dot{q} - \nabla \cdot \vec{q} + \underline{\underline{\tau}} : (\nabla \vec{u}) + \nabla \cdot \left(\rho \sum_{i=1}^{N} h_{f,i}^{0} Y_i \vec{u}_{D,i} \right) + \rho \sum_{i=1}^{N} Y_i \vec{u}_{D,i} \cdot \vec{F}_i . \tag{1.38}$$

The left side of Eq. (1.38) can be expressed as the substantial derivative of either temperature or pressure. For example, writing changes in temperature as:

$$dT = \left(\frac{\partial T}{\partial p} \right)_{\rho, Y_i} dp + \left(\frac{\partial T}{\partial \rho} \right)_{p, Y_i} d\rho + \sum_{i=1}^{N} \left(\frac{\partial T}{\partial Y_i} \right)_{p, \rho, Y_{j \neq i}} dY_i , \tag{1.39}$$

the substantial derivative of temperature may be expressed as:

$$\frac{DT}{Dt} = \frac{T}{p} \frac{Dp}{Dt} - \frac{T}{\rho} \frac{D\rho}{Dt} - T \sum_{i=1}^{N} \frac{\overline{MW}}{MW_i} \frac{DY_i}{Dt} \tag{1.40}$$

so that:

$$\begin{aligned}
&\rho \frac{Dh_{sens}}{Dt} - \frac{Dp}{Dt} \\
&\quad = \rho c_p \frac{DT}{Dt} - \frac{Dp}{Dt} \\
&\quad = \rho c_p T \left(\frac{1}{\gamma p} \frac{Dp}{Dt} + \nabla \cdot \vec{u} - \frac{\overline{MW}}{\rho} \sum_{i=1}^{N} \frac{\dot{w}_i}{MW_i} - \frac{\overline{MW}}{\rho} \sum_{i=1}^{N} \frac{\nabla \cdot (\rho \mathscr{D}_i \nabla Y_i)}{MW_i} \right) \\
&\quad = \rho c_p T \left(\frac{1}{\gamma T} \frac{DT}{Dt} + \frac{\gamma - 1}{\gamma} \left(\nabla \cdot \vec{u} - \frac{\overline{MW}}{\rho} \sum_{i=1}^{N} \frac{\dot{w}_i}{MW_i} - \frac{\overline{MW}}{\rho} \sum_{i=1}^{N} \frac{\nabla \cdot (\rho \mathscr{D}_i \nabla Y_i)}{MW_i} \right) \right) .
\end{aligned} \tag{1.41}$$

Hence, the energy equation may be written in terms of an evolution equation for the temperature as:

$$\begin{aligned}
&\frac{1}{T} \frac{DT}{Dt} + (\gamma - 1) \nabla \cdot \vec{u} \\
&\quad = \left\{ \begin{array}{l} \dfrac{\dot{q}}{\rho c_v T} + (\gamma - 1) \dfrac{\dot{n}}{n} + (\gamma - 1) \dfrac{1}{n} \displaystyle\sum_{i=1}^{N} \dfrac{\nabla \cdot (\rho \mathscr{D}_i \nabla Y_i)}{MW_i} \\ + \dfrac{1}{\rho c_v T} \left(-\nabla \cdot \vec{q} + \underline{\underline{\tau}} : (\nabla \vec{u}) + \nabla \cdot \left(\rho \displaystyle\sum_{i=1}^{N} h_{f,i}^{0} Y_i \vec{u}_{D,i} \right) + \rho \displaystyle\sum_{i=1}^{N} Y_i \vec{u}_{D,i} \cdot \vec{F}_i \right) \end{array} \right.
\end{aligned} \tag{1.42}$$

or for pressure as:

$$\begin{aligned}
&\frac{1}{\gamma p} \frac{Dp}{Dt} + \nabla \cdot \vec{u} \\
&\quad = \left\{ \begin{array}{l} \dfrac{\dot{q}}{\rho c_p T} + \dfrac{\dot{n}}{n} + \dfrac{1}{n} \displaystyle\sum_{i=1}^{N} \dfrac{\nabla \cdot (\rho \mathscr{D}_i \nabla Y_i)}{MW_i} \\ + \dfrac{1}{\rho c_p T} \left(-\nabla \cdot \vec{q} + \underline{\underline{\tau}} : (\nabla \vec{u}) + \nabla \cdot \left(\rho \displaystyle\sum_{i=1}^{N} h_{f,i}^{0} Y_i \vec{u}_{D,i} \right) + \rho \displaystyle\sum_{i=1}^{N} Y_i \vec{u}_{D,i} \cdot \vec{F}_i \right) \end{array} \right.
\end{aligned} \tag{1.43}$$

where $\dot{n}$ describes the time rate of change of the molar concentration of the gas and is defined as:

$$\dot{n} = \sum_i \frac{\dot{w}_i}{MW_i}, \quad n = \frac{\rho}{\overline{MW}}. \tag{1.44}$$

Note that

$$-\frac{1}{\overline{MW}} \frac{D}{Dt} \overline{MW} = \frac{\dot{n}}{n}, \tag{1.45}$$

so $\dot{n} = 0$ if the average molecular weight is constant.

Neglecting molecular transport and body forces, Eq. (1.43) is:

$$\frac{1}{\gamma p} \frac{Dp}{Dt} + \nabla \cdot \vec{u} = \frac{\dot{q}}{\rho c_p T} + \frac{\dot{n}}{n}. \tag{1.46}$$

The two terms on the right-hand side of this expression are source terms that describe volume production due to chemical reactions – the first because of unsteady heat release and the second due to changes in number of moles of the gas. To illustrate the relative magnitudes of these two source terms, $\dot{q}$ and $\dot{n}$, consider the ratio of product to reactant gas volume, assuming constant pressure combustion:

$$\frac{\text{Mole Production} + \text{Heat Release}}{\text{Heat Release Alone}} = \frac{\left(\dfrac{T^b}{T^u} \cdot \dfrac{\overline{MW}^u}{\overline{MW}^b} - 1\right)}{\left(\dfrac{T^b}{T^u} - 1\right)}, \tag{1.47}$$

where the superscripts u and b denote the reactant (unburned) and product (burned) values. When fuels are burned in air, the $\dot{n}$ term is small relative to the $\dot{q}$ term, because the reactive species are strongly diluted in inert nitrogen. However, there are applications – most notably, oxy-combustion – in which the molecular weight change is far more prominent. An equilibrium calculation of stoichiometric methane–air and methane–oxygen combustion shows that this ratio equals 1.01 and 1.27 for the air and oxygen systems, respectively. Consequently, for air-breathing systems, the molar production term can be neglected, as it will be in the remainder of this text. In this case, Eq. (1.46) may be written as:

$$\frac{Dp}{Dt} = -\gamma p (\nabla \cdot \vec{u}) + (\gamma - 1)\dot{q}. \tag{1.48}$$

1.6. Nomenclature

This section details the nomenclature used in the text. We have tried to maintain a consistent nomenclature across this text, which is challenging given the different uses of common symbols across the combustion, acoustics, and hydrodynamic stability communities. This uniformity in definition also makes the nomenclature admittedly complicated; the reader is encouraged to spend a few minutes understanding a few basic items.

All gas velocities are given by u. Subscripts such as x, y, and z, or r and θ, are used to denote the specific scalar component of the vector. Superscripts u and b are used to denote the value just upstream or downstream of the flame. Numbered subscripts are used to indicate perturbation quantities, using expansions detailed in