

Hydrodynamics

Alejandro Campos

January 14, 2025

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Preface

Part I

Governing equations

Chapter 1

Representations of a fluid

1.1 Eulerian vs Lagrangian

The Eulerian description of a fluid is that for which fluid properties are of the form $\mathbf{f} = \mathbf{f}(t, \mathbf{x})$, where t and \mathbf{x} denote time and position. Examples of these include density $\rho = \rho(t, \mathbf{x})$, fluid velocity $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$, and specific internal energy $e = e(t, \mathbf{x})$.

Lagrangian fields are used to describe moving particles, for which fluid properties are of the form $\mathbf{f}^+ = \mathbf{f}^+(t, \mathbf{y})$, where t denotes time and \mathbf{y} the location of the particle at an initial time. Eulerian and Lagrangian properties are related to each other according to

$$\mathbf{f}^+(t, \mathbf{y}) = \mathbf{f}(t, \mathbf{x}^+(t, \mathbf{y})). \quad (1.1)$$

There are two Lagrangian properties that deserve further attention. The position and velocity of a particle are given by $\mathbf{x}^+ = \mathbf{x}^+(t, \mathbf{y})$ and $\mathbf{v}^+ = \mathbf{v}^+(t, \mathbf{y})$, respectively. These two are related to each other according to

$$\frac{\partial \mathbf{x}^+}{\partial t} = \mathbf{v}^+. \quad (1.2)$$

1.2 Atomistic vs continuum

Eulerian and Lagrangian variables are respectively defined at every point \mathbf{x} or \mathbf{y} within the domain containing the fluid. Thus, in the fluid approach we do not account for the microscopic distribution of the fluid's atoms and molecules, which are not necessarily present at every point \mathbf{x} . That being said, we can establish a correlation between the fluid variables and atomistic variables, which define the underlying microscopic structure. Examples of these atomistic variables include m_i , \mathbf{v}_i , and ϵ_i , which are the mass, velocity, and internal energy of the i^{th} atom or molecule in the system.

Consider the total mass M_Ω in some subdomain Ω . This mass can be computed by summing up the masses m_i of the atoms or molecules in this subdomain, or by using the Eulerian field variable for density, as shown below

$$M_\Omega = \sum_{i \in \Omega} m_i = \int_\Omega \rho d\mathbf{x}. \quad (1.3)$$

In the above, $i \in \Omega$ denotes the atoms or molecules within the subdomain Ω . Now consider the total momentum \mathbf{P}_Ω in some subdomain Ω . This momentum can be computed by summing up the momentum $m_i \mathbf{u}_i$ of the atoms or molecules in this subdomain, or by using the Eulerian

field variable for velocity, as shown below

$$P_\Omega = \sum_{i \in \Omega} m_i \mathbf{v}_i = \int_\Omega \rho \mathbf{u} d\mathbf{x}. \quad (1.4)$$

Finally, consider the internal energy IE_Ω in some subdomain Ω . This internal energy can be computed by summing up the internal energies e_i of the atoms or molecules in this subdomain, or by using the Eulerian field variable for the specific internal energy, as shown below

$$IE_\Omega = \sum_{i \in \Omega} \epsilon_i = \int_\Omega \rho e d\mathbf{x}. \quad (1.5)$$

Denote the volume of domain Ω as V_Ω , which is given by

$$V_\Omega = \int_\Omega d\mathbf{x}. \quad (1.6)$$

We can now write

$$\rho = \lim_{\Omega \rightarrow \epsilon} \frac{1}{V_\Omega} \int_\Omega \rho d\mathbf{x} = \lim_{\Omega \rightarrow \epsilon} \frac{1}{V_\Omega} \sum_{i \in \Omega} m_i = \lim_{\Omega \rightarrow \epsilon} \frac{M_\Omega}{V_\Omega}. \quad (1.7)$$

Thus, the density is the mass contained in a small domain divided by the volume of that small domain as the domain becomes sufficiently small. Similarly for velocity, we have

$$\mathbf{u} = \frac{\rho \mathbf{v}}{\rho} = \lim_{\Omega \rightarrow \epsilon} \frac{\frac{1}{V_\Omega} \int_\Omega \rho \mathbf{u} d\mathbf{x}}{\frac{1}{V_\Omega} \int_\Omega \rho d\mathbf{x}} = \lim_{\Omega \rightarrow \epsilon} \frac{\sum_{i \in \Omega} m_i v^{(i)}}{\sum_{i \in \Omega} m_i} = \lim_{\Omega \rightarrow \epsilon} \frac{P_\Omega}{M_\Omega}. \quad (1.8)$$

That is, the velocity is the the momentum contained in a small domain divided by the mass contained in that small domain as the domain becomes sufficiently small. Finally, for energy we have

$$e = \frac{\rho e}{\rho} = \lim_{\Omega \rightarrow \epsilon} \frac{\frac{1}{V_\Omega} \int_\Omega \rho e d\mathbf{x}}{\frac{1}{V_\Omega} \int_\Omega \rho d\mathbf{x}} = \lim_{\Omega \rightarrow \epsilon} \frac{\sum_{i \in \Omega} e_i}{\sum_{i \in \Omega} m_i} = \lim_{\Omega \rightarrow \epsilon} \frac{IE_\Omega}{M_\Omega}. \quad (1.9)$$

That is, the specific internal energy is the internal energy contained in a small subdomain divided by the mass contained in that small subdomain as the subdomain becomes sufficiently small.

In the above, a sufficiently small subdomain is one that is small compared to the smallest length scale in the flow field but large enough that it contains a sufficiently large number of atoms or molecules.

Chapter 2

Kinematics of fluid motion

2.1 Material derivative

We are interested in knowing how $\mathbf{f}^+(t, \mathbf{y})$ for a hypothetical particle changes as we move along the particle's path. Applying the chain rule and product rule,

$$\begin{aligned}
 \frac{\partial}{\partial t} \mathbf{f}^+(t, \mathbf{y}) &= \frac{\partial}{\partial t} \mathbf{f}(t, \mathbf{x}^+(t, \mathbf{y})) \\
 &= \frac{\partial}{\partial t} \mathbf{f}(t, x_1^+(t, \mathbf{y}), x_2^+(t, \mathbf{y}), x_3^+(t, \mathbf{y})) \\
 &= \left(\frac{\partial \mathbf{f}(t, x_1, x_2, x_3)}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+(t, \mathbf{y})} + \frac{\partial x_1^+(t, \mathbf{y})}{\partial t} \left(\frac{\partial \mathbf{f}(t, x_1, x_2, x_3)}{\partial x_1} \right)_{\mathbf{x}=\mathbf{x}^+(t, \mathbf{y})} + \dots \\
 &= \left(\frac{\partial \mathbf{f}(t, x_1, x_2, x_3)}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+(t, \mathbf{y})} + v_1^+(t, \mathbf{y}) \left(\frac{\partial \mathbf{f}(t, x_1, x_2, x_3)}{\partial x_1} \right)_{\mathbf{x}=\mathbf{x}^+(t, \mathbf{y}), \dots} + \dots \quad (2.1)
 \end{aligned}$$

In abridged notation this becomes

$$\boxed{\frac{\partial \mathbf{f}^+}{\partial t} = \left(\frac{\partial \mathbf{f}}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+} + \mathbf{v}^+ \cdot (\nabla \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}} \quad (2.2)$$

For an arbitrary particle, the Lagrangian velocity \mathbf{v}^+ has an Eulerian counterpart $\mathbf{v} = \mathbf{v}(t, \mathbf{x})$ such that the following is satisfied $\mathbf{v}^+ = \mathbf{v}(t, \mathbf{x}^+)$. For this same particle, we can also introduce the Lagrangian variable $\mathbf{u}^+ = \mathbf{u}^+(t, \mathbf{y})$ and the Eulerian counterpart $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$, such that the following is satisfied $\mathbf{u}^+ = \mathbf{u}(t, \mathbf{x}^+)$. We emphasize that \mathbf{u}^+ is not the velocity of the particle, it is instead an additional particle property since \mathbf{v}^+ is the actual velocity of the particle. There is a special type of particle, referred to as a fluid particle, which is one that moves with the flow. For this particle $\mathbf{v} = \mathbf{u}$. We denote properties of a fluid particle with the subscript u , e.g. \mathbf{x}_u^+ , \mathbf{f}_u^+ , etc.

Given the the particle property $\mathbf{f}_u^+ = \mathbf{f}(t, \mathbf{x}_u^+)$, we have

$$\begin{aligned}
 \frac{\partial \mathbf{f}_u^+}{\partial t} &= \left(\frac{\partial \mathbf{f}}{\partial t} \right)_{\mathbf{x}=\mathbf{x}_u^+} + \mathbf{v}_u^+ \cdot (\nabla \mathbf{f})_{\mathbf{x}=\mathbf{x}_u^+} \\
 &= \left(\frac{\partial \mathbf{f}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{f} \right)_{\mathbf{x}=\mathbf{x}_u^+}. \quad (2.3)
 \end{aligned}$$

The term in parenthesis above is referred to as the material derivative, and it is labeled as

$$\frac{D\mathbf{f}}{Dt} = \frac{\partial \mathbf{f}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{f}. \quad (2.4)$$

An application of the above follows. Say we are given a fluid whose temperature and velocity fields are T and u , respectively. The PDE for temperature is

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \frac{\partial^2 T}{\partial x^2}. \quad (2.5)$$

We now introduce a fluid particle with Lagrangian temperature $T_u^+ = T_u^+(t, y)$. This Lagrangian property is related to its corresponding Eulerian field by $T_u^+(t, y) = T_u(t, x_u^+(t, y))$. Using eq. (2.3) we find the rate of change of T_u^+ to be

$$\frac{\partial T_u^+}{\partial t} = \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right)_{x=x_u^+} = \left(\frac{\partial^2 T}{\partial x^2} \right)_{x=x_u^+}. \quad (2.6)$$

Thus, we can interpret the PDE as describing the rate of change of a particle's property as the particle moves through space. This rate of change is given by the RHS term of eq. (2.5) evaluated at the particle's position.

2.2 The Jacobian matrix

We introduce the Jacobian matrix \mathbf{J}^+ with components $J_{ij}^+ = J_{ij}^+(t, \mathbf{y})$ defined by

$$J_{ij}^+ = \frac{\partial x_i^+}{\partial y_j}. \quad (2.7)$$

Thus, the total differential for the Lagrangian velocity can be expressed as follows

$$dx_i^+ = \frac{\partial x_i^+}{\partial t} dt + \frac{\partial x_i^+}{\partial y_j} dy_j = v_i^+ dt + J_{ij}^+ dy_j, \quad (2.8)$$

The evolution equation for the Jacobian matrix is derived as follows

$$\frac{\partial J_{ij}^+}{\partial t} = \frac{\partial}{\partial y_j} \left(\frac{\partial x_i^+}{\partial t} \right) = \frac{\partial v_i^+}{\partial y_j} = \frac{\partial v_i(t, \mathbf{x}^+)}{\partial y_j} = \frac{\partial x_k^+}{\partial y_j} \left(\frac{\partial v_i}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}^+} = J_{kj}^+ \left(\frac{\partial v_i}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}^+} \quad (2.9)$$

We now introduce $J^+ = J^+(t, \mathbf{y})$ as

$$J^+ = |\det(\mathbf{J}^+)|. \quad (2.10)$$

Jacobi's formula for some matrix $\mathbf{a} = \mathbf{a}(t)$ is as follows

$$\frac{\partial \det(\mathbf{a})}{\partial t} = \det(\mathbf{a}) \text{tr} \left(\mathbf{a}^{-1} \cdot \frac{\partial \mathbf{a}}{\partial t} \right). \quad (2.11)$$

Thus, for the Jacobian matrix, we have

$$\frac{\partial \det(\mathbf{J}^+)}{\partial t} = \det(\mathbf{J}^+) \text{tr} [(\mathbf{J}^+)^{-1} \cdot (\mathbf{G})_{\mathbf{x}=\mathbf{x}^+} \cdot \mathbf{J}^+], \quad (2.12)$$

where $G_{ij} = \partial v_i / \partial x_j$. The trace on the right-hand is a product of three matrices of the following form $a_{ij}^{-1} b_{jk} a_{ki}$. This is equivalent to b_{kk} . Thus, we finally have

$$\frac{\partial J^+}{\partial t} = J^+ \left(\frac{\partial v_k}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}^+}. \quad (2.13)$$

Consider now a fluid particle, so that

$$J_{u,ij}^+ = \frac{\partial x_{u,i}^+}{\partial y_j}, \quad (2.14)$$

and

$$J_u^+ = |\det(\mathbf{J}_u^+)|. \quad (2.15)$$

Given eq. (2.13), its evolution equation is

$$\frac{\partial J_u^+}{\partial t} = J_u^+ \left(\frac{\partial u_k}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}_u^+}. \quad (2.16)$$

2.3 Material line

A material line $l_i^+ = l_i^+(t, \mathbf{y})$ is defined as the segment that joins two fluid particles that are infinitesimally close to each other, that is

$$l_i^+(t, \mathbf{y}) = x_{u,i}^+(t, \mathbf{y} + \mathbf{f}(\mathbf{y})) - x_{u,i}^+(t, \mathbf{y}), \quad (2.17)$$

where $\mathbf{f}(\mathbf{y})$ is the initial infinitesimal displacement. The rate of change of a material line can be evaluated as follows

$$\begin{aligned} \frac{\partial l_i^+}{\partial t} &= \frac{\partial}{\partial t} x_{u,i}^+(t, \mathbf{y} + \mathbf{f}(\mathbf{y})) - \frac{\partial}{\partial t} x_{u,i}^+(t, \mathbf{y}) \\ &= u_i(t, \mathbf{x}_u^+(t, \mathbf{y} + \mathbf{f}(\mathbf{y}))) - u_i(t, \mathbf{x}_u^+(t, \mathbf{y})) \\ &= u_i(t, \mathbf{x}_u^+(t, \mathbf{y}) + \mathbf{l}^+(t, \mathbf{y})) - u_i(t, \mathbf{x}_u^+(t, \mathbf{y})), \end{aligned} \quad (2.18)$$

We now make use of Taylor's theorem to obtain

$$u_i(t, \mathbf{x}_u^+ + \mathbf{l}^+) = u_i(t, \mathbf{x}_u^+) + l_j^+ \left(\frac{\partial u_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_u^+} + \frac{1}{2} l_j^+ l_k^+ R_{ijk}(\mathbf{x}^+) \quad (2.19)$$

where

$$|R_{ijk}(\mathbf{x})| \leq \max_{j,k} \max_{\mathbf{y} \in B} \left| \left(\frac{\partial^2 u_i}{\partial x_j \partial x_k} \right)_{\mathbf{x}=\mathbf{y}} \right|, \quad \mathbf{x} \in B \quad (2.20)$$

where B is the closed ball where u_i is twice continuously spatially differentiable. Define $f(\mathbf{l}^+) = l_j^+ l_k^+ R_{ijk}$, where R_{ijk} has been evaluated at a specific \mathbf{x}^+ . Since $|l_j^+| = |\mathbf{l}^+ \cdot \mathbf{e}_j| = |\mathbf{l}^+| |\mathbf{e}_j| \cos(\theta) < |\mathbf{l}^+|$, one can easily show that

$$|f(\mathbf{l}^+)| = |l_j^+ l_k^+ R_{ijk}| < |l_j^+| |l_k^+| |R_{ijk}| < C |\mathbf{l}^+|^2 \quad (2.21)$$

Define $g(\mathbf{l}^+) = |\mathbf{l}^+|$. For any $\epsilon > 0$, there exists a neighborhood of $\mathbf{l}^+ = 0$ such that $C |\mathbf{l}^+|^2 < \epsilon |\mathbf{l}^+|$, which can be re-written as $|f(\mathbf{l}^+)| < \epsilon |g(\mathbf{l}^+)|$. Thus $f(\mathbf{l}^+) = o[g(\mathbf{l}^+)] = o[|\mathbf{l}^+|]$ as $\mathbf{l}^+ \rightarrow 0$ and we express Taylor's theorem as follows

$$u_i(t, \mathbf{x}_u^+ + \mathbf{l}^+) = u_i(t, \mathbf{x}_u^+) + l_j^+ \left(\frac{\partial u_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_u^+} + o[|\mathbf{l}^+|]. \quad (2.22)$$

(Note: In the equation above I'm always adding $f(\mathbf{l}^+)$ after the second $+$ sign, regardless of the size of \mathbf{l}^+ . By stating that $f(\mathbf{l}^+) = o(g(|\mathbf{l}^+|))$ as $\mathbf{l}^+ \rightarrow 0$, or by writing the Taylor's Theorem

as above, I only mean that $f(\mathbf{l}^+)$ is a function with a very specific behavior as $\mathbf{l}^+ \rightarrow 0$.) The equation above leads to the evolution equation for a material line, namely

$$\frac{\partial l_i^+}{\partial t} = l_j^+ \left(\frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_u^+} + o[|\mathbf{l}^+|]. \quad (2.23)$$

We apply the same reasoning used to obtain equation (2.22) but for the variable $x_i^+(t, \mathbf{y} + \mathbf{f}(\mathbf{y}))$, which gives

$$x_{u,i}^+(t, \mathbf{y} + \mathbf{f}(\mathbf{y})) = x_{u,i}^+(t, \mathbf{y}) + f_j(\mathbf{y}) \left(\frac{\partial x_{u,i}^+(t, \mathbf{z})}{\partial z_j} \right)_{\mathbf{z}=\mathbf{y}} + o[|\mathbf{f}(\mathbf{y})|]. \quad (2.24)$$

Using (eq. (2.17)), the above becomes

$$l_i^+(t, \mathbf{y}) = f_j(\mathbf{y}) \left(\frac{\partial x_i^+(t, \mathbf{z})}{\partial z_j} \right)_{\mathbf{z}=\mathbf{y}} + o[|\mathbf{f}(\mathbf{y})|]. \quad (2.25)$$

In terms of the Jacobian matrix, the above is rewritten as

$$l_i^+(t, \mathbf{y}) = f_j(\mathbf{y}) J_{ij}^+(t, \mathbf{y}) + o[|\mathbf{f}(\mathbf{y})|]. \quad (2.26)$$

Neglecting higher order terms, we have the following ODE and its proposed solution

$$\frac{\partial l_i^+}{\partial t} = l_j^+ \left(\frac{\partial u_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_u^+} \quad l_i^+ = f_j J_{ij}^+. \quad (2.27)$$

Plugging the proposed solution for l_i^+ into its ODE, and using equation (2.9) for a fluid particle, shows that this is indeed a solution, as shown below

$$\frac{\partial l_i^+}{\partial t} = \frac{\partial}{\partial t} (f_j J_{ij}^+) = f_j \frac{\partial J_{ij}^+}{\partial t} = f_j J_{kj}^+ \left(\frac{\partial u_i}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}_u^+} = l_k^+ \left(\frac{\partial u_i}{\partial x_k} \right)_{\mathbf{x}=\mathbf{x}_u^+}. \quad (2.28)$$

2.4 Reynolds transport theorem

Define the one-dimensional domain $[a_0, b_0]$. Also define the one-dimensional domain $L^+ = L^+(t, a_0, b_0)$, which is given by

$$L^+ = \{x^+ : y \in [a_0, b_0]\}. \quad (2.29)$$

Note that $L^+(0, a_0, b_0) = [a_0, b_0]$. The left boundary of this volume is given by $a^+ = a^+(t, a_0, b_0)$ and the right boundary by $b^+ = b^+(t, a_0, b_0)$. These satisfy $a^+(0, a_0, b_0) = a_0$ and $b^+(0, a_0, b_0) = b_0$.

We introduce the Lagrangian function $I^+ = I^+(t, a_0, b_0)$ and its Eulerian counterpart $I = I(t, a, b)$. These two are given by

$$I(t, a, b) = \int_a^b f(t, x) dx, \quad (2.30)$$

$$I^+(t, a_0, b_0) = I(t, a^+(t, a_0, b_0), b^+(t, a_0, b_0)). \quad (2.31)$$

We can then write

$$\begin{aligned}
\frac{\partial}{\partial t} I^+(t, a_0, b_0) &= \frac{\partial}{\partial t} I(t, a^+(t, a_0, b_0), b^+(t, a_0, b_0)) \\
&= \left[\frac{\partial I(t, a, b)}{\partial t} \right]_{\substack{a=a^+ \\ b=b^+}} + \left[\frac{\partial I(t, a, b)}{\partial a} \right]_{\substack{a=a^+ \\ b=b^+}} \frac{da^+}{dt} + \left[\frac{\partial I(t, a, b)}{\partial b} \right]_{\substack{a=a^+ \\ b=b^+}} \frac{db^+}{dt} \\
&= \left[\frac{\partial I(t, a, b)}{\partial t} \right]_{\substack{a=a^+ \\ b=b^+}} + \left[\frac{\partial I(t, a, b)}{\partial a} \right]_{\substack{a=a^+ \\ b=b^+}} v(t, a^+) + \left[\frac{\partial I(t, a, b)}{\partial b} \right]_{\substack{a=a^+ \\ b=b^+}} v(t, b^+).
\end{aligned}$$

Due to the fundamental theorem of calculus (see appendix in my PDEs notes), we can re-write the above as

$$\begin{aligned}
\frac{\partial}{\partial t} I^+(t, a_0, b_0) &= \left[\frac{\partial I(t, a, b)}{\partial t} \right]_{\substack{a=a^+ \\ b=b^+}} - [f(t, a)]_{\substack{a=a^+ \\ b=b^+}} v(t, a^+) + [f(t, b)]_{\substack{a=a^+ \\ b=b^+}} v(t, b^+) \\
&= \int_{a^+}^{b^+} \frac{\partial f(t, x)}{\partial t} dx - f(t, a^+) v(t, a^+) + f(t, b^+) v(t, b^+). \tag{2.32}
\end{aligned}$$

The analogue in 3D for the above is typically referred to as the Reynolds transport theorem. Consider the volume Ω_0 as a predefined set of \mathbf{y} vectors. The control volume $\Omega^+ = \Omega^+(t, \Omega_0)$ is then given by

$$\Omega^+ = \{\mathbf{x}^+ : \mathbf{y} \in \Omega_0\}. \tag{2.33}$$

Note that $\Omega^+(0, \Omega_0) = \Omega_0$. The boundary of this volume is denoted by $\partial\Omega^+$. The velocity of the boundary at any point $\mathbf{x} \in \partial\Omega^+$ is given by the Eulerian field $\mathbf{v} = \mathbf{v}(t, \mathbf{x})$ at such \mathbf{x} value. Similarly, the unit normal to the boundary at any $\mathbf{x} \in \partial\Omega^+$ is given by the Eulerian field $\mathbf{n} = \mathbf{n}(t, \mathbf{x})$ at such an \mathbf{x} . For this case $I^+ = I^+(t, \Omega_0)$ and its Eulerian counterpart is $I = I(t, \Omega)$. These two are then given by

$$I(t, \Omega) = \int_{\Omega} f(t, \mathbf{x}) dV_x, \tag{2.34}$$

$$I^+(t, \Omega_0) = I(t, \Omega^+(t, \Omega_0)). \tag{2.35}$$

We can then write

$$\frac{\partial I^+}{\partial t} = \frac{\partial I(t, \Omega^+)}{\partial t} = \frac{\partial}{\partial t} \int_{\Omega^+} f(t, \mathbf{x}) dV_x$$

Using integration by substitution, we have

$$\frac{\partial I^+}{\partial t} = \frac{\partial}{\partial t} \int_{\Omega_0} f(t, \mathbf{x}^+(t, \mathbf{y})) J^+ dV_y,$$

where J^+ is given by eq. (2.10). Since the domain of integration no longer depends on time, we can bring in the partial derivative inside the integral to obtain

$$\begin{aligned}
\frac{\partial I^+}{\partial t} &= \int_{\Omega_0} \frac{\partial}{\partial t} [f(t, \mathbf{x}^+(t, \mathbf{y})) J^+] dV_y \\
&= \int_{\Omega_0} \left[\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f \right]_{\mathbf{x}=\mathbf{x}^+} J^+ + f_{\mathbf{x}=\mathbf{x}^+} \frac{\partial J^+}{\partial t} dV_y
\end{aligned}$$

Using eq. (2.13) we get

$$\begin{aligned}\frac{\partial I^+}{\partial t} &= \int_{\Omega_0} \left[\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f \right]_{\mathbf{x}=\mathbf{x}^+} J^+ + (f \nabla \cdot \mathbf{v})_{\mathbf{x}=\mathbf{x}^+} J^+ dV_y \\ &= \int_{\Omega_0} \left[\frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{v}) \right]_{\mathbf{x}=\mathbf{x}^+} J^+ dV_y.\end{aligned}$$

Using integration by substitution again, the above becomes

$$\boxed{\frac{\partial I^+}{\partial t} = \int_{\Omega^+} \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{v}) dV_x.} \quad (2.36)$$

This is the analogue of eq. (2.2).

If the moving volume is attached to the fluid, then we use the notation $\Omega^+ = \Omega_u^+$ and $\mathbf{v} = \mathbf{u}$. Thus, given $I_u^+(t, \Omega_0) = I(t, \Omega_u^+(t, \Omega_0))$, we have

$$\begin{aligned}\frac{\partial I_u^+}{\partial t} &= \int_{\Omega_u^+} \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) dV_x \\ &= \left(\int_{\Omega} \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) dV_x \right)_{\Omega=\Omega_u^+}.\end{aligned} \quad (2.37)$$

This is the analogue of eq. (2.3). The term in parenthesis above is typically labeled as follows

$$\frac{DI}{Dt} = \int_{\Omega} \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) dV. \quad (2.38)$$

This is the analogue of eq. (2.4).

Chapter 3

Conservation laws

Conservation laws describe changes in mass, momentum, energy, and passive scalars. The densities of these four variables are shown in table 3.1. When each of these densities is multiplied by $\mathbf{u} \cdot \mathbf{n}$, then the resulting terms are referred to as convective fluxes.

3.1 Mass

Lagrangian C.V. Approach: Amount of mass contained in a Lagrangian C.V attached to the fluid is conserved.

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho \, dv = 0 \quad (3.1)$$

Using the identity in eq. (2.37), we obtain:

$$\left(\int_{\Omega} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \, dv \right)_{\Omega=\Omega_u^+(t)} = 0, \quad (3.2)$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0} \quad (3.3)$$

Eulerian C.V. Approach: Change of mass in an Eulerian C.V (stationary) is equivalent to: mass flow rate in – mass flow rate out.

$$\frac{d}{dt} \int_{\Omega} \rho \, dv = - \int_{\partial \Omega} \rho \mathbf{u} \cdot \mathbf{n} \, ds \quad (3.4)$$

Table 3.1: Densities of various fluid properties

Property	Corresponding density
Mass	ρ
Momentum	$\rho \mathbf{u}$
Energy	$\rho(e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u})$
Passive scalar	ρY

Since this volume is stationary, we move the derivative inside the integral for the term on the LHS and use Gauss's theorem for the term on the RHS,

$$\int_{\Omega} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) dv = 0. \quad (3.5)$$

Thus,

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0.} \quad (3.6)$$

Einstein Notation:

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0.} \quad (3.7)$$

Alternate Form: Expanding the second term above, the conservation of mass equation can be written as

$$\frac{D\rho}{Dt} + \rho \frac{\partial u_i}{\partial x_i} = 0. \quad (3.8)$$

3.2 Momentum

Lagrangian C.V. Approach: Change of momentum contained in a Lagrangian C.V. is equal to applied forces.

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho \mathbf{u} dv = \int_{\partial \Omega_u^+(t)} \mathbf{T} ds + \int_{\Omega_u^+(t)} \rho \mathbf{f} dv \quad (3.9)$$

where \mathbf{T} is the stress vector and \mathbf{f} the body force. Since $\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{n}$, where $\boldsymbol{\sigma}$ is the stress tensor, the above is written as

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho \mathbf{u} dv = \int_{\Omega_u^+(t)} \nabla \cdot \boldsymbol{\sigma} dv + \int_{\Omega_u^+(t)} \rho \mathbf{f} dv \quad (3.10)$$

We note that the ∇ operator is being applied to the second index of the stress tensor.

Using the identity in eq. (2.37), we obtain

$$\left(\int_{\Omega} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) dv \right)_{\Omega=\Omega_u^+(t)} = \int_{\Omega_u^+(t)} \nabla \cdot \boldsymbol{\sigma} dv + \int_{\Omega_u^+(t)} \rho \mathbf{f} dv \quad (3.11)$$

which gives,

$$\boxed{\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f}.} \quad (3.12)$$

Eulerian C.V. Approach: Change of momentum over fixed volume is equal to: (1) convected amount of momentum through the borders of the C.V. *plus* (2) the forces acting on the volume.

$$\frac{d}{dt} \int_{\Omega} \rho \mathbf{u} dv = - \int_{\partial \Omega} \rho \mathbf{u} \mathbf{u} \cdot \mathbf{n} ds + \int_{\Omega} \nabla \cdot \boldsymbol{\sigma} dv + \int_{\Omega} \rho \mathbf{f} dv. \quad (3.13)$$

Since this volume is stationary, we move the derivative inside the integral for the first term on the LHS and use Gauss's theorem for the first term on the RHS,

$$\int_{\Omega} \frac{\partial \rho \mathbf{u}}{\partial t} dv + \int_{\Omega} \nabla \cdot (\rho \mathbf{u} \mathbf{u}) dv = \int_{\Omega} \nabla \cdot \boldsymbol{\sigma} dv + \int_{\Omega} \rho \mathbf{f} dv. \quad (3.14)$$

Thus,

$$\boxed{\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f}.} \quad (3.15)$$

Einstein Notation:

$$\boxed{\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho f_i.} \quad (3.16)$$

Stress tensor: The stress tensor is expressed as follows:

$$\begin{aligned} \boldsymbol{\sigma} &= -p\mathbf{I} + \mathbf{t} \\ \sigma_{ij} &= -p\delta_{ij} + t_{ij} \end{aligned}$$

where \mathbf{t} is the deviatoric stress tensor.

With this expression the conservation of momentum becomes,

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{t} + \rho \mathbf{f}, \quad (3.17)$$

in vector notation and

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j} + \rho f_i, \quad (3.18)$$

in tensor notation.

Alternate Form: Using the product rule for the left terms of the conservation of momentum equation, where $\rho u_i u_j$ is the product of ρu_j and u_i , we get:

$$\frac{\partial \rho}{\partial t} u_i + \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial \rho u_j}{\partial x_j} u_i = -\frac{\partial p}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j} + \rho f_i$$

The first and last terms on the left side vanish due to continuity, and the second and third terms amount to ρ times the material derivative. Thus, the alternate form of the conservation of momentum is

$$\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j} + \rho f_i \quad (3.19)$$

Viscous stress tensor: The Navier-Stokes equations are the conservation of momentum equations with the shear stress tensor given by:

$$t_{ij} = 2\mu S_{ij} - \left(\frac{2}{3}\mu - \mu_\nu\right) \delta_{ij} S_{kk} \quad (3.20)$$

where μ is the coefficient of viscosity, μ_ν is the bulk coefficient of viscosity and S_{ij} is the rate of strain tensor.

If μ and μ_ν are constant, we can reformulate the derivative of the shear stress tensor as follows.

$$\begin{aligned} \frac{\partial}{\partial x_j} \left[2\mu S_{ij} - \left(\frac{2}{3}\mu - \mu_\nu\right) \delta_{ij} S_{kk} \right] &= \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \left(\frac{2}{3}\mu - \mu_\nu\right) \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] \\ &= \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \mu \frac{\partial^2 u_j}{\partial x_i \partial x_j} - \frac{2}{3}\mu \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \mu_\nu \frac{\partial^2 u_k}{\partial x_i \partial x_k} \\ &= \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3}\mu \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \mu_\nu \frac{\partial^2 u_k}{\partial x_i \partial x_k} \end{aligned}$$

The Navier-Stokes equations then become,

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3}\mu \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \mu_\nu \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \rho f_i$$

If the bulk viscosity is zero we obtain:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3} \mu \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \rho f_i$$

If the flow is incompressible, we obtain:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \rho f_i$$

3.3 Energy

Lagrangian C.V. Approach: The total energy per unit mass is denoted as E , which is defined as $E = e + K$, where e is the internal energy per unit mass and K the kinetic energy per unit mass. These energies are defined as $e = C_v T$ and $K = \frac{1}{2} u_i u_i$, where C_v is the specific heat at constant volume and T the temperature. The total change of E is equal to work done by forces on the C.V and heat transferred to the C.V.

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho E dv = \int_{\partial \Omega_u^+(t)} \mathbf{T} \cdot \mathbf{u} ds + \int_{\Omega_u^+(t)} \rho \mathbf{f} \cdot \mathbf{u} dv - \int_{\partial \Omega_u^+(t)} \mathbf{q} \cdot \mathbf{n} ds. \quad (3.21)$$

The first and second terms on the RHS are work done by the surface and body forces, respectively, and the third term is the heat transfer away from the body. Since $\mathbf{T} \cdot \mathbf{u} = (\boldsymbol{\sigma} \cdot \mathbf{n}) \cdot \mathbf{u} = (\mathbf{u} \cdot \boldsymbol{\sigma}) \cdot \mathbf{n}$, application of Gauss's law gives

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho E dv = \int_{\Omega_u^+(t)} \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) dv + \int_{\Omega_u^+(t)} \rho \mathbf{f} \cdot \mathbf{u} dv - \int_{\Omega_u^+(t)} \nabla \cdot \mathbf{q} dv. \quad (3.22)$$

Using the identity in eq. (2.37) we obtain,

$$\left(\int_{\Omega} \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) dv \right)_{\Omega=\Omega_u^+(t)} = \int_{\Omega_u^+(t)} \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) dv + \int_{\Omega_u^+(t)} \rho \mathbf{f} \cdot \mathbf{u} dv - \int_{\Omega_u^+(t)} \nabla \cdot \mathbf{q} dv, \quad (3.23)$$

which gives,

$$\boxed{\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}.} \quad (3.24)$$

Eulerian C.V. Approach: Change of energy over fixed volume is equal to: (1) convected energy through the borders of the C.V., *plus* (2) energy transfer due to work done by forces acting on the volume *plus*, (3) heat transfer away from the C.V.

$$\frac{d}{dt} \int_{\Omega} \rho E dv = - \int_{\partial \Omega} \rho E \mathbf{u} \cdot \mathbf{n} ds + \int_{\Omega} \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) dv + \int_{\Omega} \rho \mathbf{f} \cdot \mathbf{u} dv - \int_{\Omega} \nabla \cdot \mathbf{q} dv. \quad (3.25)$$

Since this volume is stationary, we move the derivative inside the integral for the first term on the LHS and use Gauss's theorem for the first term on the RHS,

$$\int_{\Omega} \frac{\partial \rho E}{\partial t} dv + \int_{\Omega} \nabla \cdot (\rho E \mathbf{u}) dv = \int_{\Omega} \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) dv + \int_{\Omega} \rho \mathbf{f} \cdot \mathbf{u} dv - \int_{\Omega} \nabla \cdot \mathbf{q} dv. \quad (3.26)$$

Thus,

$$\boxed{\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}.} \quad (3.27)$$

Einstein Notation:

$$\boxed{\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_j}{\partial x_j} = \frac{\partial u_i \sigma_{ij}}{\partial x_j} + \rho f_j u_j - \frac{\partial q_j}{\partial x_j}} \quad (3.28)$$

Stress tensor: As for the momentum case, we separate the stress tensor into its isotropic and deviatoric components, and thus express the conservation of energy equation as

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[\rho \left(E + \frac{p}{\rho} \right) \mathbf{u} \right] = \nabla \cdot (\mathbf{u} \cdot \mathbf{t}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q} \quad (3.29)$$

in vector notation, or

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_j} \left[\rho \left(E + \frac{p}{\rho} \right) u_j \right] = \frac{\partial u_i t_{ij}}{\partial x_j} + \rho f_j u_j - \frac{\partial q_j}{\partial x_j} \quad (3.30)$$

in tensor notation.

Alternate Forms: The definition of the enthalpy is

$$h = e + \frac{p}{\rho} \quad (3.31)$$

and the definition of the total enthalpy is

$$H = h + K. \quad (3.32)$$

Thus, the energy equation can be re-expressed as

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_j} (\rho H u_j) = \frac{\partial u_i t_{ij}}{\partial x_j} + \rho f_j u_j - \frac{\partial q_j}{\partial x_j} \quad (3.33)$$

Using the product rule for the terms on the left of eq. (3.28), where $\rho E u_j$ is the product of ρu_j and E , we get

$$\frac{\partial \rho}{\partial t} E + \rho \frac{\partial E}{\partial t} + \rho u_j \frac{\partial E}{\partial x_j} + \frac{\partial \rho u_j}{\partial x_j} E = \frac{\partial u_i \sigma_{ij}}{\partial x_j} + \rho f_j u_j - \frac{\partial q_j}{\partial x_j}. \quad (3.34)$$

The first and fourth terms on the left side vanish due to continuity, and the second and third terms amount to ρ times the material derivative of E . Thus, the alternate form of the conservation of energy is:

$$\rho \frac{DE}{Dt} = \frac{\partial u_i \sigma_{ij}}{\partial x_j} + \rho f_j u_j - \frac{\partial q_j}{\partial x_j}. \quad (3.35)$$

Heat conduction: According to Fourier's law, the heat transfer vector is expressed as follows

$$q_i = -\kappa \frac{\partial T}{\partial x_i} \quad (3.36)$$

where κ is the thermal conductivity and T the temperature. The thermal conductivity is obtained using

$$\kappa = \frac{\mu C_p}{Pr} \quad (3.37)$$

where Pr is the Prandtl number. We note here that the thermal diffusivity d is expressed in terms of the thermal conductivity through the relation $d = \kappa / \rho C_p$.

3.4 Passive Scalar

Lagrangian C.V. Approach: Define ϕ as some passive scalar per unit mass. The total amount of this passive scalar within a Lagrangian C.V. can change due to diffusion through the borders of the C.V., or due to sources and sinks within. Thus

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho \phi dv = - \int_{\partial \Omega_u^+(t)} \mathbf{J} \cdot \mathbf{n} ds + \int_{\Omega_u^+(t)} w dv. \quad (3.38)$$

\mathbf{J} is the diffusive mass flux and w a volumetric source/sink. Using Gauss's theorem, the above is rewritten as

$$\frac{d}{dt} \int_{\Omega_u^+(t)} \rho \phi dv = - \int_{\Omega_u^+(t)} \nabla \cdot \mathbf{J} dv + \int_{\Omega_u^+(t)} w dv. \quad (3.39)$$

Using the identity in eq. (2.37), we obtain

$$\left(\int_{\Omega} \frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \mathbf{u}) dv \right)_{\Omega=\Omega_u^+(t)} = - \int_{\Omega_u^+(t)} \nabla \cdot \mathbf{J} dv + \int_{\Omega_u^+(t)} w dv \quad (3.40)$$

which gives

$$\boxed{\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \mathbf{u}) = -\nabla \cdot \mathbf{J} + w.} \quad (3.41)$$

Eulerian C.V. Approach: The change in the amount of a passive scalar in an Eulerian C.V. is equal to: (1) the convected amount of the passive scalar through the borders of the C.V., *plus* (2) the diffusion of the scalar through the borders of the C.V., *plus* (3) the creation or destruction of the scalar within the C.V.

$$\frac{d}{dt} \int_{\Omega} \rho \phi dv = - \int_{\partial \Omega} \rho \phi \mathbf{u} \cdot \mathbf{n} ds - \int_{\partial \Omega} \mathbf{J} \cdot \mathbf{n} ds + \int_{\Omega} w dv. \quad (3.42)$$

Since this volume is stationary, we move the derivative inside the integral for the first term on the LHS, and use Gauss's theorem for the second term in the LHS

$$\int_v \frac{\partial \rho \phi}{\partial t} dv + \int_s \rho \phi \mathbf{u} \cdot \mathbf{n} ds = - \int_v \nabla \cdot \mathbf{J} dv + \int_v w dv. \quad (3.43)$$

Thus,

$$\boxed{\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \mathbf{u}) = -\nabla \cdot \mathbf{J} + w.} \quad (3.44)$$

Einstein Notation:

$$\boxed{\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \phi u_i}{\partial x_i} = -\frac{\partial J_i}{\partial x_i} + w.} \quad (3.45)$$

Alternate Form: Expanding the second term above, the conservation of scalar equation can be written as

$$\rho \frac{D\phi}{Dt} = -\frac{\partial J_i}{\partial x_i} + W. \quad (3.46)$$

Diffusive mass flux: According to Fick's law of diffusion, the diffusive mass flux is given by

$$J_i = -\rho D \frac{\partial \phi}{\partial x_i}, \quad (3.47)$$

where D is the diffusivity. It is obtained from

$$D = \frac{\mu}{\rho Sc}, \quad (3.48)$$

where Sc is the Schmidt number.

3.5 Additional relations

So far we have five conservation equations, one for ρ , three for the three components of \mathbf{u} and one for E . However, we have additional unknowns, such as p , T , μ and κ . Thus, additional equations are required to close the system. Some of these are the thermal equation of state and the caloric equation of state. As an example, for perfect gasses these two take the following forms, respectively

$$p = \rho RT, \quad (3.49)$$

$$e = C_v T. \quad (3.50)$$

In the above R is the gas constant, which is defined as $R = R_u/M$, where R_u is the universal gas constant and M the molar mass. C_v is the specific heat at constant volume. If we introduce the specific heat at constant pressure C_p , we have

$$R = C_p - C_v. \quad (3.51)$$

We also introduce γ , the ratio of specific heats

$$\gamma = \frac{C_p}{C_v}. \quad (3.52)$$

It's value is equal to 5/3 for monoatomic gases and 7/5 for diatomic gasses. Combining eqs. (3.51) and (3.52) leads to the following expressions for the specific heats

$$C_v = \frac{R}{\gamma - 1}, \quad (3.53)$$

$$C_p = \frac{\gamma R}{\gamma - 1}. \quad (3.54)$$

Using eqs. (3.50) and (3.53), we can express the caloric equation of state in terms of the energy density $U = \rho e$ as follows

$$U = \frac{1}{\gamma - 1} \rho RT. \quad (3.55)$$

Using eq. (3.49) in the above we get $U = \frac{1}{\gamma - 1} P$, which is the same as $P = (\gamma - 1)\rho e$.

We denote the mass of all atoms or molecules at a point as M and number of atoms or molecules at a point as N . Similarly, the volume at a point is denoted as V . Thus, the density can be expressed as

$$\rho = \frac{M}{V}. \quad (3.56)$$

We can also define a number density as

$$n = \frac{N}{V}. \quad (3.57)$$

Additionally, we denote the number of moles at a point as O . Avogadro's number N_a can thus be used to write

$$N = N_a O. \quad (3.58)$$

Similarly, with M as the molar mass, we have

$$M = M O. \quad (3.59)$$

Finally, we mention that the universal gas constant can be written as $R_u = k_B N_a$, where k_B is the Boltzman constant. Thus, using the relationships above, we can show that

$$\rho R = \frac{M}{V} \frac{R_u}{M} = \frac{O}{V} k_B N_a = \frac{N}{V} k_B = n k_B, \quad (3.60)$$

Thus, we can make the following equivalences

$$p = \rho R T \quad \longleftrightarrow \quad p = n k_B T, \quad (3.61)$$

$$U = \frac{1}{\gamma - 1} \rho R T \quad \longleftrightarrow \quad U = \frac{1}{\gamma - 1} n k_B T. \quad (3.62)$$

3.6 Summary of governing equations

Conservation equations

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0 \\ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} &= \frac{\partial \sigma_{ij}}{\partial x_j} + \rho f_i \\ \frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_i}{\partial x_i} &= \frac{\partial u_i \sigma_{ij}}{\partial x_j} + \rho f_i u_i - \frac{\partial q_i}{\partial x_i} \\ \frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \phi u_i}{\partial x_i} &= -\frac{\partial J_i}{\partial x_i} + w \end{aligned}$$

Transport models

$$\begin{aligned} t_{ij} &= 2\mu S_{ij}^* \\ q_i &= -\kappa \frac{\partial T}{\partial x_i} \\ J_i &= -\rho D \frac{\partial \phi}{\partial x_i} \end{aligned}$$

Transport coefficients

$$\begin{aligned} \mu &= \mu_0 \left(\frac{T}{T_0} \right)^n \\ \kappa &= \frac{\mu C_p}{Pr} \\ D &= \frac{\mu}{\rho Sc} \end{aligned}$$

Equations of state

$$p = \phi(\rho, T)$$

$$e = \psi(\rho, T)$$

Additional relations

$$E = e + K$$

$$K = \frac{1}{2} u_i u_i$$

$$\sigma_{ij} = -p\delta_{ij} + t_{ij}$$

$$S_{ij}^* = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

Chapter 4

Additional fluid equations

4.1 Vorticity Equation

The vorticity vector \mathbf{w} is defined as

$$\mathbf{w} = \nabla \times \mathbf{u}. \quad (4.1)$$

Using tensor notation, the cross product above can be reformulated as follows

$$\begin{aligned} w_i &= \epsilon_{ijk} \frac{\partial u_k}{\partial x_j} \\ &= \epsilon_{ijk} (S_{kj} + W_{kj}) \\ &= \frac{1}{2} (\epsilon_{ijk} S_{kj} - \epsilon_{ikj} S_{jk}) + \epsilon_{ijk} W_{kj} \\ &= \epsilon_{ijk} W_{kj}. \end{aligned} \quad (4.2)$$

A further identity is derived as follows

$$\begin{aligned} \frac{1}{2} \epsilon_{jit} w_t &= \frac{1}{2} \epsilon_{jit} \epsilon_{tpq} \frac{\partial u_q}{\partial x_p} \\ &= \frac{1}{2} (\delta_{jp} \delta_{iq} - \delta_{jq} \delta_{ip}) \frac{\partial u_q}{\partial x_p} \\ &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \\ &= W_{ij}, \end{aligned} \quad (4.3)$$

where standard relations for the levi-cevita tensors were used to expand their product.

The transport equation for vorticity is obtained by taking the curl of the momentum equation (3.19). This leads to

$$\frac{\partial \mathbf{w}}{\partial t} + \nabla \times [(\mathbf{u} \cdot \nabla) \mathbf{u}] = -\nabla \times \left(\frac{1}{\rho} \nabla p \right) + \nabla \times \left(\frac{1}{\rho} \nabla \cdot \mathbf{t} \right). \quad (4.4)$$

For the second term on the left hand side, we use a vector identity to write

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \left(\frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) - \mathbf{u} \times (\nabla \times \mathbf{u}). \quad (4.5)$$

Thus,

$$\nabla \times [(\mathbf{u} \cdot \nabla) \mathbf{u}] = -\nabla \times (\mathbf{u} \times \mathbf{w}). \quad (4.6)$$

Using a second vector identity, we have

$$\begin{aligned}\nabla \times (\mathbf{u} \times \mathbf{w}) &= \mathbf{u}(\nabla \cdot \mathbf{w}) - \mathbf{w}(\nabla \cdot \mathbf{u}) - (\mathbf{u} \cdot \nabla)\mathbf{w} + (\mathbf{w} \cdot \nabla)\mathbf{u} \\ &= -\mathbf{w}(\nabla \cdot \mathbf{u}) - (\mathbf{u} \cdot \nabla)\mathbf{w} + (\mathbf{w} \cdot \nabla)\mathbf{u}.\end{aligned}\quad (4.7)$$

Thus, the vorticity equation can be expressed as

$$\frac{D\mathbf{w}}{Dt} + \mathbf{w}(\nabla \cdot \mathbf{u}) - (\mathbf{w} \cdot \nabla)\mathbf{u} = -\nabla \times \left(\frac{1}{\rho} \nabla p \right) + \nabla \times \left(\frac{1}{\rho} \nabla \cdot \mathbf{t} \right). \quad (4.8)$$

For incompressible flows, the vorticity equation becomes

$$\frac{D\mathbf{w}}{Dt} - (\mathbf{w} \cdot \nabla)\mathbf{u} = \nu \Delta \mathbf{w}. \quad (4.9)$$

For inviscid flows, the vorticity equation becomes

$$\frac{D\mathbf{w}}{Dt} + \mathbf{w}(\nabla \cdot \mathbf{u}) - (\mathbf{w} \cdot \nabla)\mathbf{u} = -\nabla \times \left(\frac{1}{\rho} \nabla p \right). \quad (4.10)$$

Explain stream tubes, vortex tubes, vortex lines and line vortex (filament). NOTE: A vortex line is not a line vortex!

4.2 Kinetic energy equation

The kinetic energy is defined as $K = \frac{1}{2}u_i u_i$. To derive its transport equation, multiply the conservation of momentum eq. (3.16) by u_i . For example, for the left-hand side, one would proceed as follows

$$\begin{aligned}u_i \frac{\partial \rho u_i}{\partial t} + u_i \frac{\partial \rho u_i u_j}{\partial x_j} &= \frac{1}{2} \left(u_i \frac{\partial \rho u_i}{\partial t} + u_i \frac{\partial \rho u_i u_j}{\partial x_j} \right) + \frac{1}{2} \left(u_i \frac{\partial \rho u_i}{\partial t} + u_i \frac{\partial \rho u_i u_j}{\partial x_j} \right) \\ &= \frac{1}{2} \left(u_i \frac{\partial \rho u_i}{\partial t} + u_i \frac{\partial \rho u_i u_j}{\partial x_j} \right) \\ &\quad + \frac{1}{2} \left(\rho u_i \frac{\partial u_i}{\partial t} + \rho u_i u_j \frac{\partial u_i}{\partial x_j} + u_i u_i \frac{\partial \rho}{\partial t} + u_i u_i \frac{\partial \rho u_j}{\partial x_j} \right) \\ &= \frac{\partial \rho K}{\partial t} + \frac{\partial \rho K u_j}{\partial x_j} + K \left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} \right).\end{aligned}\quad (4.11)$$

Thus the transport equation for the TKE is as follows

$$\frac{\partial \rho K}{\partial t} + \frac{\partial \rho K u_j}{\partial x_j} = \frac{\partial u_i \sigma_{ij}}{\partial x_j} - \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \rho f_j u_j. \quad (4.12)$$

If using the expression for the stress tensor, we get

$$\frac{\partial \rho K}{\partial t} + \frac{\partial \rho K u_j}{\partial x_j} = -\frac{\partial u_j p}{\partial x_j} + \frac{\partial u_i t_{ij}}{\partial x_j} + p \frac{\partial u_i}{\partial x_i} - t_{ij} \frac{\partial u_i}{\partial x_j} + \rho f_j u_j. \quad (4.13)$$

4.3 Internal energy equation

The internal energy is defined as $e = C_v T$. To derive its transport equation, we subtract the kinetic energy eq. (4.12) from the total energy eq. (3.28) to obtain

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} = \sigma_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \quad (4.14)$$

If using the expression for the stress tensor, we get

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} = -p \frac{\partial u_i}{\partial x_i} + t_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \quad (4.15)$$

The last two terms are referred to as the dissipative terms, since they represent a transfer of energy away from K towards e .

Alternate forms of the internal energy equation can be derived, these are shown in the subsections below.

4.3.1 Pressure equation

We begin with the equation for internal energy, eq. (4.15), but express the internal energy in terms of the pressure using

$$\rho e = \rho C_v T = \frac{C_v}{R} p = \frac{1}{\gamma - 1} p. \quad (4.16)$$

Thus, the internal energy eq. (4.15) becomes

$$\frac{\partial}{\partial t} \left(\frac{1}{\gamma - 1} p \right) + \frac{\partial}{\partial x_j} \left(\frac{1}{\gamma - 1} p u_j \right) = -p \frac{\partial u_i}{\partial x_i} + t_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \quad (4.17)$$

which we re-write as

$$\frac{1}{\gamma - 1} \left(\frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \gamma p \frac{\partial u_i}{\partial x_i} \right) = t_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \quad (4.18)$$

We will now re-write the left-hand side of the pressure equation above into a more convenient form. Using eq. (3.8), we first show that

$$\frac{\partial u_i}{\partial x_i} = -\frac{1}{\rho} \frac{\partial \rho}{\partial t} - \frac{1}{\rho} \frac{\partial \rho}{\partial x_i} u_i = -\frac{\partial \ln \rho}{\partial t} - \frac{\partial \ln \rho}{\partial x_i} u_i, \quad (4.19)$$

and thus

$$\gamma \frac{\partial u_i}{\partial x_i} = -\frac{1}{\rho^\gamma} \frac{\partial \rho^\gamma}{\partial t} - \frac{1}{\rho^\gamma} \frac{\partial \rho^\gamma}{\partial x_i} u_i. \quad (4.20)$$

Using the above, one can then write

$$\begin{aligned} \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \gamma p \frac{\partial u_i}{\partial x_i} &= \frac{\partial p}{\partial t} - p \frac{1}{\rho^\gamma} \frac{\partial \rho^\gamma}{\partial t} + u_j \frac{\partial p}{\partial x_j} - p \frac{1}{\rho^\gamma} \frac{\partial \rho^\gamma}{\partial x_j} u_j \\ &= \rho^\gamma \left[\frac{\partial}{\partial t} \left(\frac{p}{\rho^\gamma} \right) + u_j \frac{\partial}{\partial x_j} \left(\frac{p}{\rho^\gamma} \right) \right]. \end{aligned} \quad (4.21)$$

Thus, the equation for pressure is re-written as

$$\frac{1}{\gamma - 1} \rho^\gamma \left[\frac{\partial}{\partial t} \left(\frac{p}{\rho^\gamma} \right) + u_j \frac{\partial}{\partial x_j} \left(\frac{p}{\rho^\gamma} \right) \right] = t_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \quad (4.22)$$

4.3.2 Enthalpy equation

Add to both sides of the internal energy eq. (4.15) the following terms

$$\frac{\partial p}{\partial t} + \frac{\partial p u_j}{\partial x_j}. \quad (4.23)$$

This allows us to write the internal energy equation as

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_j}{\partial x_j} = \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} - \frac{\partial q_j}{\partial x_j} + t_{ij} \frac{\partial u_i}{\partial x_j}. \quad (4.24)$$

4.3.3 Entropy equation

We first write the transport equation for internal energy eq. (4.15) in non-conservative form

$$\rho \frac{De}{Dt} = -\frac{\partial q_j}{\partial x_j} - p \frac{\partial u_i}{\partial x_i} + t_{ij} \frac{\partial u_i}{\partial x_j}. \quad (4.25)$$

To proceed we first note that

$$\frac{D\rho\vartheta}{Dt} = 0 \quad (4.26)$$

where $\vartheta = 1/\rho$, and thus

$$\frac{1}{\rho} \frac{D\rho}{Dt} = -\frac{1}{\vartheta} \frac{D\vartheta}{Dt}. \quad (4.27)$$

Using this in the non-conservative form of the continuity eq. (3.8) gives

$$\frac{\partial u_i}{\partial x_i} = \frac{1}{\vartheta} \frac{D\vartheta}{Dt}. \quad (4.28)$$

Thus, eq. (4.25) becomes

$$\rho \left(\frac{De}{Dt} + p \frac{D\vartheta}{Dt} \right) = -\frac{\partial q_j}{\partial x_j} + t_{ij} \frac{\partial u_i}{\partial x_j}. \quad (4.29)$$

We now make use of the Gibbs equation

$$Tds = de + pd\vartheta \quad (4.30)$$

to obtain

$$\rho T \frac{Ds}{Dt} = -\frac{\partial q_j}{\partial x_j} + t_{ij} \frac{\partial u_i}{\partial x_j}. \quad (4.31)$$

4.4 Kelvin's Theorem

4.5 Bernoulli's equation

We'll assume the flow is steady, inviscid, and the volume force is conservative. Thus, eq. (3.19) in vector notation becomes

$$\mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nabla G. \quad (4.32)$$

Using the vector identity $(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla(\frac{1}{2} \mathbf{u} \cdot \mathbf{u}) - \mathbf{u} \times (\nabla \times \mathbf{u})$ we have

$$\nabla \left(\frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) - \mathbf{u} \times (\nabla \times \mathbf{u}) = -\frac{1}{\rho} \nabla p + \nabla G. \quad (4.33)$$

It can be shown that

$$\frac{1}{\rho} \nabla p = \nabla \int \frac{1}{\rho} dp. \quad (4.34)$$

See, for example, Fundamental Mechanics of Fluids by I.G. Currie. Using this and dotting by \mathbf{u} , one obtains

$$\mathbf{u} \cdot \nabla \left(\int \frac{1}{\rho} dp + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} - G \right) = 0. \quad (4.35)$$

The above is equivalent to

$$\int \frac{1}{\rho} dp + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} - G = \text{constant along a streamline.} \quad (4.36)$$

This equation is referred to as the Bernoulli equation.

A similar result can be obtained if one focuses on the energy equation instead of the momentum equation. If the flow is steady, inviscid, and the volume force is conservative, the energy equation simplifies to

$$\mathbf{u} \cdot \nabla E = -\frac{1}{\rho} \nabla \cdot (\mathbf{u}p) + \nabla G \cdot \mathbf{u}. \quad (4.37)$$

For the first term on the right-hand side, we can write

$$\frac{1}{\rho} \nabla \cdot (\mathbf{u}p) = \frac{1}{\rho} \nabla \cdot \left(\rho \mathbf{u} \frac{p}{\rho} \right) = \mathbf{u} \cdot \nabla \left(\frac{p}{\rho} \right), \quad (4.38)$$

where we have used conservation of mass for the last equality. Thus, we now have

$$\mathbf{u} \cdot \nabla \left(E + \frac{p}{\rho} - G \right) = 0, \quad (4.39)$$

or in terms of enthalpy

$$\mathbf{u} \cdot \nabla (h + K - G) = 0, \quad (4.40)$$

The above is equivalent to

$$h + K - G = \text{constant along a streamline.} \quad (4.41)$$

4.6 Arbitrary Lagrangian Eulerian equations

4.6.1 Differential form

Consider an arbitrary particle—not a fluid particle—with position \mathbf{x}^+ and velocity field \mathbf{v} . Using eq. (2.2) for the density function $\rho^+ = \rho(t, \mathbf{x}^+)$ we have

$$\frac{\partial \rho^+}{\partial t} = \left(\frac{\partial \rho}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+} + (\mathbf{v} \cdot \nabla \rho)_{\mathbf{x}=\mathbf{x}^+}. \quad (4.42)$$

We evaluate eq. (3.6) at the particle's location \mathbf{x}^+ , which we express as

$$\left(\frac{\partial \rho}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+} + (\mathbf{u} \cdot \nabla \rho)_{\mathbf{x}=\mathbf{x}^+} + (\rho \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = 0.$$

Using eq. (4.42), this can be written as

$$\frac{\partial \rho^+}{\partial t} + [(\mathbf{u} - \mathbf{v}) \cdot \nabla \rho]_{\mathbf{x}=\mathbf{x}^+} + (\rho \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = 0.$$

Manipulating, we have

$$\frac{\partial \rho^+}{\partial t} + \{ \nabla \cdot [\rho(\mathbf{u} - \mathbf{v})] \}_{\mathbf{x}=\mathbf{x}^+} + (\rho \nabla \cdot \mathbf{v})_{\mathbf{x}=\mathbf{x}^+} = 0.$$

Using eq. (2.13), the above becomes

$$\frac{\partial \rho^+}{\partial t} + \{ \nabla \cdot [\rho(\mathbf{u} - \mathbf{v})] \}_{\mathbf{x}=\mathbf{x}^+} + \rho^+ \frac{1}{J^+} \frac{\partial J^+}{\partial t} = 0.$$

Multiplying by J^+ we finally obtain

$$\frac{\partial J^+ \rho^+}{\partial t} + J^+ \{ \nabla \cdot [\rho(\mathbf{u} - \mathbf{v})] \}_{\mathbf{x}=\mathbf{x}^+} = 0. \quad (4.43)$$

We follow the same procedure detailed above but for the momentum equation. Using eq. (2.2), we have

$$\frac{\partial \rho^+ \mathbf{u}^+}{\partial t} = \left(\frac{\partial \rho \mathbf{u}}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+} + (\mathbf{v} \cdot \nabla \rho \mathbf{u})_{\mathbf{x}=\mathbf{x}^+}. \quad (4.44)$$

We evaluate eq. (3.15) at the particle's location, which we express as

$$\left(\frac{\partial \rho \mathbf{u}}{\partial t} \right)_{\mathbf{x}=\mathbf{x}^+} + [\mathbf{u} \cdot \nabla (\rho \mathbf{u})]_{\mathbf{x}=\mathbf{x}^+} + (\rho \mathbf{u} \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}.$$

Using eq. (4.44), this can be written as

$$\frac{\partial \rho^+ \mathbf{u}^+}{\partial t} + [(\mathbf{u} - \mathbf{v}) \cdot \nabla (\rho \mathbf{u})]_{\mathbf{x}=\mathbf{x}^+} + (\rho \mathbf{u} \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}.$$

Manipulating, we have

$$\frac{\partial \rho^+ \mathbf{u}^+}{\partial t} + \{\nabla \cdot [\rho \mathbf{u}(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} + (\rho \mathbf{u} \nabla \cdot \mathbf{v})_{\mathbf{x}=\mathbf{x}^+} = (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}.$$

Using eq. (2.13), the above becomes

$$\frac{\partial \rho^+ \mathbf{u}^+}{\partial t} + \{\nabla \cdot [\rho \mathbf{u}(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} + \rho^+ \mathbf{u}^+ \frac{1}{J^+} \frac{\partial J^+}{\partial t} = (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}.$$

Multiplying by J^+ we finally obtain

$$\frac{\partial J^+ \rho^+ \mathbf{u}^+}{\partial t} + J^+ \{\nabla \cdot [\rho \mathbf{u}(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} = J^+ (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f})_{\mathbf{x}=\mathbf{x}^+}. \quad (4.45)$$

We now follow the previous procedure but for the energy equation. Using eq. (2.2), we have

$$\frac{\partial \rho^+ E^+}{\partial t} = \left[\frac{\partial \rho E}{\partial t} \right]_{\mathbf{x}=\mathbf{x}^+} + [\mathbf{v} \cdot \nabla (\rho E)]_{\mathbf{x}=\mathbf{x}^+}. \quad (4.46)$$

We evaluate eq. (3.27) at the particle's location, which we express as

$$\begin{aligned} \left[\frac{\partial \rho E}{\partial t} \right]_{\mathbf{x}=\mathbf{x}^+} + [\mathbf{u} \cdot \nabla (\rho E)]_{\mathbf{x}=\mathbf{x}^+} + (\rho E \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = \\ [\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}]_{\mathbf{x}=\mathbf{x}^+}. \end{aligned}$$

Using eq. (4.46), this can be written as

$$\begin{aligned} \frac{\partial \rho^+ E^+}{\partial t} + \{(\mathbf{u} - \mathbf{v}) \cdot \nabla (\rho E)\}_{\mathbf{x}=\mathbf{x}^+} + (\rho E \nabla \cdot \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} = \\ [\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}]_{\mathbf{x}=\mathbf{x}^+}. \end{aligned}$$

Manipulating, we have

$$\begin{aligned} \frac{\partial \rho^+ E^+}{\partial t} + \{\nabla \cdot [\rho E(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} + (\rho E \nabla \cdot \mathbf{v})_{\mathbf{x}=\mathbf{x}^+} = \\ [\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}]_{\mathbf{x}=\mathbf{x}^+}. \end{aligned}$$

Using eq. (2.13), the above becomes

$$\frac{\partial \rho^+ E^+}{\partial t} + \{\nabla \cdot [\rho E(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} + \rho^+ E^+ \frac{1}{J^+} \frac{\partial J^+}{\partial t} = [\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}]_{\mathbf{x}=\mathbf{x}^+}.$$

Multiplying by J^+ we finally obtain

$$\frac{\partial J^+ \rho^+ E^+}{\partial t} + J^+ \{\nabla \cdot [\rho E(\mathbf{u} - \mathbf{v})]\}_{\mathbf{x}=\mathbf{x}^+} = J^+ [\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}]_{\mathbf{x}=\mathbf{x}^+}. \quad (4.47)$$

4.6.2 Integral form

Consider an arbitrary volume—not a material volume—whose volume is given by $\Omega^+(t)$, and its boundary motion is given by \mathbf{v} . Using eq. (2.36) for the density we have

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho dv = \int_{\Omega^+(t)} \frac{\partial \rho}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho \mathbf{v}) dv. \quad (4.48)$$

We integrate eq. (3.6) over the volume $\Omega^+(t)$, which we express as

$$\int_{\Omega^+(t)} \frac{\partial \rho}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho \mathbf{u}) dv = 0.$$

Using eq. (4.48) and the divergence theorem, this can be written as

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho dv + \int_{\partial\Omega^+(t)} \rho(\mathbf{u} - \mathbf{v}) \cdot \mathbf{n} ds. \quad (4.49)$$

We follow the same procedure as detailed above but for the momentum equations. Using eq. (2.36) for momentum we have

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho \mathbf{u} dv = \int_{\Omega^+(t)} \frac{\partial \rho \mathbf{u}}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho \mathbf{u} \mathbf{v}) dv. \quad (4.50)$$

We integrate eq. (3.15) over the volume $\Omega^+(t)$, which we express as

$$\int_{\Omega^+(t)} \frac{\partial \rho \mathbf{u}}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho \mathbf{u} \mathbf{u}) dv = \int_{\Omega^+(t)} \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{f} dv.$$

Using eq. (4.50) and the divergence theorem, this can be written as

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho \mathbf{u} dv + \int_{\partial\Omega^+(t)} \rho \mathbf{u}(\mathbf{u} - \mathbf{v}) \cdot \mathbf{n} ds = \int_{\partial\Omega^+(t)} \boldsymbol{\sigma} \cdot \mathbf{n} ds + \int_{\Omega^+(t)} \rho \mathbf{f} dv. \quad (4.51)$$

We repeat the same procedure as above but for the energy equation. Using eq. (2.36) for energy we have

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho E dv = \int_{\Omega^+(t)} \frac{\partial \rho E}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho E \mathbf{v}) dv. \quad (4.52)$$

We integrate eq. (3.27) over the volume $\Omega^+(t)$, which we express as

$$\int_{\Omega^+(t)} \frac{\partial \rho E}{\partial t} dv + \int_{\Omega^+(t)} \nabla \cdot (\rho \mathbf{u} E) dv = \int_{\Omega^+(t)} \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}) + \rho \mathbf{f} \cdot \mathbf{u} - \nabla \cdot \mathbf{q} dv.$$

Using eq. (4.52) and the divergence theorem, this can be written as

$$\begin{aligned} \frac{d}{dt} \int_{\Omega^+(t)} \rho E \, dv + \int_{\partial\Omega^+(t)} \rho E (\mathbf{u} - \mathbf{v}) \cdot \mathbf{n} \, ds = \\ \int_{\partial\Omega^+(t)} \mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} \, ds + \int_{\Omega^+(t)} \rho \mathbf{f} \cdot \mathbf{u} \, ds - \int_{\partial\Omega^+(t)} \mathbf{q} \cdot \mathbf{n} \, ds. \end{aligned} \quad (4.53)$$

Chapter 5

Mixtures

5.1 Multi-material vs. multi-fluid vs. multi-species

Multi-material, multi-fluid, and multi-species refer to different aspects of a fluid model. These are not mutually exclusive, for example, one can have a multi-material multi-fluid model, or a multi-material single-fluid model. Below are some definitions:

1. Multi-species: the fluid is composed of multiple species.
2. Multi-fluid: a velocity equation is solved for each species.
3. Multi-material: the species are grouped into bunches that share some general properties, such as EOS and thermal conductivity. Either a multi-fluid or single-fluid formulation can be multi-material.

Multi-material or multi-fluid problems are always multi-species. Single-material or single-fluid problems can also be multi-species, but are not necessarily always so. Thus, we use the multi-species label only when dealing with the single-material single-fluid model, to clarify whether we are using that model for cases where there are multiple species or not.

5.2 Definition of multi-material variables

We define a material k as a collection of species s . Rather than labeling species using the single subscript s , we'll use the subscript k, i, s and k, e , where the former denotes the ion species s that belongs to material k , and the latter denotes the electron species that belongs to material k . The number of ion species within a material is denoted as \mathcal{N}_k , and the total number of materials as \mathcal{M} .

For multi-material problems there is a large number of new variables that are used. These are summarized below.

Mass densities

$$\rho = \frac{M}{V}. \quad (5.1)$$

$$\rho_k = \frac{M_k}{V_k}. \quad (5.2)$$

$$\rho_{k,i,s} = \frac{M_{k,i,s}}{V_{k,i,s}}. \quad (5.3)$$

$$\rho_{k,e} = \frac{M_{k,e}}{V_k}. \quad (5.4)$$

Number densities

$$n = \frac{N}{V}. \quad (5.5)$$

$$n_k = \frac{N_k}{V_k}. \quad (5.6)$$

$$n_{k,i,s} = \frac{N_{k,i,s}}{V_{k,i,s}}. \quad (5.7)$$

$$n_{k,e} = \frac{N_{k,e}}{V_k}. \quad (5.8)$$

Relation between mass and number densities

$$m_{k,i,s} n_{k,i,s} = \rho_{k,i,s}. \quad (5.9)$$

$$m_e n_{k,e} = \rho_{k,e}. \quad (5.10)$$

Material volume and mass fractions

$$\eta_k = \frac{V_k}{V}, \quad (5.11)$$

$$Y_k = \frac{M_k}{M}. \quad (5.12)$$

$$\rho_k = \rho \frac{Y_k}{\eta_k}. \quad (5.13)$$

Species volume and mass fractions

$$\eta_{k,i,s} = \frac{V_{k,i,s}}{V_k}. \quad (5.14)$$

$$Y_{k,i,s} = \frac{M_{k,i,s}}{M_k}. \quad (5.15)$$

$$\rho_{k,i,s} = \rho_k \frac{Y_{k,i,s}}{\eta_{k,i,s}}. \quad (5.16)$$

Energies

$$e = \frac{IE}{M}. \quad (5.17)$$

$$e_k = \frac{IE_k}{M_k}. \quad (5.18)$$

$$e_{k,i,s} = \frac{IE_{k,i,s}}{M_{k,i,s}}. \quad (5.19)$$

$$e_{k,e} = \frac{IE_{k,e}}{M_k}. \quad (5.20)$$

Total ion variables

$$\eta_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} \approx 1, \quad (5.21)$$

$$Y_{k,i} = \sum_s^{\mathcal{N}_k} Y_{k,i,s} \approx 1, \quad (5.22)$$

$$n_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} n_{k,i,s}. \quad (5.23)$$

$$e_{k,i} = \sum_s^{\mathcal{N}_k} Y_{k,i,s} e_{k,i,s}. \quad (5.24)$$

$$h_{k,i} = \sum_s^{\mathcal{N}_k} Y_{k,i,s} h_{k,i,s}. \quad (5.25)$$

$$p_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} p_{k,i,s}. \quad (5.26)$$

$$\rho_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} \rho_{k,i,s}. \quad (5.27)$$

$$\mathbf{t}_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} \mathbf{t}_{k,i,s}. \quad (5.28)$$

$$\boldsymbol{\sigma}_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s}. \quad (5.29)$$

$$\mathbf{R}_{k,i} = \sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s}. \quad (5.30)$$

$$\mathbf{q}_{k,i} = \sum_s^{\mathcal{N}_k} \mathbf{q}_{k,i,s}. \quad (5.31)$$

$$Q_{k,i} = \sum_s^{\mathcal{N}_k} Q_{k,i,s}. \quad (5.32)$$

5.3 Interpretation of multi-material variables

Consider the volume $V_{\Omega,k}$ occupied by material k in some subdomain Ω . This can be computed by using the volume fraction $\eta_k = \eta_k(t, \mathbf{x})$ as shown below

$$V_{\Omega,k} = \int_{\Omega} \eta_k d\mathbf{x}. \quad (5.33)$$

Now consider the mass $M_{\Omega,k}$ of material k in some subdomain Ω . This can be computed by summing up the masses m_i of the atoms or molecules of material k in this subdomain, or by using the mass fraction $Y_k = Y_k(t, \mathbf{x})$, as shown below

$$M_{\Omega,k} = \sum_{i \in \Omega, i \in k} m_i = \int_{\Omega} \rho Y_k d\mathbf{x}. \quad (5.34)$$

In the above $i \in \Omega, i \in k$ denotes the atoms or molecules of material k located in the subdomain Ω . Finally, consider the internal energy $IE_{\Omega,k}$ of material k in some subdomain Ω . This internal energy can be computed by summing up the internal energies ϵ_i of the atoms or molecules of material k in this subdomain, or by using the specific internal energy $e_k = e_k(t, \mathbf{x})$, as shown below

$$IE_{\Omega,k} = \sum_{i \in \Omega, i \in k} \epsilon_i = \int_{\Omega} \rho Y_k e_k d\mathbf{x}. \quad (5.35)$$

We can now write

$$\eta_k = \lim_{\Omega \rightarrow \epsilon} \frac{1}{V_{\Omega}} \int_{\Omega} \eta_k d\mathbf{x} = \lim_{\Omega \rightarrow \epsilon} \frac{V_{\Omega,k}}{V_{\Omega}}. \quad (5.36)$$

That is, the volume fraction is the volume occupied by material k within a small domain divided by the volume of that small domain as the domain becomes sufficiently small. For mass fraction, we have

$$Y_k = \frac{\rho Y_k}{\rho} = \lim_{\Omega \rightarrow \epsilon} \frac{\frac{1}{V_{\Omega}} \int_{\Omega} \rho Y_k d\mathbf{x}}{\frac{1}{V_{\Omega}} \int_{\Omega} \rho d\mathbf{x}} = \lim_{\Omega \rightarrow \epsilon} \frac{\sum_{i \in \Omega, i \in k} m_i}{\sum_{i \in \Omega} m_i} = \lim_{\Omega \rightarrow \epsilon} \frac{M_{\Omega,k}}{M_{\Omega}}. \quad (5.37)$$

That is, the mass fraction is the mass of material k contained in a small domain divided by the mass contained in that small domain as the domain becomes sufficiently small. Similarly for specific internal energy of an material, we have

$$e_k = \frac{\rho Y_k e_k}{\rho Y_k} = \lim_{\Omega \rightarrow \epsilon} \frac{\frac{1}{V_{\Omega}} \int_{\Omega} \rho Y_k e_k d\mathbf{x}}{\frac{1}{V_{\Omega}} \int_{\Omega} \rho Y_k d\mathbf{x}} = \lim_{\Omega \rightarrow \epsilon} \frac{\sum_{i \in \Omega, i \in k} \epsilon_i}{\sum_{i \in \Omega, i \in k} m_i} = \lim_{\Omega \rightarrow \epsilon} \frac{IE_{\Omega,k}}{M_{\Omega,k}}. \quad (5.38)$$

That is, the specific internal energy of an material is the internal energy of material k contained in a small domain divided by the mass of material k in that small domain as the domain becomes sufficiently small.

5.4 Multi-fluid formulation

5.4.1 Fluid equations derived from kinetic equation

The starting point are fluid equations derived from the kinetic equation (see general notes) complemented with the definitions of current and charge density as well as an ideal equation of state. These are summarized below.

- Particle density

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \mathbf{u}_s) = \hat{S}_s, \quad (5.39)$$

- Momentum

$$\frac{\partial m_s n_s \mathbf{u}_s}{\partial t} + \nabla \cdot (m_s n_s \mathbf{u}_s \mathbf{u}_s) - Z_s e n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) = \nabla \cdot \boldsymbol{\sigma}_s + \mathbf{R}_s + \hat{\mathbf{M}}_s, \quad (5.40)$$

- Internal Energy

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_s \right) + \nabla \cdot \left(\frac{3}{2} p_s \mathbf{u}_s \right) = \boldsymbol{\sigma}_s : \nabla \mathbf{u}_s - \nabla \cdot \mathbf{q}_s + Q_s + \hat{Q}_s - \mathbf{u}_s \cdot \hat{\mathbf{M}}_s + m_s K_s \hat{S}_s. \quad (5.41)$$

- Current density

$$\mathbf{J} = \sum_s^{\mathcal{N}} Z_s e n_s \mathbf{u}_s. \quad (5.42)$$

- Charge density

$$\rho_q = \sum_s^{\mathcal{N}} Z_s e n_s. \quad (5.43)$$

- Equation of state

$$p_s = n_s k_B T_s. \quad (5.44)$$

For the treatment in this section, we'll use the following assumptions:

1. No sources ($\hat{S}_s = \hat{\mathbf{M}}_s = \hat{Q}_s = 0$ for all s).

5.4.2 Multi-material multi-fluid model

We note that the number densities in section 5.4.1 use as their denominator the total volume. We would instead like to express densities using variables such as that defined in eq. (5.7), where the denominator is only the volume of the species under consideration. The correspondence between these two densities is $n_s \rightarrow \eta_k \eta_{k,i,s} n_{k,i,s}$. Using an ideal equation of state, we have

$$p_i = n_i k_B T_i \rightarrow \eta_k \eta_{k,i,s} n_{k,i,s} k_B T_{k,i,s} = \eta_k \eta_{k,i,s} p_{k,i,s}, \quad (5.45)$$

where $p_{k,i,s} = n_{k,i,s} k_B T_{k,i,s}$. The same argument above applies to the stress tensor since it is defined in terms of the pressure. Finally, the analogous is used for electron quantities as well. Thus, the governing equations in section 5.4.1 are now written as

$$\frac{\partial \eta_k \eta_{k,i,s} n_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s}) = 0, \quad (5.46)$$

$$\frac{\partial \eta_k n_{k,e}}{\partial t} + \nabla \cdot (\eta_k n_{k,e} \mathbf{u}_{k,e}) = 0, \quad (5.47)$$

$$\begin{aligned} \frac{\partial m_{k,i,s} \eta_k \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s}}{\partial t} + \nabla \cdot (m_{k,i,s} \eta_k \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}_{k,i,s}) \\ - Z_{k,i,s} e \eta_k \eta_{k,i,s} n_{k,i,s} (\mathbf{E} + \mathbf{u}_{k,i,s} \times \mathbf{B}) = \nabla \cdot (\eta_k \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s}) + \mathbf{R}_{k,i,s}, \end{aligned} \quad (5.48)$$

$$\begin{aligned} \frac{\partial m_{k,e} \eta_k n_{k,e} \mathbf{u}_{k,e}}{\partial t} + \nabla \cdot (m_{k,e} \eta_k n_{k,e} \mathbf{u}_{k,e} \mathbf{u}_{k,e}) \\ + e \eta_k n_{k,e} (\mathbf{E} + \mathbf{u}_{k,e} \times \mathbf{B}) = \nabla \cdot (\eta_k \boldsymbol{\sigma}_{k,e}) + \mathbf{R}_{k,e}, \end{aligned} \quad (5.49)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k \eta_{k,i,s} p_{k,i,s} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k \eta_{k,i,s} p_{k,i,s} \mathbf{u}_{k,i,s} \right) = \eta_k \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} : \nabla \mathbf{u}_{k,i,s} - \nabla \cdot \mathbf{q}_{k,i,s} + Q_{k,i,s}, \quad (5.50)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k p_{k,e} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,e} \mathbf{u}_{k,e} \right) = \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u}_{k,e} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e}, \quad (5.51)$$

$$\mathbf{J}_k = e\eta_k \left(\sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - n_{k,e} \mathbf{u}_{k,e} \right), \quad (5.52)$$

$$\mathbf{J} = \sum_k^{\mathcal{M}} \mathbf{J}_k \quad (5.53)$$

$$\rho_{q,k} = e\eta_k \left(\sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} - n_{k,e} \right), \quad (5.54)$$

$$\rho_q = \sum_k^{\mathcal{M}} \rho_{q,k}, \quad (5.55)$$

$$p_{k,i,s} = n_{k,i,s} k_B T_{k,i,s}, \quad (5.56)$$

$$p_{k,e} = n_{k,e} k_B T_{k,e}. \quad (5.57)$$

5.4.3 Single-material multi-fluid model

The equations are the same as the multi-material formulation, but there is only one material now and hence the k subscript can be dropped and all $\eta_k = 1$. Thus we have

$$\frac{\partial \eta_{i,s} n_{i,s}}{\partial t} + \nabla \cdot (\eta_{i,s} n_{i,s} \mathbf{u}_{i,s}) = 0, \quad (5.58)$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{u}_e) = 0, \quad (5.59)$$

$$\frac{\partial m_{i,s} \eta_{i,s} n_{i,s} \mathbf{u}_{i,s}}{\partial t} + \nabla \cdot (m_{i,s} \eta_{i,s} n_{i,s} \mathbf{u}_{i,s} \mathbf{u}_{i,s}) - Z_{i,s} e \eta_{i,s} n_{i,s} (\mathbf{E} + \mathbf{u}_{i,s} \times \mathbf{B}) = \nabla \cdot (\eta_{i,s} \boldsymbol{\sigma}_{i,s}) + \mathbf{R}_{i,s}, \quad (5.60)$$

$$\frac{\partial m_e n_e \mathbf{u}_e}{\partial t} + \nabla \cdot (m_e n_e \mathbf{u}_e \mathbf{u}_e) + e n_e (\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) = \nabla \cdot \boldsymbol{\sigma}_e + \mathbf{R}_e, \quad (5.61)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} \eta_{i,s} p_{i,s} \right) + \nabla \cdot \left(\frac{3}{2} \eta_{i,s} p_{i,s} \mathbf{u}_{i,s} \right) = \eta_{i,s} \boldsymbol{\sigma}_{i,s} : \nabla \mathbf{u}_{i,s} - \nabla \cdot \mathbf{q}_{i,s} + Q_{i,s}, \quad (5.62)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_e \right) + \nabla \cdot \left(\frac{3}{2} p_e \mathbf{u}_e \right) = \boldsymbol{\sigma}_e : \nabla \mathbf{u}_e - \nabla \cdot \mathbf{q}_e + Q_e, \quad (5.63)$$

$$\mathbf{J} = e \left(\sum_s^{\mathcal{N}} Z_{i,s} \eta_{i,s} n_{i,s} \mathbf{u}_{i,s} - n_e \mathbf{u}_e \right), \quad (5.64)$$

$$\rho_q = e \left(\sum_s^{\mathcal{N}} Z_{i,s} \eta_{i,s} n_{i,s} - n_e \right), \quad (5.65)$$

$$p_{i,s} = n_{i,s} k_B T_{i,s}, \quad (5.66)$$

$$p_e = n_e k_B T_e. \quad (5.67)$$

5.4.4 Single-material two-fluid model

If there is only one ion species, then we have the two-fluid model. For this case $\eta_{i,s}n_{i,s}$, $\eta_{i,s}p_{i,s}$, and $\eta_{i,s}\boldsymbol{\sigma}_{i,s}$ simplify to $\eta_i n_i$, $\eta_i p_i$, and $\eta_i \boldsymbol{\sigma}_i$, respectively. Since $\eta_i \approx 1$, we have

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{u}_i) = 0, \quad (5.68)$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{u}_e) = 0, \quad (5.69)$$

$$\frac{\partial m_i n_i \mathbf{u}_i}{\partial t} + \nabla \cdot (m_i n_i \mathbf{u}_i \mathbf{u}_i) - Z e n_i (\mathbf{E} + \mathbf{u}_i \times \mathbf{B}) = \nabla \cdot \boldsymbol{\sigma}_i + \mathbf{R}_i, \quad (5.70)$$

$$\frac{\partial m_e n_e \mathbf{u}_e}{\partial t} + \nabla \cdot (m_e n_e \mathbf{u}_e \mathbf{u}_e) + e n_e (\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) = \nabla \cdot \boldsymbol{\sigma}_e + \mathbf{R}_e, \quad (5.71)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_i \right) + \nabla \cdot \left(\frac{3}{2} p_i \mathbf{u}_i \right) = \boldsymbol{\sigma}_i : \nabla \mathbf{u}_i - \nabla \cdot \mathbf{q}_i + Q_i, \quad (5.72)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_e \right) + \nabla \cdot \left(\frac{3}{2} p_e \mathbf{u}_e \right) = \boldsymbol{\sigma}_e : \nabla \mathbf{u}_e - \nabla \cdot \mathbf{q}_e + Q_e, \quad (5.73)$$

$$\mathbf{J} = e(Z n_i \mathbf{u}_i - n_e \mathbf{u}_e), \quad (5.74)$$

$$\rho_q = e(Z n_i - n_e). \quad (5.75)$$

$$p_i = n_i k_B T_i, \quad (5.76)$$

$$p_e = n_e k_B T_e. \quad (5.77)$$

5.5 Single-fluid formulation

A single-fluid formulation is defined as that for which there is a single velocity vector. For the single-fluid formulation, we'll use the following assumptions

1. $m_{k,e} \approx 0$ since $m_{k,e} \ll m_{k,i,s}$.
2. Quasi-neutrality, i.e. $\sum_s \mathcal{N}_k Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} = n_{k,e}$.

5.5.1 Single-fluid variables

We now introduce the following single-fluid variables

$$\mathbf{u}_{k,i} = \sum_s \mathcal{N}_k Y_{k,i,s} \mathbf{u}_{k,i,s} \quad (5.78)$$

$$\mathbf{u} = \sum_k \mathcal{M} Y_k \mathbf{u}_{k,i}. \quad (5.79)$$

$$e_k = e_{k,i} + e_{k,e}. \quad (5.80)$$

$$e = \sum_k \mathcal{M} Y_k e_k. \quad (5.81)$$

$$h_k = h_{k,i} + h_{k,e}. \quad (5.82)$$

$$h = \sum_k \mathcal{M} Y_k h_k. \quad (5.83)$$

5.5.2 Total sum of collisional terms

In the general notes, we derived the following two expressions

$$\sum_s^{\mathcal{N}} \mathbf{R}_s = 0, \quad (5.84)$$

$$\sum_s^{\mathcal{N}} Q_s = - \sum_s^{\mathcal{N}} \mathbf{u}_s \cdot \mathbf{R}_s. \quad (5.85)$$

Using the current notation, the above two are re-written as

$$\sum_k^{\mathcal{M}} \left(\sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e} \right) = 0. \quad (5.86)$$

$$\sum_k^{\mathcal{M}} \left(\sum_s^{\mathcal{N}_k} Q_{k,i,s} + Q_{k,e} \right) = - \sum_k^{\mathcal{M}} \left(\sum_s^{\mathcal{N}_k} \mathbf{u}_{k,i,s} \cdot \mathbf{R}_{k,i,s} + \mathbf{u}_{k,e} \cdot \mathbf{R}_{k,e} \right). \quad (5.87)$$

5.5.3 The general model

Mass

Multiplying eq. (5.46) by $m_{k,i,s}$ and using eq. (5.9) gives

$$\frac{\partial \eta_k \eta_{k,i,s} \rho_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \eta_{k,i,s} \rho_{k,i,s} \mathbf{u}_{k,i,s}) = 0.$$

Using eq. (5.16), the above becomes

$$\frac{\partial \eta_k \rho_k Y_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s}) = 0.$$

We introduce the species diffusion vector

$$\mathbf{j}_{k,i,s} = \eta_k \rho_k Y_{k,i,s} \mathbf{w}_{k,i,s}, \quad (5.88)$$

where

$$\mathbf{w}_{k,i,s} = \mathbf{u}_{k,i,s} - \mathbf{u}. \quad (5.89)$$

The mass-conservation equation is then written as

$$\frac{\partial \eta_k \rho_k Y_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \rho_k Y_{k,i,s} \mathbf{u}) = - \nabla \cdot \mathbf{j}_{k,i,s}.$$

Note that adding over all s of a material gives

$$\frac{\partial \eta_k \rho_k}{\partial t} + \nabla \cdot (\eta_k \rho_k \mathbf{u}) = - \nabla \cdot \mathbf{j}_{k,i},$$

where

$$\mathbf{j}_{k,i} = \eta_k \rho_k \mathbf{w}_{k,i}, \quad (5.90)$$

and

$$\mathbf{w}_{k,i} = \mathbf{u}_{k,i} - \mathbf{u}. \quad (5.91)$$

Multiplying eq. (5.46) by $Z_{k,i,s}$ and summing over all s of a material gives

$$\frac{\partial}{\partial t} \left(\eta_k \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \right) + \nabla \cdot \left(\eta_k \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \right) = 0.$$

Subtracting eq. (5.47) from the above and using the assumption of quasi-neutrality in item 2 gives

$$\nabla \cdot \left(\eta_k \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - n_{k,e} \mathbf{u}_{k,e} \right) = 0,$$

which is equivalent to

$$\nabla \cdot \mathbf{J}_k = 0.$$

Summing over all k gives

$$\nabla \cdot \mathbf{J} = 0.$$

Momentum

We now add eqs. (5.48) and (5.49) and use item 1 to obtain

$$\begin{aligned} \frac{\partial m_{k,i,s} \eta_k \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s}}{\partial t} + \nabla \cdot (m_{k,i,s} \eta_k \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}_{k,i,s}) - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} - n_{k,e}) \mathbf{E} \\ - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - n_{k,e} \mathbf{u}_{k,e}) \times \mathbf{B} = \nabla \cdot [\eta_k (\eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e})] + \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

Using eq. (5.9) the above becomes

$$\begin{aligned} \frac{\partial \eta_k \eta_{k,i,s} \rho_{k,i,s} \mathbf{u}_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \eta_{k,i,s} \rho_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}_{k,i,s}) - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} - n_{k,e}) \mathbf{E} \\ - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - n_{k,e} \mathbf{u}_{k,e}) \times \mathbf{B} = \nabla \cdot [\eta_k (\eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e})] + \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

Using eq. (5.16) we get

$$\begin{aligned} \frac{\partial \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}_{k,i,s}) - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} - n_{k,e}) \mathbf{E} \\ - e \eta_k (Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - n_{k,e} \mathbf{u}_{k,e}) \times \mathbf{B} = \nabla \cdot [\eta_k (\eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e})] + \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

Summing over all s of a material, using the assumption of item 2 and the definition of the current in eq. (5.52) the above simplifies to

$$\begin{aligned} \frac{\partial}{\partial t} \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} + \nabla \cdot \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}_{k,i,s} - \mathbf{J}_k \times \mathbf{B} = \\ \nabla \cdot \left[\eta_k \left(\sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e} \right) \right] + \sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

We now write the momentum equation as

$$\begin{aligned} \frac{\partial}{\partial t} \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} + \nabla \cdot \sum_s^{\mathcal{N}_k} [\eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u} + \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} (\mathbf{u}_{k,i,s} - \mathbf{u})] - \mathbf{J}_k \times \mathbf{B} = \\ \nabla \cdot \left[\eta_k \left(\sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e} \right) \right] + \sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

Using the definition of $\mathbf{j}_{k,i,s}$ the above becomes

$$\begin{aligned} \frac{\partial}{\partial t} \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} + \nabla \cdot \sum_s^{\mathcal{N}_k} (\eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}) - \mathbf{J}_k \times \mathbf{B} = \\ \nabla \cdot \left[\eta_k \left(\sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e} \right) \right] - \nabla \cdot \sum_s^{\mathcal{N}_k} \mathbf{j}_{k,i,s} \mathbf{u}_{k,i,s} + \sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e}. \end{aligned}$$

We now sum over all materials to obtain

$$\begin{aligned} \frac{\partial}{\partial t} \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} + \nabla \cdot \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} (\eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \\ \nabla \cdot \sum_k^{\mathcal{M}} \left(\sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e} \right) - \nabla \cdot \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \mathbf{j}_{k,i,s} \mathbf{u}_{k,i,s} + \sum_k^{\mathcal{M}} \left(\sum_s^{\mathcal{N}_k} \mathbf{R}_{k,i,s} + \mathbf{R}_{k,e} \right). \end{aligned}$$

We note that

$$\sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \eta_k \rho_k Y_{k,i,s} \mathbf{u}_{k,i,s} = \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \rho Y_k Y_{k,i,s} \mathbf{u}_{k,i,s} = \rho \mathbf{u}. \quad (5.92)$$

Using the above and eq. (5.86) we get

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \sum_k^{\mathcal{M}} \left[\eta_k \left(\sum_s^{\mathcal{N}_k} \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} + \boldsymbol{\sigma}_{k,e} \right) \right] - \nabla \cdot \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \mathbf{j}_{k,i,s} \mathbf{u}_{k,i,s}.$$

Finally, we write the above as

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \sum_k^{\mathcal{M}} [\eta_k (\boldsymbol{\sigma}_{k,i} + \boldsymbol{\sigma}_{k,e})] - \nabla \cdot \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \mathbf{j}_{k,i,s} \mathbf{u}_{k,i,s},$$

or

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \sum_k^{\mathcal{M}} \eta_k \boldsymbol{\sigma}_k - \nabla \cdot \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \mathbf{j}_{k,i,s} \mathbf{u}_{k,i,s},$$

where $\boldsymbol{\sigma}_k = \boldsymbol{\sigma}_{k,i} + \boldsymbol{\sigma}_{k,e}$.

Given the assumption in item 1, eq. (5.49) for electron momentum becomes

$$e \eta_k n_{k,e} (\mathbf{E} + \mathbf{u}_{k,e} \times \mathbf{B}) = \nabla \cdot (\eta_k \boldsymbol{\sigma}_{k,e}) + \mathbf{R}_{k,e},$$

Using the definition of the current in eq. (5.52), the left-hand side can be re-written as

$$e \eta_k n_{k,e} (\mathbf{E} + \mathbf{u}_{k,e} \times \mathbf{B}) = e \eta_k n_{k,e} \mathbf{E} + \left(e \eta_k \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} - \mathbf{J}_k \right) \times \mathbf{B},$$

and thus the electron momentum equation becomes

$$e \eta_k n_{k,e} \mathbf{E} + e \eta_k \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \times \mathbf{B} = \mathbf{J}_k \times \mathbf{B} + \nabla \cdot (\eta_k \boldsymbol{\sigma}_{k,e}) + \mathbf{R}_{k,e},$$

Using the definition of $\mathbf{j}_{k,i,s}$, we can write

$$\begin{aligned} \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \times \mathbf{B} &= \sum_s^{\mathcal{N}_k} [Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u} + Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} (\mathbf{u}_{k,i,s} - \mathbf{u})] \times \mathbf{B} \\ &= \sum_s^{\mathcal{N}_k} \left(Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u} + Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \frac{\mathbf{j}_{k,i,s}}{\eta_k \rho_k Y_{k,i,s}} \right) \times \mathbf{B}. \end{aligned}$$

Using eq. (5.9) we get

$$\begin{aligned} \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u}_{k,i,s} \times \mathbf{B} &= \sum_s^{\mathcal{N}_k} \left(Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u} + Z_{k,i,s} \eta_{k,i,s} \frac{\rho_{k,i,s}}{m_{k,i,s}} \frac{\mathbf{j}_{k,i,s}}{\eta_k \rho_k Y_{k,i,s}} \right) \times \mathbf{B} \\ &= \sum_s^{\mathcal{N}_k} \left(Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u} + \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{m_{k,i,s} \eta_k} \right) \times \mathbf{B} \\ &= \sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} \mathbf{u} \times \mathbf{B} + \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{m_{k,i,s} \eta_k} \times \mathbf{B} \\ &= n_{k,e} \mathbf{u} \times \mathbf{B} + \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{m_{k,i,s} \eta_k} \times \mathbf{B}. \end{aligned}$$

Thus, the electron momentum equation becomes

$$e \eta_k n_{k,e} (\mathbf{E} + \mathbf{u} \times \mathbf{B}) = \mathbf{J}_k \times \mathbf{B} + \nabla \cdot (\eta_k \boldsymbol{\sigma}_{k,e}) + \mathbf{R}_{k,e} - e \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{m_{k,i,s}} \times \mathbf{B}.$$

We define the total electron density as

$$n_e = \sum_k^{\mathcal{M}} \eta_k n_{k,e}.$$

Thus, summing over all k gives

$$e n_e (\mathbf{E} + \mathbf{u} \times \mathbf{B}) = \mathbf{J} \times \mathbf{B} + \nabla \cdot \sum_k^{\mathcal{M}} \eta_k \boldsymbol{\sigma}_{k,e} + \sum_k^{\mathcal{M}} \mathbf{R}_{k,e} - e \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{m_{k,i,s}} \times \mathbf{B}.$$

or

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \frac{1}{e n_e} \left(\mathbf{J} \times \mathbf{B} + \nabla \cdot \sum_k^{\mathcal{M}} \eta_k \boldsymbol{\sigma}_{k,e} + \sum_k^{\mathcal{M}} \mathbf{R}_{k,e} \right) - \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{n_e m_{k,i,s}} \times \mathbf{B}. \quad (5.93)$$

Internal energy

Use the definition of $\mathbf{w}_{k,i,s}$ to re-write eq. (5.50) and eq. (5.51) as follows

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k \eta_{k,i,s} p_{k,i,s} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k \eta_{k,i,s} p_{k,i,s} \mathbf{u} \right) &= \\ \eta_k \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i,s} + Q_{k,i,s} - \nabla \cdot \left(\frac{3}{2} \eta_k \eta_{k,i,s} p_{k,i,s} \mathbf{w}_{k,i,s} \right) &+ \eta_k \eta_{k,i,s} \boldsymbol{\sigma}_{k,i,s} : \nabla \mathbf{w}_{k,i,s}. \\ \frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k p_{k,e} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,e} \mathbf{u} \right) &= \\ \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} - \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,e} \mathbf{w}_{k,e} \right) &+ \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{w}_{k,e}. \end{aligned}$$

5.5.4 Multi-material single-fluid model

We add two extra assumptions

1. All ions of a material k move with the same ion velocity $\mathbf{u}_{k,i}$.
2. All ions of a material k have the same temperature $T_{k,i}$

If all ions of a material move with a single ion velocity, then the definition of \mathbf{u}_k in eq. (5.78) gives

$$\mathbf{u}_{k,i,s} = \mathbf{u}_{k,i}, \quad (5.94)$$

which gives for the species diffusion vector

$$\mathbf{j}_{k,i,s} = \rho Y_k Y_{k,i,s} \mathbf{w}_{k,i,s} = \rho Y_k Y_{k,i,s} \mathbf{w}_{k,i}. \quad (5.95)$$

Adding over all ion species of a material and using expressions for total ion quantities, the ion pressure equation becomes

$$\frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k p_{k,i} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,i} \mathbf{u} \right) = \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} - \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,i} \mathbf{w}_{k,i} \right) + \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{w}_{k,i}.$$

Similarly, the ion EOS is multiplied by $\eta_{k,i,s}$ on both sides and then added over all species of a material to obtain

$$p_{k,i} = n_{k,i} k_B T_{k,i}. \quad (5.96)$$

To summarize, we have

$$\frac{\partial \eta_k \rho_k Y_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \rho_k Y_{k,i,s} \mathbf{u}) = -\nabla \cdot \mathbf{j}_{k,i,s}, \quad (5.97)$$

$$\nabla \cdot \mathbf{J} = 0, \quad (5.98)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \sum_k \eta_k \boldsymbol{\sigma}_k - \nabla \cdot \sum_k \mathbf{j}_{k,i} \mathbf{u}_{k,i}, \quad (5.99)$$

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \frac{1}{en_e} \left(\mathbf{J} \times \mathbf{B} + \nabla \cdot \sum_k \eta_k \boldsymbol{\sigma}_{k,e} + \sum_k \mathbf{R}_{k,e} \right) - \sum_k \sum_s \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{n_e m_{k,i,s}} \times \mathbf{B}, \quad (5.100)$$

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k p_{k,i} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,i} \mathbf{u} \right) = \\ \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} - \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,i} \mathbf{w}_{k,i} \right) + \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{w}_{k,i}, \end{aligned} \quad (5.101)$$

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{3}{2} \eta_k p_{k,e} \right) + \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,e} \mathbf{u} \right) = \\ \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} - \nabla \cdot \left(\frac{3}{2} \eta_k p_{k,e} \mathbf{w}_{k,e} \right) + \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{w}_{k,e}, \end{aligned} \quad (5.102)$$

$$\mathbf{J}_k = en_k n_{k,e} (\mathbf{u}_{k,i} - \mathbf{u}_{k,e}), \quad (5.103)$$

$$\mathbf{J} = \sum_k \mathbf{J}_k, \quad (5.104)$$

$$\rho_{q,k} = 0, \quad (5.105)$$

$$\rho_q = \sum_k^{\mathcal{M}} \rho_{q,k}, \quad (5.106)$$

$$p_{k,i} = n_{k,i} k_B T_{k,i}, \quad (5.107)$$

$$p_{k,e} = n_{k,e} k_B T_{k,e}. \quad (5.108)$$

Note that eq. (5.97) gives $\eta_k \rho_k Y_{k,i,s}$. Summing over all s gives $\eta_k \rho_k$. Summing over all k gives ρ . Dividing $\eta_k \rho_k Y_{k,i,s}$ by $\eta_k \rho_k$ gives $Y_{k,i,s}$. Dividing $\eta_k \rho_k$ by ρ gives Y_k .

5.5.5 Single-material single-fluid multi-species model

Assuming there is only one material, then $\mathbf{w}_{k,i} = \mathbf{u}_{k,i} - \mathbf{u} = 0$ and thus eq. (5.95) gives $\mathbf{j}_{k,i,s} = 0$. Summing over all s would then give $\mathbf{j}_{k,i} = 0$. Additionally, $\eta_k = 1$ and $\rho_k = \rho$. Thus, the model in section 5.5.4 becomes

$$\frac{\partial \rho Y_{i,s}}{\partial t} + \nabla \cdot (\rho Y_{i,s} \mathbf{u}) = 0, \quad (5.109)$$

$$\nabla \cdot \mathbf{J} = 0, \quad (5.110)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \boldsymbol{\sigma}, \quad (5.111)$$

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \frac{1}{en_e} (\mathbf{J} \times \mathbf{B} + \nabla \cdot \boldsymbol{\sigma}_e + \mathbf{R}_e), \quad (5.112)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_i \right) + \nabla \cdot \left(\frac{3}{2} p_i \mathbf{u} \right) = \boldsymbol{\sigma}_i : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_i + Q_i, \quad (5.113)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_e \right) + \nabla \cdot \left(\frac{3}{2} p_e \mathbf{u} \right) = \boldsymbol{\sigma}_e : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_e + Q_e - \nabla \cdot \left(\frac{3}{2} p_e \mathbf{w}_e \right) + \boldsymbol{\sigma}_e : \nabla \mathbf{w}_e, \quad (5.114)$$

$$\mathbf{J} = en_e (\mathbf{u} - \mathbf{u}_e), \quad (5.115)$$

$$\rho_q = 0, \quad (5.116)$$

$$p_i = n_i k_B T_i, \quad (5.117)$$

$$p_e = n_e k_B T_e. \quad (5.118)$$

5.5.6 Single-material single-fluid two-species model

If there is only one ion species, along with the electron species, then the model in section 5.5.5 simplifies to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (5.119)$$

$$\nabla \cdot \mathbf{J} = 0. \quad (5.120)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \boldsymbol{\sigma}. \quad (5.121)$$

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \frac{1}{en_e} (\mathbf{J} \times \mathbf{B} + \nabla \cdot \boldsymbol{\sigma}_e + \mathbf{R}_e). \quad (5.122)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_i \right) + \nabla \cdot \left(\frac{3}{2} p_i \mathbf{u} \right) = \boldsymbol{\sigma}_i : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_i + Q_i. \quad (5.123)$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2} p_e \right) + \nabla \cdot \left(\frac{3}{2} p_e \mathbf{u} \right) = \boldsymbol{\sigma}_e : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_e + Q_e - \nabla \cdot \left(\frac{3}{2} p_e \mathbf{w}_e \right) + \boldsymbol{\sigma}_e : \nabla \mathbf{w}_e. \quad (5.124)$$

$$\mathbf{J} = en_e (\mathbf{u} - \mathbf{u}_e). \quad (5.125)$$

$$\rho_q = 0, \quad (5.126)$$

$$p_i = n_i k_B T_i, \quad (5.127)$$

$$p_e = n_e k_B T_e. \quad (5.128)$$

5.5.7 Alternate forms of the energy equations

Thus far we've been working with plasmas that behave as ideal gasses with three degrees of freedom (the three translational degrees of freedom). For ideal gasses we also have

$$p_{k,i,s} = (\gamma - 1) \rho_{k,i,s} e_{k,i,s}, \quad (5.129)$$

$$p_{k,e} = (\gamma - 1) \rho_k e_{k,e}. \quad (5.130)$$

Multiplying both sides of eq. (5.129) by $\eta_{k,i,s}$ and summing over all s gives

$$p_{k,i} = (\gamma - 1) \rho_k e_{k,i}. \quad (5.131)$$

Since $\gamma = 5/3$ for the plasmas under consideration, the internal energy equation for ions given by eq. (5.101) can now be written as

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,i}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} \\ &\quad - \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{w}_{k,i}) + \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{w}_{k,i}. \end{aligned}$$

Similarly, the internal energy equation for electrons given by eq. (5.102) becomes

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,e}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} \\ &\quad - \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{w}_{k,e}) + \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{w}_{k,e}. \end{aligned}$$

We re-write the last term in the two equations above as

$$\begin{aligned} \eta_k \boldsymbol{\sigma}_{k,s} : \nabla \mathbf{w}_{k,s} &= \nabla \cdot (\mathbf{w}_{k,s} \cdot \eta_k \boldsymbol{\sigma}_{k,s}) - \mathbf{w}_{k,s} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,s}) \\ &= -\nabla \cdot (\eta_k p_{k,s} \mathbf{w}_{k,s}) + \nabla \cdot (\mathbf{w}_{k,s} \cdot \eta_k \mathbf{t}_{k,s}) - \mathbf{w}_{k,s} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,s}), \end{aligned}$$

where s is equal to i or e . Thus, the ion and electron internal energy equations become

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,i}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} \\ &\quad - \nabla \cdot \left[\left(e_{k,i} + \frac{p_{k,i}}{\rho_k} \right) \eta_k \rho_k \mathbf{w}_{k,i} \right] + \nabla \cdot (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i}) - \mathbf{w}_{k,i} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,i}). \end{aligned}$$

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,e}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} \\ &\quad - \nabla \cdot \left[\left(e_{k,e} + \frac{p_{k,e}}{\rho_k} \right) \eta_k \rho_k \mathbf{w}_{k,e} \right] + \nabla \cdot (\mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,e}). \end{aligned}$$

The enthalpies are given by

$$h_{k,i,s} = e_{k,i,s} + \frac{p_{k,i,s}}{\rho_{k,i,s}}, \quad (5.132)$$

$$h_{k,e} = e_{k,e} + \frac{p_{k,e}}{\rho_k}. \quad (5.133)$$

Using expressions from section 5.5.1, we can show that

$$h_{k,i} = \sum_s \mathcal{N}_k Y_{k,i,s} h_{k,i,s} = \sum_s \mathcal{N}_k Y_{k,i,s} e_{k,i,s} + \sum_s \mathcal{N}_k \frac{\eta_{k,i,s} p_{k,i,s}}{\rho_k} = e_{k,i} + \frac{p_{k,i}}{\rho_k}. \quad (5.134)$$

Using eqs. (5.133) and (5.134) for $h_{k,i}$ and $h_{k,e}$ the energy equations are written as

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,i}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} \\ &\quad - \nabla \cdot (h_{k,i} \eta_k \rho_k \mathbf{w}_{k,i}) + \nabla \cdot (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i}) - \mathbf{w}_{k,i} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,i}). \end{aligned}$$

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,e}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} \\ &\quad - \nabla \cdot (h_{k,e} \eta_k \rho_k \mathbf{w}_{k,e}) + \nabla \cdot (\mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,e}). \end{aligned}$$

Using eq. (5.90) for $\mathbf{j}_{k,i}$ and $\mathbf{j}_{k,e} = \eta_k \rho_k \mathbf{w}_{k,e}$ the internal energy equations become

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,i}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} \\ &\quad - \nabla \cdot (h_{k,i} \mathbf{j}_{k,i}) + \nabla \cdot (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i}) - \mathbf{w}_{k,i} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,i}). \end{aligned}$$

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,e}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} \\ &\quad - \nabla \cdot (h_{k,e} \mathbf{j}_{k,e}) + \nabla \cdot (\mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,e}). \end{aligned}$$

Finally, adding up the ion and electron internal energy equations and using eq. (5.80) gives

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_k}{\partial t} + \nabla \cdot (\eta_k \rho_k e_k \mathbf{u}) &= \eta_k \boldsymbol{\sigma}_k : \nabla \mathbf{u} - \nabla \cdot (\mathbf{q}_{k,i} + \mathbf{q}_{k,e}) + Q_{k,i} + Q_{k,e} \\ &\quad - \nabla \cdot (h_{k,i} \mathbf{j}_{k,i} + h_{k,e} \mathbf{j}_{k,e}) + \nabla \cdot (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i} + \mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) - \mathbf{w}_{k,i} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,i}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,e}). \end{aligned} \quad (5.135)$$

Summing eq. (5.135) over all materials and using eq. (5.81) gives

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{u}) &= \sum_k \mathcal{M} \eta_k \boldsymbol{\sigma}_k : \nabla \mathbf{u} - \nabla \cdot \sum_k \mathcal{M} (\mathbf{q}_{k,i} + \mathbf{q}_{k,e}) + \sum_k \mathcal{M} (Q_{k,i} + Q_{k,e}) \\ &\quad - \nabla \cdot \sum_k \mathcal{M} (h_{k,i} \mathbf{j}_{k,i} + h_{k,e} \mathbf{j}_{k,e}) + \nabla \cdot \sum_k \mathcal{M} (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i} + \mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) \\ &\quad - \sum_k \mathcal{M} [\mathbf{w}_{k,i} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,i}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \boldsymbol{\sigma}_{k,e})]. \end{aligned}$$

We can now re-write eq. (5.87) as

$$\sum_k \mathcal{M} (Q_{k,i} + Q_{k,e}) = - \sum_k \mathcal{M} (\mathbf{u}_{k,i} \cdot \mathbf{R}_{k,i} + \mathbf{u}_{k,e} \cdot \mathbf{R}_{k,e}). \quad (5.136)$$

Thus, the total internal energy equation becomes

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{u}) &= \sum_k^{\mathcal{M}} \eta_k \sigma_k : \nabla \mathbf{u} - \nabla \cdot \sum_k^{\mathcal{M}} (\mathbf{q}_{k,i} + \mathbf{q}_{k,e}) - \sum_k^{\mathcal{M}} (\mathbf{u}_{k,i} \cdot \mathbf{R}_{k,i} + \mathbf{u}_{k,e} \cdot \mathbf{R}_{k,e}) \\ &\quad - \nabla \cdot \sum_k^{\mathcal{M}} (h_{k,i} \mathbf{j}_{k,i} + Y_{k,e} h_{k,e} \bar{\mathbf{j}}_{k,e}) + \nabla \cdot \sum_k^{\mathcal{M}} (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i} + \mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) \\ &\quad - \sum_k^{\mathcal{M}} [\mathbf{w}_{k,i} \cdot \nabla (\eta_k \sigma_{k,i}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \sigma_{k,e})]. \end{aligned}$$

To summarize we have

$$\frac{\partial \eta_k \rho_k Y_{k,i,s}}{\partial t} + \nabla \cdot (\eta_k \rho_k Y_{k,i,s} \mathbf{u}) = -\nabla \cdot \mathbf{j}_{k,i,s}, \quad (5.137)$$

$$\nabla \cdot \mathbf{J} = 0, \quad (5.138)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mathbf{J} \times \mathbf{B} = \nabla \cdot \sum_k^{\mathcal{M}} \eta_k \sigma_k - \nabla \cdot \sum_k^{\mathcal{M}} \mathbf{j}_{k,i} \mathbf{u}_{k,i}, \quad (5.139)$$

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \frac{1}{en_e} \left(\mathbf{J} \times \mathbf{B} + \nabla \cdot \sum_k^{\mathcal{M}} \eta_k \sigma_{k,e} + \sum_k^{\mathcal{M}} \mathbf{R}_{k,e} \right) - \sum_k^{\mathcal{M}} \sum_s^{\mathcal{N}_k} \frac{Z_{k,i,s} \mathbf{j}_{k,i,s}}{n_e m_{k,i,s}} \times \mathbf{B}, \quad (5.140)$$

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,i}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,i} \mathbf{u}) &= \eta_k \sigma_{k,i} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,i} + Q_{k,i} \\ &\quad - \nabla \cdot (h_{k,i} \mathbf{j}_{k,i}) + \nabla \cdot (\mathbf{w}_{k,i} \cdot \eta_k \mathbf{t}_{k,i}) - \mathbf{w}_{k,i} \cdot \nabla (\eta_k \sigma_{k,i}). \end{aligned} \quad (5.141)$$

$$\begin{aligned} \frac{\partial \eta_k \rho_k e_{k,e}}{\partial t} + \nabla \cdot (\eta_k \rho_k e_{k,e} \mathbf{u}) &= \eta_k \sigma_{k,e} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}_{k,e} + Q_{k,e} \\ &\quad - \nabla \cdot (h_{k,e} \mathbf{j}_{k,e}) + \nabla \cdot (\mathbf{w}_{k,e} \cdot \eta_k \mathbf{t}_{k,e}) - \mathbf{w}_{k,e} \cdot \nabla (\eta_k \sigma_{k,e}). \end{aligned} \quad (5.142)$$

$$\mathbf{J}_k = e \eta_k n_{k,e} (\mathbf{u}_{k,i} - \mathbf{u}_{k,e}), \quad (5.143)$$

$$\mathbf{J} = \sum_k^{\mathcal{M}} \mathbf{J}_k, \quad (5.144)$$

$$\rho_{q,k} = 0, \quad (5.145)$$

$$\rho_q = \sum_k^{\mathcal{M}} \rho_{q,k}, \quad (5.146)$$

$$p_{k,i} = n_{k,i} k_B T_{k,i}, \quad (5.147)$$

$$p_{k,e} = n_{k,e} k_B T_{k,e}, \quad (5.148)$$

$$p_{k,i} = (\gamma - 1) \rho_k e_{k,i}, \quad (5.149)$$

$$p_{k,e} = (\gamma - 1) \rho_k e_{k,e}. \quad (5.150)$$

Some extra notes on this model:

1. As before the mass transport equation gives $\eta_k \rho_k Y_{k,i,s}$. Summing over all s gives $\eta_k \rho_k$. Dividing $\eta_k \rho_k Y_{k,i,s}$ by $\eta_k \rho_k$ gives $Y_{k,i,s}$. Summing $\eta_k \rho_k$ over all k gives ρ . Dividing $\eta_k \rho_k$ by ρ gives Y_k .
2. The ion internal energy equation gives $e_{k,i}$.
3. The electron internal energy equation gives $e_{k,e}$.
4. If η_k is known, we can compute ρ_k from $\rho_k = \rho Y_k / \eta_k$.
5. Using ρ_k and $e_{k,i}$ in eq. (5.149) we get $p_{k,i}$.
6. Using ρ_k and $e_{k,e}$ in eq. (5.150) we get $p_{k,e}$.
7. We can compute $h_{k,i}$ using eq. (5.134), which we repeat below

$$h_{k,i} = e_{k,i} + \frac{p_{k,i}}{\rho_k}.$$

8. We can compute $h_{k,e}$ using eq. (5.133), which we repeat below

$$h_{k,e} = e_{k,e} + \frac{p_{k,e}}{\rho_k}.$$

9. We can compute $n_{k,i,s}$ using eq. (5.9), which we repeat below

$$m_{k,i,s} n_{k,i,s} = \rho_k Y_{k,i,s}.$$

10. We can compute $n_{k,i}$ using eqs. (5.9) and (5.23), as shown below

$$n_{k,i} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} n_{k,i,s} = \sum_s^{\mathcal{N}_k} \eta_{k,i,s} \frac{\rho_{k,i,s}}{m_{k,i,s}} = \sum_s^{\mathcal{N}_k} \frac{\rho_k Y_{k,i,s}}{m_{k,i,s}}. \quad (5.151)$$

11. We can compute $n_{k,e}$ from quasi-neutrality, which we repeat below

$$\sum_s^{\mathcal{N}_k} Z_{k,i,s} \eta_{k,i,s} n_{k,i,s} = n_{k,e}, \quad (5.152)$$

12. Using $p_{k,i}$ and $n_{k,i}$ in eq. (5.147) we get $T_{k,i}$.
13. Using $p_{k,e}$ and $n_{k,e}$ in eq. (5.148) we get $T_{k,e}$.

Note that this model requires knowing the value of η_k . Thus the following equation is also solved

$$\frac{\partial \eta_k}{\partial t} + \mathbf{u} \cdot \nabla (\eta_k) = \alpha_k, \quad (5.153)$$

where α_k is a closure model.

5.5.8 Generic EOS

Rather than assuming ideal equations of state for each species, we can instead account for generic equations of state. To show this, we first start with

Chapter 6

Mixtures

In this chapter we focus on fluids that consist of mixtures of elements, which we sometimes refer to as species and other times as materials. There are two approaches that we'll consider, multi-species hydrodynamics, where the constituent elements in the mixture are referred to as species, and multi-material hydrodynamics, which is a higher-fidelity extension of multi-species hydrodynamics and where we refer to the constituent elements of the mixture as materials.

We introduce an additional fraction, the mole fraction $X_\alpha = X_\alpha(t, \mathbf{x})$, as shown below

$$X_\alpha = \frac{O_k}{O}, \quad (6.1)$$

where O_k is the number of moles of material k at a point in space, and O is the number of all moles at a point in space. Since $M_k = M_k O$, where M_k is the molar mass of material k , we can introduce two relationships between X_k and Y_k :

$$Y_k = \frac{M_k O_k}{\sum_l M_l O_l} = \frac{M_k X_k}{\sum_l M_l X_l} \quad (6.2)$$

$$X_k = \frac{M_k / M_k}{\sum_l M_l / M_l} = \frac{Y_k / M_k}{\sum_l Y_l / M_l} \quad (6.3)$$

6.1 Multi-species hydrodynamics

The multi-species fluid model consists of the Navier-Stokes equations augmented with multiple scalars, where each scalar is the mass fraction of a species in the system. For this case, the species mass fractions are no longer passive scalars. For ideal gases, for example, they affect the value of R , which in turns affects the pressure, density, and temperature of the whole mixture. They also affect the enthalpy diffusion, which then alters the heat flux and internal energy.

6.1.1 Equations of state and thermodynamic variables

We introduce the partial pressure p_α such that the total pressure is obtained from

$$p = \sum_\alpha p_\alpha. \quad (6.4)$$

We'll also introduce the secondary partial pressure \hat{p}_α which satisfies

$$p_\alpha = \eta_\alpha \hat{p}_\alpha. \quad (6.5)$$

The thermal equation of state is now expressed as

$$\hat{p}_\alpha = \phi_\alpha(\rho_\alpha, T_\alpha), \quad (6.6)$$

and the caloric equation of state as

$$e_\alpha = \psi_\alpha(\rho_\alpha, T_\alpha). \quad (6.7)$$

There are two relations that can be derived from ???. One is obtained by first performing the sum

$$\sum_\alpha \eta_\alpha \rho_\alpha = \sum_\alpha \rho Y_\alpha, \quad (6.8)$$

which leads to

$$\rho = \sum_\alpha \eta_\alpha \rho_\alpha. \quad (6.9)$$

The other relation is obtained by performing the sum

$$\sum_\alpha \frac{\eta_\alpha}{\rho} = \sum_\alpha \frac{Y_\alpha}{\rho_\alpha}, \quad (6.10)$$

which leads to

$$\frac{1}{\rho} = \sum_\alpha \frac{Y_\alpha}{\rho_\alpha}. \quad (6.11)$$

Using eqs. (1.9), (5.37) and (5.38) we have

$$e = \sum_\alpha Y_\alpha e_\alpha. \quad (6.12)$$

The species enthalpy h_α is defined in terms of the other species variables as follows

$$h_\alpha = e_\alpha + \frac{\hat{p}_\alpha}{\rho_\alpha}. \quad (6.13)$$

We can now show that

$$\begin{aligned} \sum_\alpha Y_\alpha h_\alpha &= \sum_\alpha Y_\alpha e_\alpha + \sum_\alpha \frac{Y_\alpha \hat{p}_\alpha}{\rho_\alpha} \\ &= \sum_\alpha Y_\alpha e_\alpha + \sum_\alpha \frac{\eta_\alpha \hat{p}_\alpha}{\rho} \\ &= \sum_\alpha Y_\alpha e_\alpha + \sum_\alpha \frac{p_\alpha}{\rho} \\ &= e + \frac{p}{\rho} \\ &= h \end{aligned} \quad (6.14)$$

In the absence of chemical reactions, condensation, or other processes, Y_i is independent of temperature. For these cases, differentiating eq. (6.12) and eq. (6.14) gives (differentiating with respect to what temperature? T_α , some common temperature T ? I think this requires temperature equilibration across all α !!!)

$$C_v = \sum_\alpha Y_\alpha C_{v,\alpha}, \quad (6.15)$$

$$C_p = \sum_\alpha Y_\alpha C_{p,\alpha}. \quad (6.16)$$

6.1.2 The pressure-temperature (PT) equilibration model

The thermodynamic variables that we'll be solving for are ρ_α , e_α , \hat{p}_α , and T_α , for a total of $4N$ variables, where N is the number of species. We now assume an equilibrium state in which $\hat{p}_\alpha = p$ and $T_\alpha = T$ for all α . Thus, the total number of unknowns is reduced to $2N + 2$. The equations to be solved are then

$$p = \phi_\alpha(\rho_\alpha, T), \quad (6.17)$$

$$e_\alpha = \psi_\alpha(\rho_\alpha, T). \quad (6.18)$$

$$\frac{1}{\rho} = \sum_\alpha \frac{Y_\alpha}{\rho_\alpha}, \quad (6.19)$$

$$e = \sum_\alpha Y_\alpha e_\alpha. \quad (6.20)$$

For the above, ρ , Y_α , and e are known variables provided by the fluid transport equations, and hence they are the inputs to the equilibration algorithm. Equations (6.17) to (6.20) constitute $2N + 2$ equations for the $2N + 2$ unknowns ρ_α , e_α , p , and T . Note that, after solving the system of equations above, one can compute η_α using ??.

If we plug in ?? into eqs. (6.17) to (6.19) then the equations for the equilibration algorithm can be written as

$$p = \phi_\alpha(\rho Y_\alpha / \eta_\alpha, T), \quad (6.21)$$

$$e_\alpha = \psi_\alpha(\rho Y_\alpha / \eta_\alpha, T). \quad (6.22)$$

$$1 = \sum_\alpha \eta_\alpha \quad (6.23)$$

$$e = \sum_\alpha Y_\alpha e_\alpha. \quad (6.24)$$

For the above ρ , Y_α , and e are still the inputs, and η_α , e_α , p and T are the $2N + 2$ unknowns. Note that, after solving the system of equations above, one can compute ρ_α using ??.

6.1.3 The PT equilibration model for perfect gasses

For an ideal gas, eq. (6.6) and eq. (6.7) are given by

$$\hat{p}_\alpha = \rho_\alpha R_\alpha T_\alpha, \quad (6.25)$$

and

$$e_\alpha = C_{v,\alpha} T_\alpha. \quad (6.26)$$

In the above, $R_\alpha = R_u / M_\alpha$ is the ideal gas constant of each species and it satisfies $R_\alpha = C_{p,\alpha} - C_{v,\alpha}$. For the species enthalpy, we have

$$h_\alpha = e_\alpha + \frac{\hat{p}_\alpha}{\rho_\alpha} = e_\alpha + R_\alpha T_\alpha = C_{v,\alpha} T_\alpha + (C_{p,\alpha} - C_{v,\alpha}) T_\alpha = C_{p,\alpha} T_\alpha. \quad (6.27)$$

The thermal equation of state for the entire mixture can be derived from the thermal equation of state for each species. We first multiply eq. (6.25) by Y_α , divide by ρ_α , and sum over all α . That is

$$\sum_\alpha p \frac{Y_\alpha}{\rho_\alpha} = \sum_\alpha Y_\alpha R_\alpha T. \quad (6.28)$$

The above can be expressed as

$$p = \rho \sum_{\alpha} \frac{Y_{\alpha}}{M_{\alpha}} R_u T. \quad (6.29)$$

We now define the the average molar mass of the mixture as $M = \sum_{\alpha} X_{\alpha} M_{\alpha}$. Using eq. (6.2), this can be rewritten as

$$\frac{1}{M} = \sum_{\alpha} \frac{Y_{\alpha}}{M_{\alpha}} \quad (6.30)$$

Thus, the thermal equation of state for the entire mixture can be expressed as

$$p = \rho R T \quad (6.31)$$

where

$$R = \frac{R_u}{M} \quad (6.32)$$

Using the above, we can easily show that

$$R = \sum_{\alpha} Y_{\alpha} \frac{R_u}{M_{\alpha}} = \sum_{\alpha} Y_{\alpha} R_{\alpha} = \sum_{\alpha} Y_{\alpha} (C_{p,\alpha} - C_{v,\alpha}) = C_p - C_v. \quad (6.33)$$

6.1.4 Summary of governing equations

Conservation equations

$$\begin{aligned} \frac{\partial \rho Y_{\alpha}}{\partial t} + \frac{\partial \rho Y_{\alpha} u_i}{\partial x_i} &= -\frac{\partial j_{\alpha,i}}{\partial x_i} + w_{\alpha} \\ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} &= \frac{\partial \sigma_{ij}}{\partial x_j} + \rho f_i \\ \frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} &= \sigma_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}. \end{aligned}$$

Transport models

$$\begin{aligned} t_{ij} &= 2\mu S_{ij}^* \\ q_i &= -\kappa \frac{\partial T}{\partial x_i} + \sum_{\alpha} h_{\alpha} j_{\alpha,i} \\ j_{\alpha,i} &= -\rho \left(D_{\alpha} \frac{\partial Y_{\alpha}}{\partial x_i} - Y_{\alpha} \sum_{\beta} D_{\beta} \frac{\partial Y_{\beta}}{\partial x_i} \right) \end{aligned}$$

Transport coefficients

$$\begin{aligned} \mu &= \mu_0 \left(\frac{T}{T_0} \right)^n \\ \kappa &= \frac{\mu C_p}{Pr} \\ D_{\alpha} &= \frac{\mu}{\rho Sc_{\alpha}} \end{aligned}$$

Equations of state

$$\begin{aligned}
p &= \phi_\alpha(\rho_\alpha, T), \\
e_\alpha &= \psi_\alpha(\rho_\alpha, T). \\
\frac{1}{\rho} &= \sum_\alpha \frac{Y_\alpha}{\rho_\alpha}, \\
e &= \sum_\alpha Y_\alpha e_\alpha.
\end{aligned}$$

Additional relations

$$\begin{aligned}
\sigma_{ij} &= -p\delta_{ij} + t_{ij} \\
S_{ij}^* &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \\
h_\alpha &= e_\alpha + \frac{p}{\rho_\alpha} \\
1 &= \sum_\alpha Y_\alpha
\end{aligned}$$

6.1.5 Mass-fraction equations

There are two methods that are often used to compute the total density ρ and the mass fractions Y_α . These two methods are equivalent in paper, as will be shown below, but when implemented numerically can lead to different behavior. Since ρ and Y_α constitute $1 + N$ unknowns, $1 + N$ equations are required.

Method 1

This is the method shown in section 6.1.4, that is, one first solves for ρY_α using

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_i}{\partial x_i} = -\frac{\partial j_{\alpha,i}}{\partial x_i} + w_\alpha.$$

and assumes the following constraint

$$\sum_\alpha Y_\alpha = 1.$$

The densities then follow from $\rho = \sum_\alpha \rho Y_\alpha$ and the mass fractions from $Y_\alpha = \rho Y_\alpha / \rho$. We can then write

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= \frac{\partial}{\partial t} \sum_\alpha \rho Y_\alpha + \frac{\partial}{\partial x_i} \sum_\alpha \rho Y_\alpha u_i \\
&= \sum_\alpha \left(\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_i}{\partial x_i} \right) \\
&= \sum_\alpha \left(-\frac{\partial j_{\alpha,i}}{\partial x_i} + w_\alpha \right).
\end{aligned}$$

Assuming $\sum_\alpha j_{\alpha,i} = 0$ and $\sum_\alpha w_\alpha = 0$, we have

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0.$$

Table 6.1: Variables for multi-species and multi-material hydrodynamics.

Variable	M-S solution	M-M solution
ρ	method 1 or 2 from section 6.1.5	method 1 or 2 from section 6.1.5
Y_α	method 1 or 2 from section 6.1.5	method 1 or 2 from section 6.1.5
e	PDE given by eq. (4.14)	from Y_α and e_α using eq. (6.12)
p_α	equal to p	thermal eos, eq. (6.6)
T_α	equal to T	caloric eos, eq. (6.7)
p	PT-equilibration algorithm	n/a
T	PT-equilibration algorithm	n/a
ρ_α	PT-equilibration algorithm	algebraic relation given by ??
e_α	PT-equilibration algorithm	PDE given by ??
η_α	algebraic relation given by ??	PDE given by ??

Method 2

In this method one first solves for ρ and ρY_α using

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0,$$

and

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_i}{\partial x_i} = -\frac{\partial j_{\alpha,i}}{\partial x_i} + w_\alpha.$$

The mass fractions then follow from $Y_\alpha = \rho Y_\alpha / \rho$. We can write

$$\begin{aligned} \frac{\partial Y_\alpha}{\partial t} + u_i \frac{\partial Y_\alpha}{\partial x_i} &= \frac{1}{\rho^2} \left(\frac{\partial \rho Y_\alpha}{\partial t} \rho - \frac{\partial \rho}{\partial t} \rho Y_\alpha \right) + u_i \frac{1}{\rho^2} \left(\frac{\partial \rho Y_\alpha}{\partial x_i} \rho - \frac{\partial \rho}{\partial x_i} \rho Y_\alpha \right) \\ &= \frac{1}{\rho} \left[\left(\frac{\partial \rho Y_\alpha}{\partial t} + u_i \frac{\partial \rho Y_\alpha}{\partial x_i} \right) - Y_\alpha \left(\frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i} \right) \right] \\ &= \frac{1}{\rho} \left(\frac{\partial \rho Y_\alpha}{\partial t} + u_i \frac{\partial \rho Y_\alpha}{\partial x_i} + \rho Y_\alpha \frac{\partial u_i}{\partial x_i} \right) \\ &= \frac{1}{\rho} \left(-\frac{\partial j_{\alpha,i}}{\partial x_i} + w_\alpha \right). \end{aligned}$$

If we assume $\sum_\alpha j_{\alpha,i} = 0$ and $\sum_\alpha w_\alpha = 0$, then we have

$$\frac{\partial}{\partial t} \sum_\alpha Y_\alpha + u_i \frac{\partial}{\partial x_i} \sum_\alpha Y_\alpha = 0. \quad (6.34)$$

That is, $\sum_\alpha Y_\alpha$ is conserved along a streamline. If the initial and boundary conditions satisfy $\sum_\alpha Y_\alpha = 1$, then this equality holds for all time and space.

Part II

Compressible Flow

Chapter 7

Thermodynamics of fluid flows

7.1 Thermodynamic variables

We will focus on a basic set of thermodynamic variables, namely

ρ	density
p	pressure
T	temperature
e	internal energy
s	entropy.

Additional thermodynamic variables that are defined in terms of those above will also be used, namely the enthalpy $h = e + p/\rho$ and the specific volume $\vartheta = 1/\rho$.

There are two more relevant thermodynamic variables that need to be introduced, which are referred to as heat capacities or specific heats. The specific heat at constant volume is

$$C_v = \left(\frac{\partial e}{\partial T} \right)_{\vartheta} \quad (7.1)$$

and the specific heat at constant pressure is

$$C_p = \left(\frac{\partial h}{\partial T} \right)_p. \quad (7.2)$$

Their ratio is labelled as γ .

7.2 Equation of state

According to the state principle only two thermodynamic variables are required to know any of the thermodynamic variables (as long as the chemical composition of the fluid is not changed by mixing or diffusion). Thus, for example, if p and T are the independent variables, then $e = \xi(p, T)$, or if ρ and s are the independent variables, then $e = \chi(\rho, s)$. These two expressions can be equated in the following manner

$$e = \xi(p, T) = \chi(\rho(p, T), s(p, T)). \quad (7.3)$$

Expression in which a thermodynamic variable is written in terms of two others are known as equations of state. We will focus on two particular equations of state, namely a thermal equation of state

$$p = \phi(\rho, T), \quad (7.4)$$

and a caloric equations of state

$$e = \psi(\rho, T). \quad (7.5)$$

Given that ρ and e are provided by the conservation of mass and conservation of energy equations, we now have four equations for the four unknowns ρ , p , T , and e .

7.3 The Gibb's equations

7.3.1 Definitions

An axiom of thermodynamics is the Gibbs equation, which is

$$de = Tds - pd\vartheta. \quad (7.6)$$

Using the definition of enthalpy, the above can also be expressed as

$$dh = Tds + \vartheta dp. \quad (7.7)$$

If we also introduce the Helmholtz function $a = e - Ts$ and the Gibbs function $g = h - Ts$, then the Gibb's equation can be written as

$$da = -sdT - pd\vartheta, \quad (7.8)$$

$$dg = -sdT + \vartheta dp. \quad (7.9)$$

7.3.2 Additional relationships

From the Gibb's equation, a wide variety of relationships between the thermodynamics variables can be derived. Some of these include the Maxwell relations

$$\left(\frac{\partial T}{\partial \vartheta}\right)_s = -\left(\frac{\partial p}{\partial s}\right)_\vartheta, \quad (7.10)$$

$$\left(\frac{\partial T}{\partial p}\right)_s = \left(\frac{\partial \vartheta}{\partial s}\right)_p, \quad (7.11)$$

$$\left(\frac{\partial s}{\partial \vartheta}\right)_T = \left(\frac{\partial p}{\partial T}\right)_\vartheta, \quad (7.12)$$

$$\left(\frac{\partial s}{\partial p}\right)_T = -\left(\frac{\partial \vartheta}{\partial T}\right)_p. \quad (7.13)$$

An additional important relationship is the following

$$\left(\frac{\partial p}{\partial \rho}\right)_s = \gamma \left(\frac{\partial p}{\partial \rho}\right)_T. \quad (7.14)$$

To derive the above we start with

$$\gamma = \frac{C_p}{C_v} = \frac{\left(\frac{\partial h}{\partial T}\right)_p}{\left(\frac{\partial e}{\partial T}\right)_\vartheta} = \frac{\left(\frac{\partial h}{\partial s}\right)_p \left(\frac{\partial s}{\partial T}\right)_p}{\left(\frac{\partial e}{\partial s}\right)_\vartheta \left(\frac{\partial s}{\partial T}\right)_\vartheta} \quad (7.15)$$

Equations (7.6) and (7.7) can be used to show that

$$\left(\frac{\partial h}{\partial s}\right)_p = \left(\frac{\partial e}{\partial s}\right)_\vartheta. \quad (7.16)$$

We then write

$$\gamma = \frac{\left(\frac{\partial s}{\partial T}\right)_p}{\left(\frac{\partial s}{\partial T}\right)_\rho} = \frac{\left(\frac{\partial s}{\partial \rho}\right)_p \left(\frac{\partial \rho}{\partial T}\right)_p}{\left(\frac{\partial s}{\partial p}\right)_\rho \left(\frac{\partial p}{\partial T}\right)_\rho} = \frac{\left(\frac{\partial s}{\partial \rho}\right)_p \left(\frac{\partial p}{\partial s}\right)_\rho}{\left(\frac{\partial T}{\partial \rho}\right)_p \left(\frac{\partial p}{\partial T}\right)_\rho}. \quad (7.17)$$

By calculus

$$\left(\frac{\partial s}{\partial \rho}\right)_p \left(\frac{\partial \rho}{\partial p}\right)_s \left(\frac{\partial p}{\partial s}\right)_\rho = -1, \quad (7.18)$$

$$\left(\frac{\partial T}{\partial \rho}\right)_p \left(\frac{\partial \rho}{\partial p}\right)_T \left(\frac{\partial p}{\partial T}\right)_\rho = -1. \quad (7.19)$$

Thus,

$$\gamma = \frac{\left(\frac{\partial p}{\partial \rho}\right)_s}{\left(\frac{\partial p}{\partial \rho}\right)_T}, \quad (7.20)$$

as required.

7.3.3 Applications of the Gibb's equation

Crocco's equation

Consider the momentum eq. (3.19), which for inviscid flows with no body forces becomes

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p. \quad (7.21)$$

Using the Gibb's equation, the above becomes

$$\frac{D\mathbf{u}}{Dt} = T\nabla s - \nabla h. \quad (7.22)$$

The above is referred to as Crocco's equation. Using the vector identity

$$(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \left(\frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) - \mathbf{u} \times (\nabla \times \mathbf{u}), \quad (7.23)$$

Crocco's equation is typically written as

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \left(\frac{1}{2} \mathbf{u} \cdot \mathbf{u} + h \right) = \mathbf{u} \times \mathbf{w} + T\nabla s. \quad (7.24)$$

Vorticity equation

Consider the vorticity eq. (4.10) for inviscid flows, which we re-write below

$$\frac{D\mathbf{w}}{Dt} + \mathbf{w}(\nabla \cdot \mathbf{u}) - (\mathbf{w} \cdot \nabla)\mathbf{u} = -\nabla \times \left(\frac{1}{\rho} \nabla p \right). \quad (7.25)$$

The right-hand side can be re-written using the alternate form of the Gibbs equation, namely eq. (7.7). Thus,

$$\nabla \times \left(\frac{1}{\rho} \nabla p \right) = -\nabla \times (T\nabla s) = -\nabla T \times \nabla s. \quad (7.26)$$

Additionally, we note that

$$\frac{1}{\rho}(\nabla \cdot \mathbf{u}) = \frac{1}{\rho} \left(-\frac{1}{\rho} \frac{D\rho}{Dt} \right) = \frac{D}{Dt} \left(\frac{1}{\rho} \right). \quad (7.27)$$

and thus

$$\frac{D\mathbf{w}}{Dt} \frac{1}{\rho} + \frac{\mathbf{w}}{\rho}(\nabla \cdot \mathbf{u}) = \frac{D\mathbf{w}}{Dt} \frac{1}{\rho} + \mathbf{w} \frac{D}{Dt} \left(\frac{1}{\rho} \right) = \frac{D}{Dt} \left(\frac{\mathbf{w}}{\rho} \right). \quad (7.28)$$

Using eqs. (7.26) and (7.28) the vorticity eq. (7.25) for inviscid flows becomes

$$\frac{D}{Dt} \left(\frac{\mathbf{w}}{\rho} \right) = \left(\frac{\mathbf{w}}{\rho} \cdot \nabla \right) \mathbf{u} + \frac{1}{\rho} \nabla T \times \nabla s. \quad (7.29)$$

For flows where $\nabla s = 0$ everywhere, we obtain

$$\frac{D}{Dt} \left(\frac{\mathbf{w}}{\rho} \right) = \left(\frac{\mathbf{w}}{\rho} \cdot \nabla \right) \mathbf{u} \quad (7.30)$$

If we evaluate the above at the position \mathbf{x}_u^+ of a fluid particle, we can re-write it as follows

$$\frac{\partial}{\partial t} \left(\frac{w_{u,i}^+}{\rho_u^+} \right) = \frac{w_{j,u}^+}{\rho_u^+} \left(\frac{\partial u_i}{\partial x_j} \right)_{\mathbf{x}=\mathbf{x}_u^+}. \quad (7.31)$$

This equation is identical to that shown on the left of (2.27), and thus its solution is

$$\frac{w_{u,i}^+(t, \mathbf{y})}{\rho_u^+(t, \mathbf{y})} = \frac{w_{u,j}^+(0, \mathbf{y})}{\rho_u^+(0, \mathbf{y})} J_{ij}^+. \quad (7.32)$$

7.3.4 Energy dependence on temperature

Consider the functional dependence for energy $e = e(p, T)$. We are interested in knowing when energy depends on temperature only, that is, $e = e(T)$. For that we need to know when

$$\left(\frac{\partial e}{\partial p} \right)_T = 0 \quad (7.33)$$

Using eq. (7.6), we have

$$\left(\frac{\partial e}{\partial p} \right)_T = T \left(\frac{\partial s}{\partial p} \right)_T - p \left(\frac{\partial \vartheta}{\partial p} \right)_T.$$

Using eq. (7.13), we re-write the above as

$$\left(\frac{\partial e}{\partial p} \right)_T = -T \left(\frac{\partial \vartheta}{\partial T} \right)_p - p \left(\frac{\partial \vartheta}{\partial p} \right)_T. \quad (7.34)$$

Let's now assume that $\vartheta = f(p/T)$, for any function f . Then,

$$\left(\frac{\partial \vartheta}{\partial T} \right)_p = -f' \left(\frac{p}{T} \right) \frac{p}{T^2}, \quad (7.35)$$

and

$$\left(\frac{\partial \vartheta}{\partial p} \right)_T = f' \left(\frac{p}{T} \right) \frac{1}{T}. \quad (7.36)$$

Plugging the above two in eq. (7.34) gives eq. (7.33).

7.4 Ideal gasses

An ideal gas is defined as one whose thermal equation of state, i.e. eq. (7.4), is

$$p = \rho RT. \quad (7.37)$$

Since the above signifies ϑ depends on p and T in the form p/T only, we can use the result from section 7.3.4 to write

$$e = e(T).$$

Since the enthalpy for an ideal gas can be written as $h = e + RT$,

$$h = h(T).$$

The specific heats can now be expressed as

$$C_v = \frac{de}{dT}, \quad (7.38)$$

$$C_p = \frac{dh}{dT}. \quad (7.39)$$

The internal energy and enthalpy can be computed from

$$e(T) - e(T_0) = \int_{T_0}^T C_v(\alpha) d\alpha, \quad (7.40)$$

$$h(T) - h(T_0) = \int_{T_0}^T C_p(\alpha) d\alpha \quad (7.41)$$

We can also now show that

$$C_p - C_v = \frac{dh}{dT} - \frac{de}{dT} = \frac{d}{dT}(h - e) = R \quad (7.42)$$

For perfect gasses, C_v and C_p are constant. Thus, $e(T) - e(T_0) = C_v(T - T_0)$ and $h(T) - h(T_0) = C_p(T - T_0)$. If one assumes that at $T = 0$, $e = 0$, we obtain the familiar expressions

$$e = C_v T, \quad (7.43)$$

$$h = C_p T. \quad (7.44)$$

7.5 Isentropic flow

7.5.1 Definitions and governing equations

We begin with the equation for entropy derived in section 4.3, namely eq. (4.31), which is repeated below

$$\rho T \frac{Ds}{Dt} = -\frac{\partial q_j}{\partial x_j} + t_{ij} \frac{\partial u_i}{\partial x_j}. \quad (4.31)$$

We re-write the following term as follows

$$\frac{1}{T} \frac{\partial q_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{q_j}{T} \right) + \frac{q_j}{T^2} \frac{\partial T}{\partial x_j},$$

to thus obtain

$$\rho \frac{Ds}{Dt} - \frac{\partial}{\partial x_j} \left(\frac{q_j}{T} \right) = \frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \frac{t_{ij}}{T} \frac{\partial u_i}{\partial x_j}.$$

Using the continuity equation this is equivalent to

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \rho s u_j}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{q_j}{T} \right) = \frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \frac{t_{ij}}{T} \frac{\partial u_i}{\partial x_j}.$$

Integrating this equation over a control volume $\Omega^+ = \Omega^+(t, \Omega_0)$ and using the Reynolds transport theorem (eq. (2.36)) allows us to write

$$\frac{d}{dt} \int_{\Omega^+} \rho s \, dv - \int_{\Omega^+} \frac{\partial}{\partial x_j} \left(\frac{q_j}{T} \right) \, dv = \int_{\Omega^+} \frac{\partial}{\partial x_j} \rho s (v_j - u_j) \, dv + \int_{\Omega^+} \frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \frac{t_{ij}}{T} \frac{\partial u_i}{\partial x_j} \, dv.$$

Using Gauss's theorem this is equivalent to

$$\frac{d}{dt} \int_{\Omega^+(t)} \rho s \, dv - \int_{\partial \Omega^+(t)} \frac{q_j}{T} n_j \, ds = \int_{\partial \Omega^+(t)} \rho s (v_j - u_j) n_j \, dv + \int_{\Omega^+(t)} \frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \frac{t_{ij}}{T} \frac{\partial u_i}{\partial x_j} \, dv.$$

Consider now a control volume $\Omega_u^+ = \Omega_u^+(t, \Omega_0)$ moving with the flow. Then

$$\frac{d}{dt} \int_{\Omega_u^+} \rho s \, dv - \int_{\partial \Omega_u^+} \frac{q_j}{T} n_j \, ds = \int_{\Omega_u^+} \frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \frac{t_{ij}}{T} \frac{\partial u_i}{\partial x_j} \, dv. \quad (7.45)$$

We define a reversible flow as one for which the right-hand side above is zero. We define an adiabatic flow as one for which q_j is zero at the boundary, and thus the second term on the left-hand side above is zero. An isentropic flow is a reversible adiabatic flow, and thus satisfies

$$\frac{d}{dt} \int_{\Omega_u^+} \rho s \, dv = 0. \quad (7.46)$$

An alternate definition of an isentropic flow can be given by focusing on a fluid particle, rather than a material volume. If q_j and $t_{ij} \partial u_i / \partial x_j$ can be neglected, then eq. (4.31) gives $Ds/Dt = 0$. That is, the entropy is constant along a streamline. This is an isentropic flow. If *in addition* the entropy is the same in all directions (i.e. $\nabla s = 0$), then the flow is homentropic.

$$\text{isentropic flow: } \frac{Ds}{Dt} = 0, \quad (7.47)$$

$$\text{homentropic flow: } \frac{\partial s}{\partial t} = \nabla s = 0. \quad (7.48)$$

We also note that for an inviscid fluid $\mu = \mu_\nu = \kappa = 0$. Thus, if the stress tensor is given by

$$t_{ij} = 2\mu S_{ij} - \left(\frac{2}{3}\mu - \mu_\nu \right) \delta_{ij} S_{kk} \quad (7.49)$$

and the heat conduction by

$$q_i = -\kappa \frac{\partial T}{\partial x_i} \quad (7.50)$$

then both of the above are zero for an inviscid fluid, and thus the flow is isentropic.

7.5.2 Isentropic stagnation variables

An isentropic stagnation variable is used to describe the value a flow variable would reach as the flow decelerates to a stagnation point in an isentropic fashion.

We re-write eq. (4.41), without a body force, below

$$h + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} = \text{constant along a streamline.} \quad (7.51)$$

This equation was obtained by assuming steady inviscid flow along a streamline, i.e. isentropic flow. If a fluid particle decelerates to stagnation isentropically, we have

$$h_t = h + \frac{1}{2} u_i u_i, \quad (7.52)$$

where h_t is the stagnation enthalpy. This definition of stagnation enthalpy holds true even if we relax the assumptions of eq. (4.41), namely inviscid steady-state flow. This is because at any point in the domain, one can always imagine a hypothetical path that a particle follows as it decelerates to stagnation isentropically. At the end of this hypothetical path, the stagnation enthalpy would be computed as in eq. (7.52). It is also interesting to note that the isentropic enthalpy reached as the particle isentropically decelerates to stagnation is independent of the path taken by the particle.

7.5.3 Isentropic flow for a perfect gas

If we compare eq. (4.22) (the pressure evolution equation for a perfect gas) with eq. (4.31) (the entropy evolution equation) we can write

$$\frac{1}{\gamma - 1} \rho^\gamma \frac{D}{Dt} \left(\frac{p}{\rho^\gamma} \right) = \rho T \frac{Ds}{Dt}.$$

We now substitute $p = \rho R T$ on the right-hand side to obtain,

$$\frac{1}{\gamma - 1} \rho^\gamma \frac{D}{Dt} \left(\frac{p}{\rho^\gamma} \right) = \frac{p}{R} \frac{Ds}{Dt}.$$

Re-arranging, we have

$$\frac{\rho^\gamma}{p} \frac{D}{Dt} \left(\frac{p}{\rho^\gamma} \right) = \frac{\gamma - 1}{R} \frac{Ds}{Dt},$$

or

$$\frac{D}{Dt} \ln \left(\frac{p}{\rho^\gamma} \right) = \frac{\gamma - 1}{R} \frac{Ds}{Dt}.$$

The solution to the PDE above is

$$\ln \left(\frac{p}{\rho^\gamma} \right) = c + \frac{\gamma - 1}{R} s, \quad (7.53)$$

where $c = c(\mathbf{x}, t)$ satisfies $Dc/Dt = 0$. One can confirm this is the solution by simply taking D/Dt of both sides.

Let's assume isentropic flow, that is

$$\frac{Ds}{Dt} = 0.$$

Taking the D/Dt derivative of eq. (7.53) gives

$$\frac{D}{Dt} \left(\frac{p}{\rho^\gamma} \right) = 0. \quad (7.54)$$

The solution to the above is $p = C\rho^\gamma$, where $C = C(\mathbf{x}, t)$ satisfies $DC/Dt = 0$. One can confirm this is the solution by simply substituting it in the equation above.

We now assume homentropic flow, that is

$$\frac{\partial s}{\partial t} = \nabla s = 0. \quad (7.55)$$

Additionally assume that flow enters through the domain boundary, and that at each point of the boundary we have

$$\left. \frac{\partial}{\partial t} \left(\frac{p}{\rho^\gamma} \right) \right|_{\partial\Omega} = \left. \nabla \left(\frac{p}{\rho^\gamma} \right) \right|_{\partial\Omega} = 0.$$

Using each of the two equalities above in eq. (7.53) we get

$$\left. \frac{\partial c}{\partial t} \right|_{\partial\Omega} = \left. \nabla c \right|_{\partial\Omega} = 0.$$

Since $Dc/Dt = 0$, we can make the stronger statement that

$$\frac{\partial c}{\partial t} = \nabla c = 0. \quad (7.56)$$

Using eqs. (7.55) and (7.56) in eq. (7.53) we finally obtain

$$\frac{\partial}{\partial t} \left(\frac{p}{\rho^\gamma} \right) = \nabla \left(\frac{p}{\rho^\gamma} \right) = 0. \quad (7.57)$$

The solution to the above is $p = C\rho^\gamma$, where C is a constant across space and time.

If we have isentropic flow, then the flow variables at two different states can be linked as follows

$$\frac{p_2}{p_1} = \left(\frac{\rho_2}{\rho_1} \right)^\gamma. \quad (7.58)$$

Using the equation of state, this can be rewritten as

$$\frac{p_2}{p_1} = \left(\frac{T_2}{T_1} \right)^{\gamma/(\gamma-1)}, \quad (7.59)$$

and

$$\frac{\rho_2}{\rho_1} = \left(\frac{T_2}{T_1} \right)^{1/(\gamma-1)}. \quad (7.60)$$

Equation (7.52) for a perfect gas can be written as

$$C_p T_t = C_p T + \frac{1}{2} u_i u_i, \quad (7.61)$$

which we further re-write as

$$C_p T_t = C_p T + \frac{1}{2} \gamma R T M^2. \quad (7.62)$$

Dividing both sides by $C_p T$ gives

$$\frac{T_t}{T} = 1 + \frac{1}{2} \frac{\gamma R}{C_p} M^2, \quad (7.63)$$

which, given $R = C_p(\gamma - 1)/\gamma$, finally becomes

$$\frac{T_t}{T} = 1 + \frac{\gamma - 1}{2} M^2. \quad (7.64)$$

Using eqs. (7.59) and (7.60) we also obtain

$$\frac{p_t}{p} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\gamma/(\gamma-1)}, \quad (7.65)$$

$$\frac{\rho_t}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/(\gamma-1)}. \quad (7.66)$$

7.5.4 Acoustic waves

Express the density, pressure, and velocity as

$$\rho = \rho_0 + \hat{\rho}, \quad (7.67)$$

$$p = p_0 + \hat{p}, \quad (7.68)$$

$$\mathbf{u} = \mathbf{u}_0 + \hat{\mathbf{u}}. \quad (7.69)$$

For the above, ρ_0 and p are constant, and $\mathbf{u}_0 = 0$. Additionally, $\hat{\rho}$, \hat{p} , and $\hat{\mathbf{u}}$ are small.

We assume the flow to be inviscid and homentropic. Since the entropy is constant, the state principle (section 7.2) states that the thermodynamic variables will depend on one quantity only. A Taylor expansion for the pressure then gives

$$p = p_0 + \left[\left(\frac{\partial p}{\partial \rho} \right)_s \right]_{\rho=\rho_0} (\rho - \rho_0) + h.o.t.. \quad (7.70)$$

We rewrite the above as

$$\hat{p} = c_0^2 \hat{\rho}, \quad (7.71)$$

where

$$c_0^2 = \left[\left(\frac{\partial p}{\partial \rho} \right)_s \right]_{\rho=\rho_0}. \quad (7.72)$$

The assumption that $\hat{\rho}$ be small can be formally stated as $\hat{\rho} \ll \rho_0$. Using eq. (7.71), the assumption that \hat{p} is small is formally stated as $\hat{p} \ll \rho_0 c_0^2$.

Assuming products of two small quantities can be neglected, the density equation gives

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= \frac{\partial(\rho_0 + \hat{\rho})}{\partial t} + \nabla \cdot [(\rho_0 + \hat{\rho})(\mathbf{u}_0 + \hat{\mathbf{u}})] \\ &= \frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot (\rho_0 \hat{\mathbf{u}}) = 0. \end{aligned} \quad (7.73)$$

The momentum equation gives

$$\begin{aligned} \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p &= (\rho_0 + \hat{\rho}) \frac{\partial(\mathbf{u}_0 + \hat{\mathbf{u}})}{\partial t} + (\rho_0 + \hat{\rho})[(\mathbf{u}_0 + \hat{\mathbf{u}}) \cdot \nabla](\mathbf{u}_0 + \hat{\mathbf{u}}) + \nabla(p_0 + \hat{p}) \\ &= (\rho_0 + \hat{\rho}) \frac{\partial \hat{\mathbf{u}}}{\partial t} + (\rho_0 + \hat{\rho})(\hat{\mathbf{u}} \cdot \nabla) \hat{\mathbf{u}} + \nabla(p_0 + \hat{p}) \\ &= \rho_0 \frac{\partial \hat{\mathbf{u}}}{\partial t} + \nabla \hat{p} \\ &= \rho_0 \frac{\partial \hat{\mathbf{u}}}{\partial t} + c_0^2 \nabla \hat{\rho} = 0. \end{aligned} \quad (7.74)$$

Taking the time derivative of eq. (7.73) and using eq. (7.74) leads to the wave equation for density

$$\frac{\partial^2 \hat{\rho}}{\partial t^2} - c_0^2 \nabla^2 \hat{\rho} = 0. \quad (7.75)$$

Similarly, taking the time derivative of eq. (7.74) and using eq. (7.73) leads to

$$\frac{\partial^2 \hat{\mathbf{u}}}{\partial t^2} - c_0^2 \nabla(\nabla \cdot \hat{\mathbf{u}}) = 0. \quad (7.76)$$

Using a vector identity, we have

$$\nabla(\nabla \cdot \hat{\mathbf{u}}) = \nabla \times (\nabla \times \hat{\mathbf{u}}) + \nabla^2 \hat{\mathbf{u}}. \quad (7.77)$$

Taking the curl of eq. (7.74) we see that if the flow is initially irrotational it remains so for all time. Thus, the wave equation for velocity takes the form

$$\frac{\partial^2 \hat{\mathbf{u}}}{\partial t^2} - c_0^2 \nabla^2 \hat{\mathbf{u}} = 0. \quad (7.78)$$

In fact, one can show that all flow variables satisfy the wave equation given the conditions specified above: inviscid, homentropic, irrotational, with $\hat{\rho}$, \hat{p} , and $\hat{\mathbf{u}}$ small.

A more general expression for eq. (7.72) is

$$c^2 = \left(\frac{\partial p}{\partial \rho} \right)_s, \quad (7.79)$$

which represents the speed of sound. Using eq. (7.14), and assuming an ideal gas, we have

$$c^2 = \gamma RT. \quad (7.80)$$

Chapter 8

Shock waves and related discontinuities

Shock jump relations; Prandtl relation and Shock equations; Oblique shocks, theta-beta curve; Shock wave boundary layer interaction.

8.1 Shock waves

Shock waves are thin regions through which flow variables change drastically. For inviscid flows, these thin regions become actual discontinuities. We will label flow variables before the shock with the underscript 1, and variables after the shock with the underscript 2. We also define the unit vector normal to the shock and pointing towards the outgoing flow as \mathbf{n} , and the shock velocity as \mathbf{b} . Then, we can define the relative velocities normal to the shock as

$$\begin{aligned}w_1 &= (\mathbf{u}_1 - \mathbf{b}) \cdot \mathbf{n}, \\w_2 &= (\mathbf{u}_2 - \mathbf{b}) \cdot \mathbf{n}.\end{aligned}\tag{8.1}$$

The relative velocities tangent to the shock are given by

$$\begin{aligned}v_1 &= (\mathbf{u}_1 - \mathbf{b}) \cdot (1 - \mathbf{nn}), \\v_2 &= (\mathbf{u}_2 - \mathbf{b}) \cdot (1 - \mathbf{nn}).\end{aligned}\tag{8.2}$$

The shock jump conditions, assuming negligible viscous stresses and heat flux on either side of the shock, are then given by

$$\rho_1 w_1 = \rho_2 w_2,\tag{8.3}$$

$$\rho_1 w_1^2 + P_1 = \rho_2 w_2^2 + P_2,\tag{8.4}$$

$$v_1 = v_2,\tag{8.5}$$

$$h_1 + \frac{1}{2}w_1^2 = h_2 + \frac{1}{2}w_2^2.\tag{8.6}$$

Combining eqs. (8.3), (8.4) and (8.6) (see Thompson (1988)), the Rankine-Hugoniot equation is obtained

$$h_2 - h_1 = \frac{1}{2}(P_2 - P_1)(\vartheta_2 + \vartheta_1).\tag{8.7}$$

Given an equation of state, we can write $h_2 = \xi(P_2, \vartheta_2)$ and $h_1 = \xi(P_1, \vartheta_1)$. Thus, the Rankine-Hugoniot equation is an expression that relates ϑ_1 , P_1 , ϑ_2 , and P_2 . If we assume that ϑ_1 and

P_1 are known, the Rankine-Hugoniot equation is simply an expression of the form $P_2 = f(\vartheta_2)$. The function f is known as a shock adiabat, and is different for each equation of state used. Lets consider for example a perfect gas. Then, eq. (8.7) becomes

$$\frac{P_2}{P_1} = \frac{\frac{\gamma+1}{\gamma-1} - \frac{\vartheta_2}{\vartheta_1}}{\frac{\gamma+1}{\gamma-1} \frac{\vartheta_2}{\vartheta_1} - 1}. \quad (8.8)$$

In fig. 8.1 an arbitrary shock adiabat $P_2 = f(\vartheta_2)$ is shown. One thing to note is that for $\vartheta_2 = \vartheta_1$ (no real shock), the shock adiabat naturally gives $P_2 = P_1$. Thus, the state corresponding to the flow upstream of the shock, i.e. (P_1, ϑ_1) , is a point in the shock adiabat line. One can then draw a straight line to various possible states after the shock, as shown in fig. 8.1. The slope of any of these lines is $(P_2 - P_1)/(\vartheta_2 - \vartheta_1)$, which as shown in Thompson (1988) is equal to $-J^2$, where $J = \rho_1 w_1 = \rho_2 w_2$.

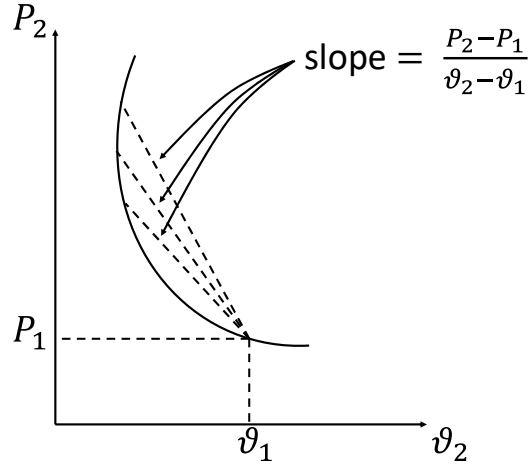


Figure 8.1: Shock adiabat for an arbitrary equation of state.

A few extra notes on shock waves:

- The shock Mach number M_{1n} is defined as

$$M_{1n} = \frac{w_1}{c_1}. \quad (8.9)$$

- The speed of sound is independent of the reference frame. Thus, whether you are in the shock reference frame, or in a stationary reference frame, the speeds of sound before and after the shock are invariant.
- The relative velocities satisfy

$$\begin{aligned} w_1 &\geq c_1 \\ w_2 &\leq c_2. \end{aligned} \quad (8.10)$$

- The shock strength Π is defined as (see Thompson (1988) for derivation):

$$\Pi = \frac{P_2 - P_1}{\rho_1 c_1^2}. \quad (8.11)$$

- Strong and weak shocks are defined according to

$$\begin{aligned} \Pi &\ll 1 && \text{weak shock} \\ \Pi &\gg 1 && \text{strong shock.} \end{aligned} \quad (8.12)$$

- For weak shocks the entropy increase across a shock is so weak, they might as well be considered isentropic.
- In the limit of vanishing strength, shock waves become acoustic discontinuities, propagating with speed c relative to the fluid.

8.1.1 Normal shocks

Following the derivations in Thompson (1988) for a perfect gas, one can express shock jump conditions as a function of γ and M_{1n} only. These are

$$\frac{P_2}{P_1} = \frac{\frac{2\gamma}{\gamma-1}M_{1n}^2 - 1}{\frac{\gamma+1}{\gamma-1}}, \quad (8.13)$$

$$\frac{w_2}{w_1} = \frac{1 + \frac{\gamma-1}{2}M_{1n}^2}{\frac{\gamma+1}{2}M_{1n}^2}, \quad (8.14)$$

$$\frac{\rho_2}{\rho_1} = \frac{\frac{\gamma+1}{2}M_{1n}^2}{1 + \frac{\gamma-1}{2}M_{1n}^2}. \quad (8.15)$$

Additionally, combining the three above one obtains

$$M_{2n}^2 = \frac{M_{1n}^2 + \frac{2}{\gamma-1}}{\frac{2\gamma}{\gamma-1}M_{1n}^2 - 1}. \quad (8.16)$$

According to eq. (8.6) $h_{t2} = h_{t1}$ (this holds not only for normal shocks but all shocks). Thus, $T_{t2} = T_{t1}$. For the stagnation pressure, we have

$$\frac{P_{t2}}{P_{t1}} = \frac{P_{t2}}{P_2} \frac{P_1}{P_{t1}} \frac{P_2}{P_1}. \quad (8.17)$$

Using eqs. (7.65), (8.13) and (8.16), and rearranging, one obtains

$$\frac{P_{t2}}{P_{t1}} = \left(\frac{\frac{\gamma+1}{\gamma-1}}{\frac{2\gamma}{\gamma-1}M_{1n}^2 - 1} \right)^{1/(\gamma-1)} \left(\frac{\frac{\gamma+1}{2}M_{1n}^2}{1 + \frac{\gamma-1}{2}M_{1n}^2} \right)^{\gamma/(\gamma-1)}. \quad (8.18)$$

Finally, entropy change across a normal shock is

$$s_2 - s_1 = -R \ln \frac{P_{t2}}{P_{t1}}, \quad (8.19)$$

as shown in Thompson (1988).

8.1.2 Oblique shocks

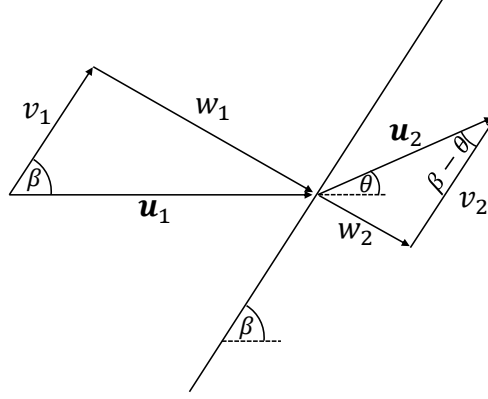


Figure 8.2: Oblique-shock geometry, β is the shock angle and θ the turning angle.

The normal shock jump conditions given by eqs. (8.13) to (8.16) and (8.18) still apply, but it is again emphasized that w_1 and w_2 are the components normal to the shock, as defined in eq. (8.1). For the tangential components, defined by eq. (8.2), we have $v_1 = v_2$ as mentioned in section 8.1. As shown in fig. 8.2, the relationship between w_1 , w_2 and \mathbf{u}_1 , \mathbf{u}_2 is

$$\begin{aligned} w_1 &= |\mathbf{u}_1| \sin \beta, \\ w_2 &= |\mathbf{u}_2| \sin(\beta - \theta). \end{aligned} \quad (8.20)$$

Similarly, the relationship between v_1 , v_2 and \mathbf{u}_1 , \mathbf{u}_2 is

$$\begin{aligned} v_1 &= |\mathbf{u}_1| \cos \beta, \\ v_2 &= |\mathbf{u}_2| \cos(\beta - \theta). \end{aligned} \quad (8.21)$$

If the upstream state is known (ρ_1 , \mathbf{u}_1 , P_1 , P_{t1}), along with the shock angle β , then the downstream state can be determined using the above relationships and the normal shock jump conditions.

Using the shock jump condition for velocity (eq. (8.14)), and some trigonometric identities, one can derive an equation for θ in terms of β , for a given inflow Mach number $M_1 = |\mathbf{u}_1|/c_1$, (see Thompson (1988)). This relationship is

$$\tan \theta = \frac{\cot \beta (M_1^2 \sin^2 \beta - 1)}{1 + \left(\frac{\gamma+1}{2}\right) M_1^2 - M_1^2 \sin^2 \beta}. \quad (8.22)$$

The information contained in the above relationship is quite vast, and can best be understood by looking at θ profiles as a function of β —for different Mach numbers—obtained from the equation above. A plot of these profiles is given in fig. 8.3. Starting from the right-most point on the x -axis, labelled as “a”, is a normal shock with a shock angle of 90° . Moving along the blue line as the shock angle decreases, we see that the turning angle increases until a maximum, labeled as “b”, is reached. A further decrease in shock angle leads to point “c”, which corresponds to turning angles for which the flow behind the shock becomes subsonic. Smaller shock angles lead to even smaller turning angles, until point “d” is reached, which corresponds to a Mach wave, to be described in a subsequent section. It is important to note that there are two shock angles that can give the same turning angle. The turning angle corresponding to the smaller shock

angle is referred to as the weak solution, whereas the turning angle corresponding to the larger shock angle is the strong solution. This nomenclature has no direct connection to that defined in eq. (8.12). The black dashed line in fig. 8.3 corresponds to the peak value for each Mach number, and thus demarcates the weak and strong solutions. A more pictorial representation of this behavior, for the specific case of a shock in front of a cylinder, is given in fig. 8.4.

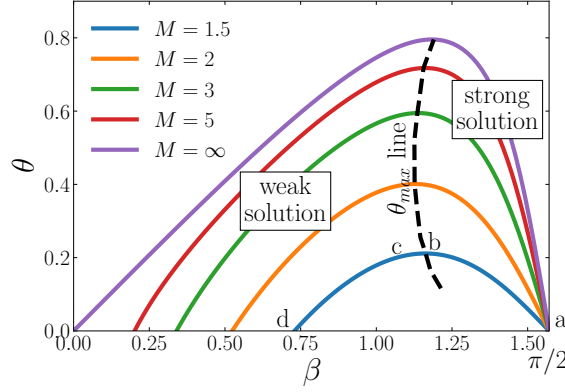


Figure 8.3: θ - β curve for a perfect gas with $\gamma = 1.4$.

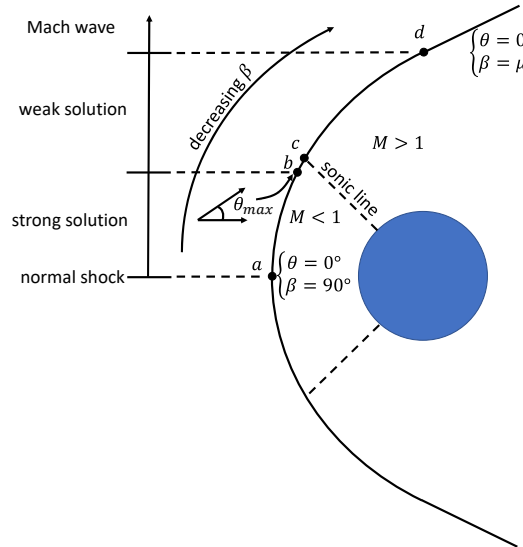


Figure 8.4: Representation of different shock waves for different shock angles β .

Given the information above, it is relevant to ask what happens when a compressible fluid flows over a wedge or a some similar object, whose wedge angle is so large that the turning angle needs to be larger than θ_{max} . Given that, as fig. 8.3 shows, there is no turning angle greater than θ_{max} , it seems like an inconsistency has been found. In reality, when the flow encounters a wedge whose angle is not that large and the turning angle can be lower than θ_{max} , then the weak solution is the one that occurs and the shock is attached to the leading edge of the wedge. As the wedge angle increases and the flow needs to be deflected by an angle greater than θ_{max} ,

the shock detaches from the wedge leading edge, as shown in fig. 8.4, and both strong and weak solutions occur along the shock. For this case, there will be a section behind the shock that will be subsonic, and thus the flow there can be turned by any angle greater than θ_{max} .

8.1.3 Weak shocks

By definition, weak shocks are those for which Π , defined in eq. (8.11), is very small. Assuming that $\rho_1 c_1^2$ is not excessively large, the definition of Π indicates that $P_2 - P_1$ is small for weak shocks. We can use the fact that $P_2 - P_1$ is small for weak shocks to show that $(s_2 - s_1) \propto (P_2 - P_1)^3$, which then indicates weak shocks have negligible entropy changes.

We begin by adding and subtracting $(P_2 - P_1)\vartheta_1$ on the right-hand side of the Rankine-Hugoniot eq. (8.7) to obtain

$$h_2 - h_1 = (P_2 - P_1)\vartheta_1 + \frac{1}{2}(P_2 - P_1)(\vartheta_2 - \vartheta_1). \quad (8.23)$$

We now use Taylor-series expansions for h and ϑ , each as a function of s and P , and plug them into the equation above to obtain the scaling of s as a function of P . For an arbitrary function $f(s, P)$ the Taylor-series expansion can symbolically be expressed as

$$\begin{aligned} f_2 - f_1 = & \left[(s_2 - s_1) \left(\frac{\partial}{\partial s} \right)_1 + (P_2 - P_1) \left(\frac{\partial}{\partial P} \right)_1 \right] f \\ & + \frac{1}{2!} \left[(s_2 - s_1) \left(\frac{\partial}{\partial s} \right)_1 + (P_2 - P_1) \left(\frac{\partial}{\partial P} \right)_1 \right]^2 f \\ & + \frac{1}{3!} \left[(s_2 - s_1) \left(\frac{\partial}{\partial s} \right)_1 + (P_2 - P_1) \left(\frac{\partial}{\partial P} \right)_1 \right]^3 f + \dots \end{aligned}$$

Since we are interested in the leading-order expression for $(s_2 - s_1)$, terms of higher-order than $(s_2 - s_1)$ will be neglected, i.e. $(s_2 - s_1)^2$, $(s_2 - s_1)^3$, $(s_2 - s_1)(P_2 - P_1)$, etc.

The Taylor-series expansion for enthalpy is

$$h_2 - h_1 = (s_2 - s_1) \left(\frac{\partial h}{\partial s} \right)_1 + (P_2 - P_1) \left(\frac{\partial h}{\partial P} \right)_1 + \frac{1}{2}(P_2 - P_1)^2 \left(\frac{\partial^2 h}{\partial P^2} \right)_1 + \frac{1}{6}(P_2 - P_1)^3 \left(\frac{\partial^3 h}{\partial P^3} \right)_1 + \dots \quad (8.24)$$

Using the Gibbs equation shown in eq. (7.7), we have $(\partial h / \partial s)_p = T$ and $(\partial h / \partial P)_s = \vartheta$. Using this in the above gives

$$h_2 - h_1 = (s_2 - s_1)T_1 + (P_2 - P_1)\vartheta_1 + \frac{1}{2}(P_2 - P_1)^2 \left(\frac{\partial \vartheta}{\partial P} \right)_1 + \frac{1}{6}(P_2 - P_1)^3 \left(\frac{\partial^2 \vartheta}{\partial P^2} \right)_1 + \dots \quad (8.25)$$

The Taylor-series expansion for the specific volume is

$$\vartheta_2 - \vartheta_1 = (s_2 - s_1) \left(\frac{\partial \vartheta}{\partial s} \right)_1 + (P_2 - P_1) \left(\frac{\partial \vartheta}{\partial P} \right)_1 + \frac{1}{2}(P_2 - P_1)^2 \left(\frac{\partial^2 \vartheta}{\partial P^2} \right)_1 + \frac{1}{6}(P_2 - P_1)^3 \left(\frac{\partial^3 \vartheta}{\partial P^3} \right)_1 + \dots \quad (8.26)$$

Plugging in the two Taylor-series expansions above in eq. (8.23), gives

$$\begin{aligned} (s_2 - s_1)T_1 + (P_2 - P_1)\vartheta_1 + \frac{1}{2}(P_2 - P_1)^2 \left(\frac{\partial \vartheta}{\partial P} \right)_1 + \frac{1}{6}(P_2 - P_1)^3 \left(\frac{\partial^2 \vartheta}{\partial P^2} \right)_1 = \\ (P_2 - P_1)\vartheta_1 + \frac{1}{2}(P_2 - P_1)^2 \left(\frac{\partial \vartheta}{\partial P} \right)_1 + \frac{1}{4}(P_2 - P_1)^3 \left(\frac{\partial^2 \vartheta}{\partial P^2} \right)_1 + \dots \quad (8.27) \end{aligned}$$

Simplifying the above finally gives

$$s_2 - s_1 = \frac{1}{12T_1} \left(\frac{\partial^2 \vartheta}{\partial P^2} \right)_1 (P_2 - P_1)^3 + \dots \quad (8.28)$$

that is, $(s_2 - s_1) \propto (P_2 - P_1)^3$.

8.1.4 Strong shocks

Strong shocks are defined as those for which $\Pi \gg 1$. In general, it seems that $P < \rho c^2$, and thus

$$\Pi = \frac{P_2}{\rho_1 c_1^2} - \frac{P_1}{\rho_1 c_1^2} \gg 1 \quad (8.29)$$

becomes

$$\frac{P_2}{\rho_1 c_1^2} \gg 1, \quad (8.30)$$

or

$$P_2 \gg \rho_1 c_1^2. \quad (8.31)$$

The above in turn implies $P_2 \gg P_1$, that is, P_1 is negligible.

Consider the normal shock jump condition for pressure given by eq. (8.13). It can be rearranged to give

$$P_2 = \frac{\frac{2\gamma}{\gamma-1} \frac{\rho_1 w_1^2}{\gamma} - P_1}{\frac{\gamma+1}{\gamma-1}}. \quad (8.32)$$

Since P_1 can be neglected, this gives

$$P_2 = \frac{2}{\gamma+1} \rho_1 w_1^2. \quad (8.33)$$

Additionally, since $M_{1n}^2 = \rho_1 w_1^2 / \gamma P_1$, a negligible P_1 leads to $M_{1n}^2 \gg 1$. Thus, eqs. (8.14) to (8.16) give

$$\frac{w_2}{w_1} = \frac{\gamma-1}{\gamma+1}, \quad (8.34)$$

$$\frac{\rho_2}{\rho_1} = \frac{\gamma+1}{\gamma-1}, \quad (8.35)$$

and

$$M_{2n}^2 = \frac{\gamma-1}{2\gamma}. \quad (8.36)$$

8.2 Mach Waves

Assume a vehicle is moving at a Mach number greater than one. In fig. 8.5, the black line represents a section of the surface of the vehicle moving at supersonic speeds. At each instance in time, each infinitesimal point on this surface slightly distorts the stationary fluid and thus produces acoustic waves (blue line). These waves, by definition, expand at the speed of sound. The green line, which is aligned with the front of the acoustic waves, is referred to as a Mach wave or Mach line. The angle of inclination of this Mach wave, labeled μ , is called the Mach angle and satisfies

$$\sin(\mu) = \frac{1}{M}. \quad (8.37)$$

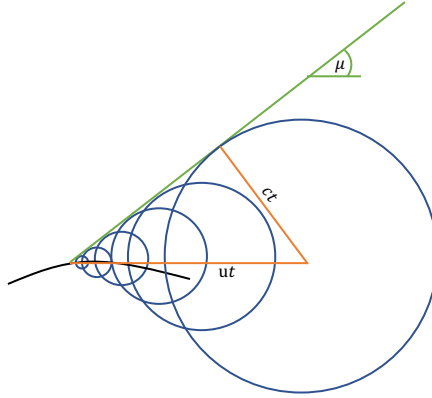


Figure 8.5: Mach wave

8.3 Contact discontinuities

A contact discontinuity is defined as a surface that separates two fluids of different properties or at different states. A defining condition is that there is no flow of matter across a contact discontinuity, that is, $w_1 = w_2 = 0$. Using this in the integral momentum conservation equation for a thin box bounding the discontinuity, and assuming negligible viscous stresses and heat fluxes, leads to $P_1 = P_2$. However, other flow properties, such as ρ , T , and v can change across the discontinuity.

Chapter 9

Quasi 1-D steady and unsteady flow

Quasi 1-D eqs; mass balance, $f(M)$, and PAFMT; Fanno flow, Rayleigh flow.

Local acoustic speed, Expansion and Compression wave, Shock tube.

Chapter 10

2-D Compressible flow

Prandtl-Meyer (Compressive, Expansive); Shock-Expansion Theory: 2D Airfoil Calculations, Shock Reflection, Isentropic flow in curved channel, Nozzle exit flows.

Part III

Flow Instabilities

Chapter 11

Hydrodynamic Instabilities

11.1 Linear Stability

Consider the following system of PDEs for a two-dimensional problem

$$\frac{\partial w}{\partial t} = \frac{\partial \phi}{\partial y} \frac{\partial w}{\partial x} - \frac{\partial \phi}{\partial x} \frac{\partial w}{\partial y}, \quad (11.1)$$

$$w = \nabla^2 \phi. \quad (11.2)$$

In the above, $\phi = \phi(x, y, t)$ is the electrostatic potential and $w = w(x, y, t)$ the vorticity.

The analysis begins by splitting the variables into equilibrium and fluctuating components, namely

$$\phi = \phi_0 + \phi_1, \quad (11.3)$$

$$w = w_0 + w_1. \quad (11.4)$$

For the above, $\phi_0 = \phi_0(x)$, $w_0 = w_0(x)$, and $\phi_1 = \phi_1(x, y, t)$, $w_1 = w_1(x, y, t)$. We now introduce a Fourier series decomposition for the fluctuating variables, and focus on a single Fourier mode as follows

$$\phi_1(x, y, t) = F(x, k_y, t)e^{ik_y y} = \tilde{\phi}(x, k_y)e^{\gamma t + ik_y y}, \quad (11.5)$$

$$w_1(x, y, t) = G(x, k_y, t)e^{ik_y y} = \tilde{w}(x, k_y)e^{\gamma t + ik_y y}. \quad (11.6)$$

In the above, γ , which can be complex, is the growth rate factor, and $\tilde{\phi} = \tilde{\phi}(x, k_y)$, $\tilde{w} = \tilde{w}(x, k_y)$ are the remaining part of the Fourier coefficient.

We then plug in the decompositions for ϕ and w in the governing PDEs. Collecting the lowest order terms leads to equations for the equilibrium solution. For example, the Poisson equation to lowest order is

$$w_0 = \nabla^2 \phi_0 = \frac{\partial^2 \phi_0}{\partial x^2}. \quad (11.7)$$

Combining terms up to next order gives

$$\frac{\partial w_1}{\partial t} = \frac{\partial \phi_0}{\partial y} \frac{\partial w_1}{\partial x} + \frac{\partial \phi_1}{\partial y} \frac{\partial w_0}{\partial x} - \frac{\partial \phi_0}{\partial x} \frac{\partial w_1}{\partial y} - \frac{\partial \phi_1}{\partial x} \frac{\partial w_0}{\partial y}, \quad (11.8)$$

$$w_1 = \nabla^2 \phi_1. \quad (11.9)$$

Using the expression for ϕ_1 in the Poisson equation above leads to

$$w_1 = \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) e^{\gamma t + ik_y y}, \quad (11.10)$$

or

$$\tilde{w} = \frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi}. \quad (11.11)$$

We'll now evaluate each of the terms in eq. (11.8).

$$\begin{aligned} \frac{\partial w_1}{\partial t} &= \gamma \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) e^{\gamma t + i k_y y}, \\ \frac{\partial \phi_0}{\partial y} \frac{\partial w_1}{\partial x} &= 0, \\ \frac{\partial \phi_1}{\partial y} \frac{\partial w_0}{\partial x} &= i k_y \tilde{\phi} e^{\gamma t + i k_y y} \frac{\partial^3 \phi_0}{\partial x^3}, \\ \frac{\partial \phi_0}{\partial x} \frac{\partial w_1}{\partial y} &= \frac{\partial \phi_0}{\partial x} i k_y \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) e^{\gamma t + i k_y y}, \\ \frac{\partial \phi_1}{\partial x} \frac{\partial w_0}{\partial y} &= 0. \end{aligned} \quad (11.12)$$

Combining all of the above, we obtain

$$\gamma \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) = i k_y \tilde{\phi} \frac{\partial^3 \phi_0}{\partial x^3} - \frac{\partial \phi_0}{\partial x} i k_y \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right). \quad (11.13)$$

This is re-written as

$$\gamma \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) = -i k_y \left[\frac{\partial \phi_0}{\partial x} \left(\frac{\partial^2 \tilde{\phi}}{\partial x^2} - k_y^2 \tilde{\phi} \right) - \frac{\partial^3 \phi_0}{\partial x^3} \tilde{\phi} \right]. \quad (11.14)$$

Appendix A

Vectors in rotating reference frames

A.1 Basic properties

A.1.1 Position

Consider the Euclidean transformation

$$\tilde{x}_i^+(\tilde{t}) = Q_{ij}(\tilde{t} - c)x_j^+(\tilde{t} - c) + b_i(\tilde{t} - c) \quad (\text{A.1})$$

where $x^+(t)$ is the Lagrangian position of a fluid particle, and $\tilde{x}^+(\tilde{t})$ is the Lagrangian position of the same particle but in a rotating reference frame. The transformation above amounts to a rotation of the reference frame determined by the orthogonal matrix $\mathbf{Q}(t)$, a translation of the reference frame determined by the vector $\mathbf{b}(t)$, and a translation in time given by $\tilde{t} = t + c$.

A.1.2 Velocity

Since the velocity of a fluid particle is given by

$$u_i^+(t) = \frac{dx_i^+(t)}{dt}, \quad (\text{A.2})$$

the components of velocity in the non-inertial reference frame are defined as

$$\tilde{u}_i^+(\tilde{t}) = \frac{d\tilde{x}_i^+(\tilde{t})}{d\tilde{t}}. \quad (\text{A.3})$$

Thus, the relationship between the velocity components in the different reference frames is given by

$$\begin{aligned} \tilde{u}_i^+(\tilde{t}) &= \frac{d}{d\tilde{t}}[Q_{ij}(\tilde{t} - c)x_j^+(\tilde{t} - c) + b_i(\tilde{t} - c)] \\ &= Q_{ij}(\tilde{t} - c)U_j^+(\tilde{t} - c) + \dot{Q}_{ij}(\tilde{t} - c)x_j^+(\tilde{t} - c) + \dot{b}_i(\tilde{t} - c). \end{aligned} \quad (\text{A.4})$$

If we assume there is no translation in space or time, the above reduces to

$$\tilde{u}_i^+ = Q_{ij}u_j^+ + \dot{Q}_{ij}x_j^+, \quad (\text{A.5})$$

where each quantity above depends on time t . Multiplying by Q_{ki}^{-1} we obtain

$$Q_{ik}\tilde{u}_i^+ = u_k^+ + Q_{ik}\dot{Q}_{ij}x_j^+. \quad (\text{A.6})$$

Noting that the tensor $Q_{ik}\dot{Q}_{ij}$ is antisymmetric, we obtain

$$u_k^+ = Q_{ik}\tilde{u}_i^+ + Q_{ij}\dot{Q}_{ik}x_j^+. \quad (\text{A.7})$$

We now define the angular velocity tensor Ω_{ij} and the angular velocity vector Ω_i using the following relationship

$$\Omega_{ij} = \epsilon_{jik}\Omega_k = Q_{kj}\dot{Q}_{ki}. \quad (\text{A.8})$$

Thus (A.7) can be expressed in terms of the angular velocity tensor as

$$u_k^+ = Q_{ik}\tilde{u}_i^+ + \Omega_{kj}x_j^+, \quad (\text{A.9})$$

or in terms of the angular velocity vector as

$$u_k^+ = Q_{ik}\tilde{u}_i^+ + \epsilon_{jki}\Omega_jx_k^+. \quad (\text{A.10})$$

A.1.3 Acceleration

We assume again no translation in space or time. Taking the derivative of both sides of eq. (A.7)

$$\frac{du_k^+}{dt} = \dot{Q}_{ik}\tilde{u}_i^+ + Q_{ik}\frac{d\tilde{u}_i^+}{dt} + \dot{Q}_{ik}\frac{dQ_{ij}x_j^+}{dt} + Q_{ij}\ddot{Q}_{ik}x_j^+. \quad (\text{A.11})$$

Using eq. (A.1) the above is re-written as

$$\frac{du_k^+}{dt} = Q_{ik}\frac{d\tilde{u}_i^+}{dt} + 2\dot{Q}_{ik}\tilde{u}_i^+ + Q_{ij}\ddot{Q}_{ik}x_j^+. \quad (\text{A.12})$$

Re-writing the last term on the right-hand-side above leads to

$$\frac{du_k^+}{dt} = Q_{ik}\frac{d\tilde{u}_i^+}{dt} + 2\dot{Q}_{ik}\tilde{u}_i^+ + \frac{dQ_{ij}\dot{Q}_{ik}}{dt}x_j^+ - \dot{Q}_{ij}\dot{Q}_{ik}x_j^+. \quad (\text{A.13})$$

We now show that

$$\begin{aligned} \dot{Q}_{ij}\dot{Q}_{ik} &= \delta_{pi}\dot{Q}_{pj}\dot{Q}_{ik} \\ &= Q_{pq}Q_{qi}^{-1}\dot{Q}_{pj}\dot{Q}_{ik} \\ &= Q_{pq}\dot{Q}_{pj}Q_{iq}\dot{Q}_{ik}. \end{aligned} \quad (\text{A.14})$$

Thus, in terms of the angular velocity tensor, we have

$$\frac{du_k^+}{dt} = Q_{ik}\frac{d\tilde{u}_i^+}{dt} + 2\dot{Q}_{ik}\tilde{u}_i^+ + \frac{d\Omega_{kj}}{dt}x_j^+ - \Omega_{kq}\Omega_{jq}x_j^+. \quad (\text{A.15})$$

In terms of the angular velocity vector, the above becomes

$$\frac{du_k^+}{dt} = Q_{ik}\frac{d\tilde{u}_i^+}{dt} + 2\dot{Q}_{ik}\tilde{u}_i^+ + \epsilon_{jki}\frac{d\Omega_j}{dt}x_k^+ - \epsilon_{qki}\Omega_i\epsilon_{qjp}\Omega_px_j^+, \quad (\text{A.16})$$

which, upon a simple re-arrangement of indices, gives

$$\frac{du_k^+}{dt} = Q_{ik}\frac{d\tilde{u}_i^+}{dt} + 2\dot{Q}_{ik}\tilde{u}_i^+ + \epsilon_{kij}\frac{d\Omega_i}{dt}x_j^+ + \epsilon_{kij}\Omega_i\epsilon_{qpj}\Omega_px_j^+. \quad (\text{A.17})$$

A.2 Unit vectors

Let the orthogonal basis for the inertial reference frame be denoted by $\hat{a}^{(1)}$, $\hat{a}^{(2)}$, and $\hat{a}^{(3)}$, and the orthogonal basis for the rotating reference frame by $\hat{b}^{(1)}$, $\hat{b}^{(2)}$, and $\hat{b}^{(3)}$. We know that the unit vector $\hat{b}^{(i)}$ has components $\tilde{b}_j^{(i)}$ in the rotating reference frame, and components $b_j^{(i)}$ in the inertial reference frame. The vector is the same whether expressed in the rotating or inertial reference frames, that is

$$\tilde{b}_k^{(i)} \hat{b}^{(k)} = b_k^{(i)} \hat{a}^{(k)} \quad (\text{A.18})$$

Since $\tilde{b}_k^{(i)} = \delta_{ik}$, we rewrite the above as

$$\hat{b}^{(i)} = b_k^{(i)} \hat{a}^{(k)} = Q_{jk} \tilde{b}_j^{(i)} \hat{a}^{(k)} = Q_{ik} \hat{a}^{(k)}. \quad (\text{A.19})$$

Doting both sides by $\hat{a}^{(j)}$ shows that

$$Q_{ij} = \hat{a}^{(j)} \cdot \hat{b}^{(i)}. \quad (\text{A.20})$$

One can also multiply both sides of eq. (A.10) by $\hat{a}^{(k)}$ and use eq. (A.19) to obtain

$$u_k^+ \hat{a}^{(k)} = \tilde{u}_i^+ \hat{b}^{(i)} + \epsilon_{jki} \Omega_i x_j^+ \hat{a}^{(k)}. \quad (\text{A.21})$$

If we introduce the following notation

$$\vec{u}_{ine}^+ = u_k^+ \hat{a}^{(k)}, \quad (\text{A.22})$$

$$\vec{u}_{rot}^+ = \tilde{u}_i^+ \hat{b}^{(i)}, \quad (\text{A.23})$$

$$\vec{\Omega} = \Omega_i \hat{a}^{(i)}, \quad (\text{A.24})$$

$$\vec{x}^+ = x_i^+ \hat{a}^{(i)}. \quad (\text{A.25})$$

then the eq. (A.21) is written as

$$\vec{u}_{ine}^+ = \vec{u}_{rot}^+ + \vec{\Omega} \times \vec{x}^+. \quad (\text{A.26})$$

Similarly, multiplying both sides of eq. (A.17) gives

$$\frac{du_k^+}{dt} \hat{a}^{(k)} = \frac{d\tilde{u}_i^+}{dt} \hat{b}^{(i)} + 2\dot{Q}_{ik} \tilde{u}_i^+ \hat{a}^{(k)} + \epsilon_{kij} \frac{d\Omega_i}{dt} x_j^+ \hat{a}^{(k)} + \epsilon_{kij} \Omega_i \epsilon_{qpj} \Omega_p x_j^+ \hat{a}^{(k)}. \quad (\text{A.27})$$

Using eq. (A.8) one can show that $\dot{Q}_{ik} = \epsilon_{pj k} \Omega_p Q_{ij}$. Thus, the second term on the left-hand-side above can be written as

$$\begin{aligned} 2\dot{Q}_{ik} \tilde{u}_i^+ \hat{a}^{(k)} &= 2\epsilon_{pj k} \Omega_p Q_{ij} \tilde{u}_i^+ \hat{a}^{(k)} \\ &= 2\Omega_p Q_{ij} \tilde{u}_i^+ \hat{a}^{(p)} \times \hat{a}^{(j)} \\ &= 2\Omega_p \hat{a}^{(p)} \times \tilde{u}_i^+ \hat{b}^{(i)}. \end{aligned} \quad (\text{A.28})$$

Therefore, in vector notation eq. (A.27) becomes

$$\vec{a}_{ine}^+ = \vec{a}_{rot}^+ + 2\vec{\Omega} \times \vec{u}_{rot}^+ + \dot{\vec{\Omega}} \times \vec{x}^+ + \vec{\Omega} \times (\vec{\Omega} \times \vec{x}^+), \quad (\text{A.29})$$

where $\vec{a}_{ine}^+ = \frac{du_k^+}{dt} \hat{a}^{(k)}$, $\vec{a}_{rot}^+ = \frac{d\tilde{u}_i^+}{dt} \hat{b}^{(i)}$, and $\dot{\vec{\Omega}} = \frac{d\Omega_i}{dt} \hat{a}^{(i)}$.

A.3 Eulerian variables

We now introduce the Eulerian counterpart to the Lagrangian variables. In the inertial reference frame these are $\rho(t, \mathbf{x})$, $u_i(t, \mathbf{x})$, and $p(t, \mathbf{x})$. They are defined by the following expressions

$$\rho^+ = \rho(t, \mathbf{x}^+) \quad (\text{A.30})$$

$$u_i^+ = u_i(t, \mathbf{x}^+) \quad (\text{A.31})$$

$$p^+ = p(t, \mathbf{x}^+). \quad (\text{A.32})$$

Similarly for the rotating reference frame, we have $\tilde{\rho}(t, \tilde{\mathbf{x}})$, $\tilde{u}_i(t, \tilde{\mathbf{x}})$, and $\tilde{p}(t, \tilde{\mathbf{x}})$. These are defined by

$$\tilde{\rho}^+ = \tilde{\rho}(t, \tilde{\mathbf{x}}^+) \quad (\text{A.33})$$

$$\tilde{u}_i^+ = \tilde{u}_i(t, \tilde{\mathbf{x}}^+) \quad (\text{A.34})$$

$$\tilde{p}^+ = \tilde{p}(t, \tilde{\mathbf{x}}^+). \quad (\text{A.35})$$

We now use the transformation rules for the Lagrangian variables to derive the transformation rules for the Eulerian variables. The transformation rules for the Lagrangian variables are

$$\rho^+ = \tilde{\rho}^+ \quad (\text{A.36})$$

$$u_k^+ = Q_{ik}\tilde{u}_i^+ + Q_{ij}\dot{Q}_{ik}x_j^+ \quad (\text{A.37})$$

$$p^+ = \tilde{p}^+. \quad (\text{A.38})$$

The second equation above is the previously derived eq. (A.7). Using the definition of the Eulerian variables, the above is re-written as

$$\rho(t, \mathbf{x}^+) = \tilde{\rho}(t, \tilde{\mathbf{x}}^+) \quad (\text{A.39})$$

$$u_i(t, \mathbf{x}^+) = Q_{ik}\tilde{u}_i(t, \tilde{\mathbf{x}}^+) + Q_{ij}\dot{Q}_{ik}x_j^+ \quad (\text{A.40})$$

$$p(t, \mathbf{x}^+) = \tilde{p}(t, \tilde{\mathbf{x}}^+). \quad (\text{A.41})$$

Using eq. (A.1), we get

$$\rho(t, \mathbf{x}^+) = \tilde{\rho}(t, \mathbf{Q}\mathbf{x}^+) \quad (\text{A.42})$$

$$u_i(t, \mathbf{x}^+) = Q_{ik}\tilde{u}_i(t, \mathbf{Q}\mathbf{x}^+) + Q_{ij}\dot{Q}_{ik}x_j^+ \quad (\text{A.43})$$

$$p(t, \mathbf{x}^+) = \tilde{p}(t, \mathbf{Q}\mathbf{x}^+) + . \quad (\text{A.44})$$

Since the above holds for any \mathbf{x}^+ , we finally re-write it as

$$\rho(t, \mathbf{x}) = \tilde{\rho}(t, \mathbf{Q}\mathbf{x}) \quad (\text{A.45})$$

$$u_i(t, \mathbf{x}) = Q_{ik}\tilde{u}_i(t, \mathbf{Q}\mathbf{x}) + Q_{ij}\dot{Q}_{ik}x_j \quad (\text{A.46})$$

$$p(t, \mathbf{x}) = \tilde{p}(t, \mathbf{Q}\mathbf{x}). \quad (\text{A.47})$$

A.4 Rotating Navier-Stokes equations

We first obtain a few set of relationships that will later be used in deriving the rotating Navier-Stokes equations. Taking the derivative of eq. (A.47) gives

$$\begin{aligned}
\frac{\partial p(t, \mathbf{x})}{\partial x_i} &= \frac{\partial \tilde{p}(t, \mathbf{Q}\mathbf{x})}{\partial x_i} \\
&= \frac{\partial}{\partial x_i} \tilde{p}(t, Q_{1j}x_j, Q_{2j}x_j, Q_{3j}x_3) \\
&= \frac{\partial Q_{1j}x_j}{\partial x_i} \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_1} \right]_{\tilde{\mathbf{x}}=\mathbf{Q}\mathbf{x}} + \frac{\partial Q_{2j}x_j}{\partial x_i} \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_2} \right]_{\tilde{\mathbf{x}}=\mathbf{Q}\mathbf{x}} + \frac{\partial Q_{3j}x_j}{\partial x_i} \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_3} \right]_{\tilde{\mathbf{x}}=\mathbf{Q}\mathbf{x}} \\
&= Q_{ji} \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\mathbf{Q}\mathbf{x}}
\end{aligned} \tag{A.48}$$

If we evaluate the above at $\mathbf{x} = \mathbf{x}^+$, we get

$$\left[\frac{\partial p(t, \mathbf{x})}{\partial x_i} \right]_{\mathbf{x}=\mathbf{x}^+} = Q_{ji} \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+}. \tag{A.49}$$

Multiplying both sides by $\hat{a}^{(i)}$ gives

$$\left[\frac{\partial p(t, \mathbf{x})}{\partial x_i} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} = \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(j)}. \tag{A.50}$$

For the shear-stress tensor, we have

$$\left[\frac{\partial \tau_{ij}(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} = \left[\frac{\partial \tilde{\tau}_{ij}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)}. \tag{A.51}$$

We also use eq. (A.29) to write

$$\begin{aligned}
\frac{du_i^+}{dt} \hat{a}^{(i)} &= \frac{d\tilde{u}_i^+}{dt} \hat{b}^{(i)} + 2\vec{\Omega} \times \left(\tilde{u}_i^+ \hat{b}^{(i)} \right) + \dot{\vec{\Omega}} \times \vec{x}^+ + \vec{\Omega} \times \left(\vec{\Omega} \times \vec{x}^+ \right) \\
&= \frac{d\tilde{u}_i^+}{dt} \hat{b}^{(i)} + 2\vec{\Omega} \times \left(\tilde{u}_i^+ \hat{b}^{(i)} \right) + \dot{\vec{\Omega}} \times \left(\tilde{x}_i^+ \hat{b}^{(i)} \right) + \vec{\Omega} \times \left[\vec{\Omega} \times \left(\tilde{x}_i^+ \hat{b}^{(i)} \right) \right]
\end{aligned} \tag{A.52}$$

Expressing the above in terms of Eulerian quantities gives

$$\begin{aligned}
\left[\frac{\partial u_i(t, \mathbf{x})}{\partial t} + u_j(t, \mathbf{x}) \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} &= \left[\frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial t} + \tilde{u}_j(t, \tilde{\mathbf{x}}) \frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \\
&+ 2\vec{\Omega} \times \left\{ [\tilde{u}_i(t, \tilde{\mathbf{x}})]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right\} + \dot{\vec{\Omega}} \times \left[(\tilde{x}_i)_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right] + \vec{\Omega} \times \left\{ \vec{\Omega} \times \left[(\tilde{x}_i)_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right] \right\}
\end{aligned} \tag{A.53}$$

The conservation of momentum equation is given by

$$\rho(t, \mathbf{x}) \left[\frac{\partial u_i(t, \mathbf{x})}{\partial t} + u_j(t, \mathbf{x}) \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right] = - \frac{\partial p(t, \mathbf{x})}{\partial x_i} + \frac{\partial \tau_{ij}(t, \mathbf{x})}{\partial x_j}. \tag{A.54}$$

Evaluating the above at $\mathbf{x} = \mathbf{x}^+$ can be written as

$$\rho(t, \mathbf{x}^+) \left[\frac{\partial u_i(t, \mathbf{x})}{\partial t} + u_j(t, \mathbf{x}) \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} = - \left[\frac{\partial p(t, \mathbf{x})}{\partial x_i} \right]_{\mathbf{x}=\mathbf{x}^+} + \left[\frac{\partial \tau_{ij}(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+}. \tag{A.55}$$

Multiplying both sides by $\hat{a}^{(i)}$ gives

$$\begin{aligned} \rho(t, \mathbf{x}^+) \left[\frac{\partial u_i(t, \mathbf{x})}{\partial t} + u_j(t, \mathbf{x}) \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} \\ = - \left[\frac{\partial p(t, \mathbf{x})}{\partial x_i} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} + \left[\frac{\partial \tau_{ij}(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)}. \end{aligned} \quad (\text{A.56})$$

Using eqs. (A.39), (A.50) and (A.51) gives

$$\begin{aligned} [\tilde{\rho}(t, \tilde{\mathbf{x}})]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \left[\frac{\partial u_i(t, \mathbf{x})}{\partial t} + u_j(t, \mathbf{x}) \frac{\partial u_i(t, \mathbf{x})}{\partial x_j} \right]_{\mathbf{x}=\mathbf{x}^+} \hat{a}^{(i)} \\ = - \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_i} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} + \left[\frac{\partial \tilde{\tau}_{ij}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)}. \end{aligned} \quad (\text{A.57})$$

Using eq. (A.53) we obtain

$$\begin{aligned} [\tilde{\rho}(t, \tilde{\mathbf{x}})]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \left(\left[\frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial t} + \tilde{u}_j(t, \tilde{\mathbf{x}}) \frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} + 2\vec{\Omega} \times \left\{ [\tilde{u}_i(t, \tilde{\mathbf{x}})]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right\} \right. \\ \left. + \dot{\vec{\Omega}} \times \left[(\tilde{x}_i)_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right] + \vec{\Omega} \times \left\{ \vec{\Omega} \times \left[(\tilde{x}_i)_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} \right] \right\} \right) = - \left[\frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_i} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)} + \left[\frac{\partial \tilde{\tau}_{ij}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right]_{\tilde{\mathbf{x}}=\tilde{\mathbf{x}}^+} \hat{b}^{(i)}. \end{aligned} \quad (\text{A.58})$$

Finally, since this holds for any $\tilde{\mathbf{x}}^+$, we get

$$\begin{aligned} \tilde{\rho}(t, \tilde{\mathbf{x}}) \left\{ \left[\frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial t} + \tilde{u}_j(t, \tilde{\mathbf{x}}) \frac{\partial \tilde{u}_i(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \right] \hat{b}^{(i)} + 2\vec{\Omega} \times \left[\tilde{u}_i(t, \tilde{\mathbf{x}}) \hat{b}^{(i)} \right] \right. \\ \left. + \dot{\vec{\Omega}} \times \left(\tilde{x}_i \hat{b}^{(i)} \right) + \vec{\Omega} \times \left[\vec{\Omega} \times \left(\tilde{x}_i \hat{b}^{(i)} \right) \right] \right\} = - \frac{\partial \tilde{p}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_i} \hat{b}^{(i)} + \frac{\partial \tilde{\tau}_{ij}(t, \tilde{\mathbf{x}})}{\partial \tilde{x}_j} \hat{b}^{(i)}. \end{aligned} \quad (\text{A.59})$$

Appendix B

Multi-component fluid flows in thermochemical non-equilibrium

In this chapter we describe the governing equations for a system of species in thermochemical non-equilibrium. The total number of molecular species is nms and the total number of species (atomic + molecular) is ns .

B.1 Conservation equations

The conservation equations that govern the dynamics of a compressible gas in thermochemical non-equilibrium are the following:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (\text{B.1})$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j} + \rho f_i \quad (\text{B.2})$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} [\rho E u_i] = \frac{\partial u_i \sigma_{ij}}{\partial x_j} + \rho f_i u_i - \frac{\partial q_i}{\partial x_i} \quad (\text{B.3})$$

$$\frac{\partial \rho e^{(v)}}{\partial t} + \frac{\partial \rho e^{(v)} u_i}{\partial x_i} = -\frac{\partial q_i^{(v)}}{\partial x_i} + Q^{(v)} \quad (\text{B.4})$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_i}{\partial x_i} = -\frac{\partial J_{\alpha,i}}{\partial x_i} + w_\alpha \quad \alpha \in [1, ns] \quad (\text{B.5})$$

B.2 Transport models

B.2.1 Shear stress, heat fluxes, and diffusive flux

The shear stress, heat flux, and diffusive flux are given by

$$t_{ij} = 2\mu S_{ij}^* \quad (\text{B.6})$$

$$q_i = -\kappa^{(t,r)} \frac{\partial T^{(t,r)}}{\partial x_i} - \kappa^{(v)} \frac{\partial T^{(v)}}{\partial x_i} + \sum_{\alpha=1}^{nms} h_\alpha J_{\alpha,i} \quad (\text{B.7})$$

$$q_i^{(v)} = -\kappa^{(v)} \frac{\partial T^{(v)}}{\partial x_i} + \sum_{\alpha=1}^{nms} e_\alpha^{(v)} J_{\alpha,i} \quad (\text{B.8})$$

$$J_{\alpha,i} = -\rho \left(D_{\alpha} \frac{\partial Y_{\alpha}}{\partial x_i} - Y_{\alpha} \sum_{\beta}^{ns} D_{\beta} \frac{\partial Y_{\beta}}{\partial x_i} \right) \quad \alpha \in [1, ns] \quad (\text{B.9})$$

B.2.2 Transport coefficients

The transport coefficients μ , $\kappa^{(t,r)}$, $\kappa^{(v)}$, and D_{α} required by the models above still need to be specified. There are a wide variety of models for these transport coefficients, and a few of these are detailed below.

The species viscosity μ_{α} is computed using a Blottner curve fit Blottner et al. (1971),

$$\mu_{\alpha} = 0.1 \exp \left[\left(A_{\alpha}^{\mu} \ln T^{(t,r)} + B_{\alpha}^{\mu} \right) \ln T^{(t,r)} + C_{\alpha}^{\mu} \right] \quad (\text{B.10})$$

The coefficients A_{α}^{μ} , B_{α}^{μ} , and C_{α}^{μ} are listed in Blottner et al. (1971). The species translational-rotational thermal conductivity is computed using the Eucken relation

$$\kappa_{\alpha} = \mu_{\alpha} \left(\frac{f}{2} + 2.25 \right) R, \quad (\text{B.11})$$

where f is the number of translational and rotational degrees of freedom (3 for monatomic gas and 5 for diatomic gas). The species vibrational thermal conductivity is computed as follows

$$\kappa_{\alpha}^{(v)} = \mu_{\alpha} C_{v,\alpha}^{(v)}, \quad (\text{B.12})$$

where $C_{v,\alpha}^{(v)}$ is the heat capacity at constant volume for the vibrational energy of a given species α (i.e. $C_{v,\alpha}^{(v)} = de_{\alpha}^{(v)} / dT^{(v)}$).

$$D_{\alpha} = \frac{\mu}{\rho S c_{\alpha}} \quad \alpha \in [1, ns] \quad (\text{B.13})$$

The viscosity μ for the whole mixture is obtained from the viscosity of each species μ_{α} using the Wilke mixing rule Wilke (1950)

$$\mu = \sum_{\alpha=1}^{ns} \frac{X_{\alpha} \mu_{\alpha}}{\phi_{\alpha}}, \quad (\text{B.14})$$

where ϕ_{α} is computed using

$$\phi_{\alpha} = \sum_{\beta=1}^{ns} X_{\beta} \frac{\left[1 + \left(\frac{\mu_{\alpha}}{\mu_{\beta}} \right)^{1/2} \left(\frac{M_{\beta}}{M_{\alpha}} \right)^{1/4} \right]^2}{\left[8 \left(1 + \frac{M_{\alpha}}{M_{\beta}} \right) \right]^{1/2}}. \quad (\text{B.15})$$

Note that the equation for the Wilke mixing rule given in Palmer and Wright (2003) differs from the above since it doesn't include the X_{β} shown in eq. (B.15).

B.3 Equation of state

B.3.1 Perfect gas

$$p = \rho R T \quad (\text{B.16})$$

$$R = \frac{R_u}{M} \quad (\text{B.17})$$

$$\frac{1}{M} = \sum_{\alpha} \frac{Y_{\alpha}}{M_{\alpha}} \quad (\text{B.18})$$

B.3.2 Ideal gas

B.4 Thermal non-equilibrium

B.4.1 Energy definitions

The total internal energy of the system $E = e$ is expressed as follows

$$e = e^{(t)} + e^{(r)} + e^{(v)} + e^{(el)} + e^{(e)} + \sum_{\alpha=1}^{ns} Y_{\alpha} h_{\alpha}^o. \quad (\text{B.19})$$

In the above, $e^{(t)}$ is the translation energy, $e^{(v)}$ the vibration energy, $e^{(el)}$ the electronic energy, and $e^{(e)}$ the electron energy. h_{α}^o denotes the heat of formation for each species. Each of the energies can be computed in terms of its single-species counterpart, as follows

$$e^{(t)} = \sum_{\alpha=1}^{ns} Y_{\alpha} e_{\alpha}^{(t)} \quad (\text{B.20})$$

$$e^{(r)} = \sum_{\alpha=1}^{nms} Y_{\alpha} e_{\alpha}^{(r)} \quad (\text{B.21})$$

$$e^{(v)} = \sum_{\alpha=1}^{nms} Y_{\alpha} e_{\alpha}^{(v)} \quad (\text{B.22})$$

$$e^{(el)} = \sum_{\alpha=1}^{nms} Y_{\alpha} e_{\alpha}^{(el)}. \quad (\text{B.23})$$

The translational energy for each single species is computed using

$$e_{\alpha}^{(t)} = \frac{3}{2} R_{\alpha} T^{(t,r)} \quad \alpha \in [1, ns]. \quad (\text{B.24})$$

The rotational energy for each single species is computed using

$$e_{\alpha}^{(r)} = R_{\alpha} T^{(t,r)} \quad \alpha \in [1, nms]. \quad (\text{B.25})$$

The vibrational energy for each single species is computed using

$$e_{\alpha}^{(v)} = \sum_{\beta=1}^{nvm} g_{\alpha,\beta} R_{\alpha} \frac{\theta_{\alpha,\beta}^{(v)}}{\exp\left(\theta_{\alpha,\beta}^{(v)} / T^{(v)}\right) - 1} \quad \alpha \in [1, nms]. \quad (\text{B.26})$$

In the above, nvm is the number of vibrational modes, $g_{\alpha,\beta}$ is the degeneracy of each vibrational mode, and $\theta_{\alpha,\beta}^{(v)}$ is the characteristic vibrational temperature of each vibrational mode. The characteristic temperatures for N_2 , O_2 , and NO can be found in Park (1990), for C_3 in Dolton et al. (1968), and for CO_2 , C_2 , CO , and CN in McBride et al. (1963). For our current purposes, both the electronic and electron energy are not accounted for, i.e.,

$$e_{\alpha}^{(el)} = 0 \quad \alpha \in [1, nms], \quad (\text{B.27})$$

$$e^{(e)} = 0. \quad (\text{B.28})$$

B.4.2 Temperature equilibration

The source term for the vibrational energy is

$$Q^{(v)} = \sum_{\alpha=1}^{nms} Q_{\alpha}^{(t,r-v)} + w_{\alpha} e_{\alpha}^{(v)}. \quad (\text{B.29})$$

In the above, $Q_{t-v,\alpha}$ represents the exchange of energy between translation-rotation and vibration energies. It is modeled using the Landau-Teller formulation

$$Q_{\alpha}^{(t,r-v)} = \rho Y_{\alpha} \frac{e_{\alpha}^{(v)}(T^{(t,r)}) - e_{\alpha}^{(v)}(T^{(v)})}{\langle \tau_{\alpha} \rangle + \tau_{\alpha}^{(c)}} \quad \alpha \in [1, nms]. \quad (\text{B.30})$$

The Landau-Teller relaxation time given by Lee (1985) is

$$\langle \tau_{\alpha} \rangle = \frac{\sum_{\beta=1}^{ns} X_{\beta}}{\sum_{\beta=1}^{ns} X_{\beta} / \tau_{\alpha,\beta}}. \quad (\text{B.31})$$

The expression used for $\tau_{\alpha,\beta}$ is that from Millikan and White (1963)

$$\tau_{\alpha,\beta} = \frac{1}{p} \exp \left[A_{\alpha,\beta} \left(T^{(t,r)}{}^{-1/3} - B_{\alpha,\beta} \right) - 18.42 \right], \quad p \text{ in atm} \quad (\text{B.32})$$

$$A_{\alpha,\beta} = 1.16 \times 10^{-3} \mu_{\alpha,\beta}^{1/2} \theta_{\alpha,1}^{(v) 4/3} \quad (\text{B.33})$$

$$B_{\alpha,\beta} = 0.015 \mu_{\alpha,\beta}^{1/4} \quad (\text{B.34})$$

$$\mu_{\alpha,\beta} = \frac{M_{\alpha} M_{\beta}}{M_{\alpha} + M_{\beta}} \times 1000 \quad (\text{B.35})$$

The relaxation time correction is that defined in Park (1990), which is given by

$$\tau_{\alpha}^{(c)} = \frac{1}{C_{\alpha} \sigma_v n} \quad (\text{B.36})$$

In the above, n is the mixture particle density, and C_{α} and σ_v are computed as follows

$$C_{\alpha} = \sqrt{\frac{8}{\pi} R_{\alpha} T^{(t,r)}}, \quad (\text{B.37})$$

$$\sigma_v = 3 \times 10^{-21} \left(\frac{50000}{T^{(t,r)}} \right)^2. \quad (\text{B.38})$$

B.5 Chemical non-equilibrium

The reaction rate for each species α is given by

$$w_{\alpha} = \sum_{\beta=1}^{nr} w_{\alpha,\beta}, \quad (\text{B.39})$$

where $w_{\alpha,\beta}$ is the reaction rate for species α due only to the chemical reaction β , and nr is the total number of reactions. The reaction rates $w_{\alpha,\beta}$ are usually expressed in terms of the progress rate \mathcal{Q}_{β} as follows

$$w_{\alpha,\beta} = M_{\alpha} \nu_{\alpha,\beta} \mathcal{Q}_{\beta}. \quad (\text{B.40})$$

In the above, $\nu_{\alpha,\beta} = \nu''_{\alpha,\beta} - \nu'_{\alpha,\beta}$, where $\nu'_{\alpha,\beta}$ and $\nu''_{\alpha,\beta}$ are the molar stoichiometric coefficients on the left and right hand side of a reaction, respectively.

The progress rate \mathcal{Q}_β of reaction β is given by

$$\mathcal{Q}_\beta = K_\beta^{(f)} \prod_{\alpha=1}^{ns} [X_\alpha]^{\nu'_{\alpha,\beta}} - K_\beta^{(b)} \prod_{\alpha=1}^{ns} [X_\alpha]^{\nu''_{\alpha,\beta}}, \quad (\text{B.41})$$

where $K_\beta^{(f)}$ and $K_\beta^{(b)}$ are the forward and backward rate constants, and $[X_\alpha]$ is the molar concentration ($[X_\alpha] = \rho Y_\alpha / M_\alpha$). The forward rate constant is computed using the empirical Arrhenius law

$$K_\beta^{(f)} = A_\beta \left(T^{(c)} \right)^{\eta_\beta} \exp \left(-\frac{\theta_\beta}{T^{(c)}} \right). \quad (\text{B.42})$$

For the above, A_β is the pre-exponential factor, η_β is the temperature exponent, and θ_β is the activation temperature—these are obtained from tables for each reaction β , and can be found, for example, in Park (1993). $T^{(c)}$ is the controlling temperature, which depends on the type of reaction under consideration. For example, for dissociation reactions $T^{(c)}$ is typically of the form $T^{(c)} = \sqrt{T^{(t,r)} T^{(v)}}$, whereas for exchange reactions $T^{(c)} = T^{(t,r)}$. The backward rate constant $K_\beta^{(b)}$ is often computed from the forward rate constant using $K_\beta^{(b)} = K_\beta^{(f)} / K_{eq}$. Multiple forms for K_{eq} are available, see Thierry and Veynante (2012); Knisely (2018).

B.6 Additional relations

$$\sigma_{ij} = -p\delta_{ij} + t_{ij} \quad (\text{B.43})$$

$$S_{ij}^* = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (\text{B.44})$$

Appendix C

Aerodynamics

To compute total forces and moments on an aerodynamic body, integration over its surface is performed. Thus, at each point of the surface s , the contribution to the total force or moment due to the local stress vector \mathbf{T} is added. That is,

- total force vector

$$\mathbf{F} = \int_s \mathbf{T} ds, \quad (\text{C.1})$$

- total moment about the leading edge

$$\mathbf{M}_{le} = \int_s \mathbf{r} \times \mathbf{T} ds. \quad (\text{C.2})$$

In the above, \mathbf{r} points from the leading edge to the point on the surface at which we are evaluating the stress vector. Note that the stress vector is given by $\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{n}$ (where \mathbf{n} is the normal to the surface) and that the stress tensor is given by $\boldsymbol{\sigma} = -p\mathbf{I} + \mathbf{t}$. The moment about an arbitrary point, rather than the leading edge, can be written as

$$\mathbf{M}_{ap} = \int_s (\mathbf{r} - \mathbf{r}_{ap}) \times \mathbf{T} ds = \mathbf{M}_{le} - \mathbf{r}_{ap} \times \int_s \mathbf{T} ds, \quad (\text{C.3})$$

where \mathbf{r}_{ap} is the vector pointing from the leading edge to the arbitrary point.

Consider the two dimensional case, as shown in fig. C.1. We label the normal force as

$$F_N = \int_s T_y ds, \quad (\text{C.4})$$

and the tangential force as

$$F_T = \int_s T_x ds. \quad (\text{C.5})$$

The moment about the leading edge, which points only along the z direction only, can be written as

$$M_{le} = \int_s (x\hat{\mathbf{x}} + y\hat{\mathbf{y}}) \times (T_x\hat{\mathbf{x}} + T_y\hat{\mathbf{y}}) ds = \int_s xT_y - yT_x ds. \quad (\text{C.6})$$

Note that, for this convention, a positive moment decreases the angle of attach, and a negative moment increases the angle of attack—this is the opposite convention of Anderson. If we choose to compute the moment along an arbitrary point on the chord of the body, then Equation (C.3) becomes

$$M_{ap} = M_{le} - x_{ap}F_N. \quad (\text{C.7})$$

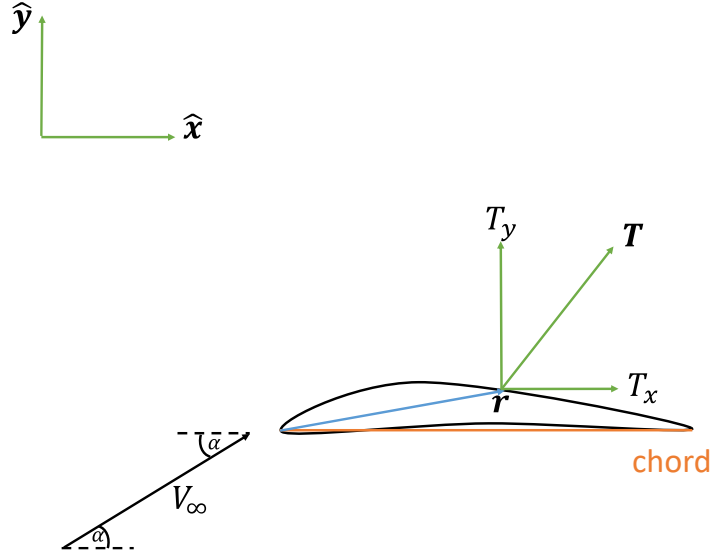


Figure C.1: Coordinate system and representative forces on an airfoil.

The center of pressure is defined as the point along the chord for which the total moment becomes zero. Thus, its location x_{cp} is given by

$$x_{cp} = \frac{M_{le}}{F_N}. \quad (\text{C.8})$$

The drag is defined as the force aligned with the free stream velocity, whereas the lift is the force normal to the free stream velocity. For 2D geometries, the direction of lift is well defined, whereas for 3D geometries, we pick the component of the force normal to the free stream velocity that points in the “up” direction. In terms for the normal and tangential force, the lift and drag for a 2D geometry are given by

$$\begin{bmatrix} L \\ D \end{bmatrix} = \begin{bmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix} \begin{bmatrix} A \\ N \end{bmatrix}. \quad (\text{C.9})$$

Given the aerodynamics pressure

$$q_\infty = \frac{1}{2} \rho_\infty V_\infty^2, \quad (\text{C.10})$$

a reference surface S , and a reference length l , the lift coefficient is given by

$$C_L = \frac{L}{q_\infty S}, \quad (\text{C.11})$$

the drag coefficient by

$$C_D = \frac{D}{q_\infty S}, \quad (\text{C.12})$$

and the moment coefficient by

$$C_M = \frac{M}{q_\infty S l}. \quad (\text{C.13})$$

Appendix D

Non-dimensionalization for compressible flows

Non-dimensionalization

$$\begin{aligned}
 x_i &= x_i^* L_0 & T &= T^* T_0 \\
 t &= t^* \frac{L_0}{u_0} & p &= p^* \rho_0 u_0^2 \\
 \rho &= \rho^* \rho_0 & \mu &= \mu^* \mu_0 \\
 u_i &= u_i^* u_0 & e &= e^* u_0^2
 \end{aligned} \tag{D.1}$$

Non-dimensional parameters

$$M_0 = \frac{u_0}{c_0} \quad \text{where } c_0 = \sqrt{\gamma R T_0} \tag{D.2}$$

$$Re_0 = \frac{\rho_0 u_0 l_0}{\mu_0} \tag{D.3}$$

$$Pr_0 = \frac{\mu_0 c_p}{\kappa_0}. \tag{D.4}$$

Parameters

$$M_t = \frac{\sqrt{\langle u_i u_i \rangle}}{\langle c \rangle} = \frac{\sqrt{\langle u_i u_i \rangle}}{\langle \sqrt{\gamma R T} \rangle} = \frac{\sqrt{\langle u_i^* u_i^* \rangle}}{\langle \sqrt{T^*} \rangle} \frac{u_0}{c_0} = \frac{\sqrt{\langle u_i^* u_i^* \rangle}}{\langle \sqrt{T^*} \rangle} M_0 \tag{D.5}$$

$$Re_\lambda = \frac{\langle \rho \rangle u_{rms} \lambda}{\langle \mu \rangle} = \frac{\langle \rho^* \rangle u_{rms}^* \lambda^*}{\langle \mu^* \rangle} \frac{\rho_0 c_0 L_0}{\mu_0} = \frac{\langle \rho^* \rangle u_{rms}^* \lambda^*}{\langle \mu^* \rangle} Re_0 \tag{D.6}$$

$$Pr = \frac{\mu c_p}{\kappa} = \frac{\mu^*}{\kappa^*} \frac{\mu_0 c_p}{\kappa_0} = \frac{\mu^*}{\kappa^*} Pr_0. \tag{D.7}$$

Dimensional Navier-Stokes

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (\text{D.8})$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (\text{D.9})$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_j}{\partial x_j} = -\frac{\partial u_j p}{\partial x_j} + \frac{\partial u_i \tau_{ij}}{\partial x_j} - \frac{\partial q_j}{\partial x_j} \quad (\text{D.10})$$

$$\tau_{ij} = 2\mu \left(S_{ij} - \frac{1}{3} S_{kk} \delta_{ij} \right) \quad (\text{D.11})$$

$$p = \rho R T \quad (\text{D.12})$$

$$e = c_v T \quad (\text{D.13})$$

$$K = \frac{1}{2} u_i u_i \quad (\text{D.14})$$

$$q_j = -\kappa \frac{\partial T}{\partial x_j} \quad (\text{D.15})$$

Non-dimensional Navier-Stokes

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial \rho^* u_i^*}{\partial x_i^*} = 0 \quad (\text{D.16})$$

$$\frac{\partial \rho^* u_i^*}{\partial t^*} + \frac{\partial \rho^* u_i^* u_j^*}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{\partial \tau_{ij}^*}{\partial x_j^*} \quad (\text{D.17})$$

$$\frac{\partial \rho^* (e^* + K^*)}{\partial t^*} + \frac{\partial \rho^* (e^* + K^*) u_j^*}{\partial x_j^*} = -\frac{\partial u_j^* p^*}{\partial x_j^*} + \frac{\partial u_i^* \tau_{ij}^*}{\partial x_j^*} - \frac{\partial q_j^*}{\partial x_j^*} \quad (\text{D.18})$$

$$\tau_{ij}^* = 2 \frac{\mu^*}{Re_0} \left(S_{ij}^* - \frac{1}{3} S_{kk}^* \delta_{ij} \right) \quad (\text{D.19})$$

$$p^* = \frac{\rho^* T^*}{\gamma M_0^2} \quad (\text{D.20})$$

$$e^* = \frac{1}{\gamma(\gamma - 1) M_0^2} T^* \quad (\text{D.21})$$

$$K^* = e^* + \frac{1}{2} u_i^* u_i^* \quad (\text{D.22})$$

$$q_i^* = -\frac{\kappa^*}{(\gamma - 1) Pr_0 Re_0 M_0^2} \frac{\partial T^*}{\partial x_i^*} \quad (\text{D.23})$$

The variables needed are $\rho, u_i, T, R, \gamma, \mu, \kappa$.
Initial non-dimensional values

$$\begin{aligned}
\rho^* &= 1 \\
u_i^* &= \text{spectrum with } \langle u_1^* u_1^* \rangle = \frac{1}{3} \\
T^* &= \text{follows from } M_t \\
\mu^* &= (T^*)^{0.76}
\end{aligned} \tag{D.24}$$

Reference values

$$\begin{aligned}
L_0 &= 2\pi \\
\rho_0 &= 1 \\
c_0 &= 1 \\
T_0 &= \text{from } c_0 \\
\mu_0 &= \text{from } Re_0
\end{aligned} \tag{D.25}$$

We then set $\gamma = 1.4$, $R = \frac{1}{\gamma}$ and compute κ from Pr .

Appendix E

Helmholtz Decomposition

$$\mathbf{u} = \mathbf{u}^{(s)} + \mathbf{u}^{(d)} + \mathbf{u}^{(h)} \quad (\text{E.1})$$

We require

$$\nabla \times \mathbf{u}^{(s)} = \mathbf{w} \quad \nabla \cdot \mathbf{u}^{(s)} = 0 \quad \mathbf{u}^{(s)} = 0 \text{ on } \partial\Omega \quad (\text{E.2})$$

$$\nabla \times \mathbf{u}^{(d)} = 0 \quad \nabla \cdot \mathbf{u}^{(d)} = d \quad \mathbf{u}^{(d)} = 0 \text{ on } \partial\Omega \quad (\text{E.3})$$

$$\nabla \times \mathbf{u}^{(h)} = 0 \quad \nabla \cdot \mathbf{u}^{(h)} = 0 \quad \mathbf{u}^{(h)} = \mathbf{u} \text{ on } \partial\Omega \quad (\text{E.4})$$

In other words, $\mathbf{u}^{(s)}$ accounts for the vorticity, $\mathbf{u}^{(d)}$ accounts for the dilatation, and $\mathbf{u}^{(h)}$ accounts for the boundary conditions.

The above requirements allow us to write

$$\mathbf{u}^{(s)} = \nabla \times \boldsymbol{\psi} \quad \mathbf{u}^{(d)} = \nabla \phi \quad \mathbf{u}^{(h)} = \nabla \varphi \quad (\text{E.5})$$

These potentials in turn can be solved using

$$\begin{cases} \nabla^2 \boldsymbol{\psi} = -\mathbf{w} & \text{in } \Omega \\ \nabla \times \boldsymbol{\psi} = 0 & \text{on } \partial\Omega \end{cases} \quad (\text{E.6})$$

$$\begin{cases} \nabla^2 \phi = d & \text{in } \Omega \\ \nabla \phi = 0 & \text{on } \partial\Omega \end{cases} \quad (\text{E.7})$$

$$\begin{cases} \nabla^2 \varphi = 0 & \text{in } \Omega \\ \nabla \varphi = \mathbf{u} & \text{on } \partial\Omega \end{cases} \quad (\text{E.8})$$

assuming $\nabla \cdot \boldsymbol{\psi} = 0$.

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