Chapter 1

Fluid Flow Modeling

Physics distinguishes four basic forms of matter: solids, liquids, gases, and plasmas. The last three forms fall in the category of *fluids*. Fluid is a material that can flow, meaning fluids cannot sustain stress in the equilibrium state. Any time a force is applied to a fluid, the latter starts and keeps moving even when the force is no longer active. Fluid mechanics studies flows of fluids under the principal laws of mechanics. Examples of real fluid flows are numerous ranging from oceans and atmosphere to gaseous stars. The relevant applications include meteorology, engineering, and astrophysics to name only a few.

There are several qualitative levels of models studied in *mathematical fluid mechanics*. The main conceptual idea is the fundamental hypothesis that matter is made of atoms and molecules, viewed as solid objects with several degrees of freedom, that obey the basic principles of *classical mechanics*.

- MOLECULAR DYNAMICS (MD) studies typically a very large number of ordinary differential equations that govern the time evolution of each single particle of the fluid coupled through the interaction forces of different kinds. Numerical simulations based on (MD) are of fundamental importance when determining the physical properties of "macroscopic" fluids, for instance their interaction with a solid wall. Models based on (MD) are fully *reversible* in time.
- KINETIC MODELS are based on *averaging* with respect to particles having the same velocity. The basic state variable is the *density* of the fluid particles at a given time and spatial position with the same velocity. Accordingly, the evolution is governed by a transport equation of Boltzmann's type including the so-called collision operator. The presence of collisions results in *irreversibility* of the process in time.
- CONTINUUM FLUID MECHANICS is a phenomenological theory based on macroscopic (observable) state variables such as density, fluid velocity, and temperature. The time evolution of these quantities is described through a

system of *partial differential equations.* The objective *existence* of the macroscopic quantities (fields) is termed the *continuum hypothesis.* The theory is widely used in numerical analysis and real world applications. The processes, in general, are irreversible in time.

- MODELS OF TURBULENCE are based on further averaging of the macroscopic models studied in continuum fluid mechanics. According to the present state of knowledge, there is no universally accepted theory of turbulence. The evolution of state variables is described by a system of partial differential equations and is irreversible in time.

The mathematical theory of *continuum fluid mechanics* developed in this book is based on fundamental physical principles that can be expressed in terms of *balance laws.* These may be written by means of either a Lagrangian or a Eulerian reference system. In Lagrangian coordinates, the description is associated to particles moving in space and time. The Eulerian reference system is based on a fixed frame attached to the underlying physical space. We will use systematically the *Eulerian description* more suitable for fluids which undergo unlimited displacements. Accordingly, the independent variables are associated to the physical space represented by a spatial domain $\Omega \subset \mathbb{R}^3$, and a time interval $I \subset \mathbb{R}$, typically, $I = (0, T)$, $T > 0$.

1.1 Fluids in continuum mechanics

We adopt the standard mathematical description of a *fluid* as found in many classical textbooks on continuum fluid mechanics. Unlike certain recently proposed alternative theories based on a largely *extended number* of state variables, we assume the *state* of a fluid at a given instant can be characterized by its density and temperature distribution whereas the *motion* is completely determined by a velocity field. Simplifying further we focus on chemically inert homogeneous fluids that may be characterized through the following quantities.

■ FLUIDS IN CONTINUUM MECHANICS:

(a) a domain $\Omega \subset \mathbb{R}^3$ occupied by a fluid in an ambient space;

(b) a non-negative measurable function $\varrho = \varrho(t, x)$ defined for $t \in (0, T)$, $x \in \Omega$, yielding the *mass density*;

(c) a vector field $\mathbf{u} = \mathbf{u}(t, x)$, $t \in (0, T)$, $x \in \Omega$, defining the *velocity* of the fluid;

(d) a positive measurable function $\vartheta = \vartheta(t, x)$, $t \in (0, T)$, $x \in \Omega$, describing the distribution of *temperature* measured in the absolute Kelvin scale;

(e) the *thermodynamic functions*: the *pressure* $p = p(\varrho, \vartheta)$, the specific *internal energy* $e = e(\varrho, \vartheta)$, and the specific *entropy* $s = s(\varrho, \vartheta)$;

(f) a *stress tensor* $\mathbb{T} = \{T_{i,j}\}_{i,j=1}^3$ yielding the force per unit surface that the part of a fluid in contact with an ideal surface element imposes on the part of the fluid on the other side of the same surface element;

(g) a vector field $\mathbf{q}$ giving the *flux of the internal energy*;

(h) a vector field $\mathbf{f} = \mathbf{f}(t, x)$, $t \in (0, T)$, $x \in \Omega$, defining the distribution of a *volume force* acting on a fluid;

(i) a function $\mathcal{Q} = \mathcal{Q}(t, x)$, $t \in (0, T)$, $x \in \Omega$, yielding the rate of *production of internal energy.*

The trio $\{\varrho, \mathbf{u}, \vartheta\}$ introduced in (b)–(d) represents the basic *state variables* characterizing completely the state of a fluid at a given instant t. The remaining quantities are determined in terms of the state variables by means of a set of constitutive relations.

Fluids are characterized among other materials through *Stokes' law*

$$\mathbb{T} = \mathbb{S} - p\mathbb{I}, \tag{1.1}$$

where $\mathbb{S}$ denotes the *viscous stress tensor*. Viscosity is a property associated to the relative motion of different parts of the fluid; whence $\mathbb{S}$ is always interrelated with the velocity gradient $\nabla_x \mathbf{u}$ or rather its symmetric part $\nabla_x \mathbf{u} + \nabla_x^T \mathbf{u}$. In particular, the viscous stress vanishes whenever $\nabla_x \mathbf{u} + \nabla_x^T \mathbf{u} = 0$, that means, when the fluid exhibits a rigid motion with respect to a fixed coordinate system. In accordance with the *Second law of thermodynamics*, viscosity is responsible for the irreversible transfer of the mechanical energy associated to the motion into heat. Although omitted in certain mathematical idealizations (Euler system), viscosity is always present and must be taken into account when modeling the motion of fluids in the long run.

The *pressure* p, similarly to the *specific energy* e and the *specific entropy* s, are typical thermostatic variables attributed to a system in thermodynamic equilibrium and as such can be evaluated as numerical functions of the density and the absolute temperature. Moreover, in accordance with the *Second law of thermodynamics*, $p = p(\varrho, \vartheta)$, $e = e(\varrho, \vartheta)$, and $s = s(\varrho, \vartheta)$ are interrelated through

■ GIBBS' EQUATION:

$$\vartheta D s(\varrho, \vartheta) = De(\varrho, \vartheta) + p(\varrho, \vartheta) D\Big(\frac{1}{\varrho}\Big). \tag{1.2}$$

The symbol D in (1.2) stands for the differential with respect to the variables ϱ, ϑ. A common hypothesis tacitly assumed in many mathematical models asserts that the time scale related to the macroscopic motion of a fluid is so large that the latter can be considered at thermodynamic equilibrium at any instant t of the "real" time, in particular, the temperature ϑ is well determined and can be taken as a state variable even if the system may be quite far from the equilibrium state (see Öttinger [168]).

Gibbs' equation (1.2) can be equivalently written in the form of *Maxwell's relation*

$$\frac{\partial e(\varrho,\vartheta)}{\partial \varrho} = \frac{1}{\varrho^2}\Big(p(\varrho,\vartheta) - \vartheta \frac{\partial p(\varrho,\vartheta)}{\partial \vartheta}\Big). \tag{1.3}$$

The precise meaning of (1.3) is that the expression $1/\vartheta(De + pD(1/\varrho))$ is a perfect gradient of a scalar function termed *entropy.*

1.2 Balance laws

Classical continuum mechanics describes a fluid by means of a family of *state variables* – observable and measurable macroscopic quantities – a representative sample of which has been introduced in the preceding part. The basic physical principles are then expressed through a system of *balance laws.* A general *balance law* takes the form of an integral identity

$$\begin{aligned}\int_B d(t_2,x)\ \mathrm{d}x - \int_B d(t_1,x)\ \mathrm{d}x + \int_{t_1}^{t_2}\int_{\partial B} \mathbf{F}(t,x)\cdot \mathbf{n}(x)\ \mathrm{dS}_x\ \mathrm{d}t \\ = \int_{t_1}^{t_2}\int_B \sigma(t,x)\ \mathrm{d}x\ \mathrm{d}t \end{aligned}\tag{1.4}$$

to be satisfied for any $t_1 \le t_2$ and any subset $B \subset \Omega$, where the symbol d stands for the volumetric (meaning per unit volume) density of an observable property, $\mathbf{F}$ denotes its flux, $\mathbf{n}$ is the outer normal vector to ∂B, and σ denotes the rate of production of d per unit volume. The principal idea, pursued and promoted in this book, asserts that (1.4) is the most natural and correct mathematical formulation of any balance law in continuum mechanics.

The expression on the left-hand side of (1.4) can be interpreted as the integral mean of the *normal trace* of the four-component vector field $[d, \mathbf{F}]$ on the boundary of the time-space cylinder $(t_1,t_2)\times B$. On the other hand, by means of the Gauss-Green theorem, we can write

$$\begin{aligned}&\int_B d(t_2,x)\varphi(t_2,x)\ \mathrm{d}x - \int_B d(t_1,x)\varphi(t_1,x)\ \mathrm{d}x + \int_{t_1}^{t_2}\int_{\partial B} \mathbf{F}(t,x)\cdot\mathbf{n}(x)\varphi(t,x)\mathrm{dS}_x\ \mathrm{d}t \\ &= \int_{t_1}^{t_2}\int_B \Big(\partial_t d(t,x) + \mathrm{div}_x \mathbf{F}(t,x)\Big)\varphi(t,x)\ \mathrm{d}x\ \mathrm{d}t \\ &\quad + \int_{t_1}^{t_2}\int_B \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\ \mathrm{d}x\ \mathrm{d}t\end{aligned}\tag{1.5}$$

for any smooth test function φ defined on $\mathbb{R}\times\mathbb{R}^3$. If all quantities are continuously differentiable, it is easy to check that relations (1.4), (1.5) are compatible as soon as

$$\partial_t d(t,x) + \mathrm{div}_x \mathbf{F}(t,x) = \sigma(t,x) \tag{1.6}$$

yielding

$$\int_B d(t_2,x)\varphi(t_2,x)\ \mathrm{d}x - \int_B d(t_1,x)\varphi(t_1,x)\ \mathrm{d}x + \int_{t_1}^{t_2}\int_{\partial B} \mathbf{F}(t,x)\cdot\mathbf{n}(x)\varphi(t,x)\mathrm{dS}_x\ \mathrm{d}t$$
$$= \int_{t_1}^{t_2}\int_B \sigma(t,x)\varphi(t,x)\,\mathrm{d}x\,\mathrm{d}t + \int_{t_1}^{t_2}\int_B \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\,\mathrm{d}x\,\mathrm{d}t. \tag{1.7}$$

The integral identity (1.7) can be used as a proper *definition* of the *normal trace* of the field $[d,\mathbf{F}]$ as long as

$$\int_0^T\int_\Omega \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\ \mathrm{d}x\ \mathrm{d}t$$
$$+ \int_0^T\int_\Omega \sigma(t,x)\varphi(t,x)\ \mathrm{d}x\ \mathrm{d}t = 0 \tag{1.8}$$

for any $\varphi \in C_c^\infty((0,T)\times\Omega)$. In the terminology of the modern theory of partial differential equations, relation (1.8) represents a *weak formulation* of the differential equation (1.6). If (1.8) holds for any test function $\varphi \in C_c^\infty((0,T)\times\Omega)$, we say that equation (1.6) is satisfied in $\mathcal{D}'((0,T)\times\Omega)$, or, in the sense of distributions.

The satisfaction of the initial condition $d(0,\cdot) = d_0$, together with the prescribed normal component of the flux $F_b = \mathbf{F}\cdot\mathbf{n}|_{\partial\Omega}$ on the boundary, can be incorporated into the weak formulation by means of the integral identity

$$-\int_\Omega d_0(x)\varphi(0,x)\ \mathrm{d}x + \int_0^T\int_{\partial\Omega} F_b(t,x)\varphi(t,x)\mathrm{dS}_x\ \mathrm{d}t \tag{1.9}$$
$$= \int_0^T\int_\Omega \sigma(t,x)\varphi(t,x)\ \mathrm{d}x\,\mathrm{d}t + \int_0^T\int_\Omega \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\ \mathrm{d}x\,\mathrm{d}t$$

to be satisfied for any $\varphi \in C_c^\infty([0,T)\times\overline{\Omega})$.

As a matter of fact, the source term σ need not be an integrable function. The normal trace of $[d,\mathbf{F}]$ is still well defined through (1.7) even if σ is merely a signed measure, more specifically, $\sigma = \sigma^+ - \sigma^-$, where $\sigma^+,\sigma^- \in \mathcal{M}^+([0,T]\times\overline{\Omega})$ are non-negative regular Borel measures defined on the compact set $[0,T]\times\overline{\Omega}$. Accordingly, relation (1.9) takes the form of a general

■ BALANCE LAW:

$$\langle\sigma;\varphi\rangle_{[\mathcal{M};C]([0,T]\times\overline{\Omega})} + \int_0^T\int_\Omega \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\ \mathrm{d}x\ \mathrm{d}t$$
$$= \int_0^T\int_{\partial\Omega} F_b(t,x)\varphi(t,x)\ \mathrm{dS}_x\ \mathrm{d}t - \int_\Omega d_0(x)\varphi(0,x)\ \mathrm{d}x \tag{1.10}$$

for any test function $\varphi \in C_c^\infty([0,T)\times\overline{\Omega})$.

If (1.10) holds, the (outer) normal trace of the field $[d, \mathbf{F}]$ can be identified through (1.7), in particular, the *instantaneous values* of d at a time t can be defined. However, these may exhibit jumps if the rate of production σ is not absolutely continuous with respect to the Lebesgue measure. Specifically, using (1.7), (1.10), we can define the *left instantaneous value* of d at a time $\tau \in (0, T]$ as

$$\begin{aligned} &\langle d(\tau-, \cdot); \varphi \rangle_{[\mathcal{M};C](\overline{\Omega})} \qquad (1.11) \\ &= \int_\Omega d_0(x) \varphi(x)\ \mathrm{d}x + \int_0^\tau \int_\Omega \mathbf{F}(t,x) \cdot \nabla_x \varphi(x)\ \mathrm{d}x\,\mathrm{d}t + \lim_{\delta \to 0+} \langle \sigma; \psi_\delta \varphi \rangle_{[\mathcal{M},C]([0,T]\times\overline{\Omega})}, \end{aligned}$$

for any $\varphi \in C_c^\infty(\Omega)$, where $\psi_\delta = \psi_\delta(t)$ is non-increasing,

$$\psi_\delta \in C^1(\mathbb{R}),\ \ \psi_\delta(t) = \left\{ \begin{array}{l} 1 \text{ for } t \in (-\infty, \tau - \delta], \\ 0 \text{ for } t \in [\tau, \infty). \end{array} \right.$$

Similarly, we define the *right instantaneous value* of d at a time $\tau \in [0, T)$ as

$$\begin{aligned} &\langle d(\tau+, \cdot); \varphi \rangle_{[\mathcal{M};C](\overline{\Omega})} \qquad (1.12) \\ &= \int_\Omega d_0(x) \varphi(x)\ \mathrm{d}x + \int_0^\tau \int_\Omega \mathbf{F}(t,x) \cdot \nabla_x \varphi(x)\ \mathrm{d}x\,\mathrm{d}t + \lim_{\delta \to 0+} \langle \sigma; \psi_\delta \varphi \rangle_{[\mathcal{M},C]([0,T]\times\overline{\Omega})}, \end{aligned}$$

where $\psi_\delta = \psi_\delta(t)$ is non-increasing,

$$\psi_\delta \in C^1(\mathbb{R}),\ \ \psi_\delta(t) = \left\{ \begin{array}{l} 1 \text{ for } t \in (-\infty, \tau], \\ 0 \text{ for } t \in [\tau + \delta, \infty). \end{array} \right.$$

Note that, at least for $d \in L^\infty(0, T; L^1(\Omega))$, the left and right instantaneous values are represented by signed measures on Ω that coincide with $d(\tau, \cdot) \in L^1(\Omega)$ at any Lebesgue point of the mapping $\tau \mapsto d(\tau, \cdot)$. Moreover, $d(\tau-, \cdot) = d(\tau+, \cdot)$ for any $\tau \in [0, T]$ and the mapping $\tau \mapsto d(\tau, \cdot)$ is weakly-(*) continuous as soon as σ is absolutely continuous with respect to the standard Lebesgue measure on $(0, T) \times \Omega$.

Under certain circumstances, notably when identifying the *entropy production rate*, the piece of information that is provided by the available mathematical theory enables us only to show that

$$\int_0^T \int_\Omega d(t,x) \partial_t \varphi(t,x) + \mathbf{F}(t,x) \cdot \nabla_x \varphi(t,x)\ \mathrm{d}x \le 0 \tag{1.13}$$

for any *non-negative* test function $\varphi \in C_c^\infty([0, T) \times \overline{\Omega})$. Intuitively, this means

$$\partial_t d + \mathrm{div}_x(\mathbf{F}) \ge 0$$

though a rigorous verification requires differentiability of d and $\mathbf{F}$.

Let us show that (1.13) is in fact *equivalent* to the integral identity

$$\int_0^T \int_\Omega d(t,x)\partial_t \varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x \varphi(t,x) \,\mathrm{d}x\,\mathrm{d}t + \langle \sigma; \varphi\rangle_{[\mathcal{M}^+;C]([0,T]\times\Omega)} = 0 \tag{1.14}$$

for any $\varphi \in C_c^\infty([0,T)\times\overline{\Omega})$, where $\sigma \in \mathcal{M}^+([0,T]\times\overline{\Omega})$ is a non-negative regular Borel measure on the set $[0,T]\times\overline{\Omega}$. This fact may be viewed as a variant of the well-known statement that any non-negative distribution is representable by a measure.

In order to see (1.14), assume that

$$d \in L^\infty(0,T;L^1(\Omega)) \text{ and } \mathbf{F} \in L^p((0,T)\times\Omega;R^3) \text{ for a certain } p > 1.$$

Consider a linear form

$$\langle \sigma; \varphi\rangle = -\int_0^T \int_\Omega \Big(d(t,x)\partial_t\varphi(t,x) + \mathbf{F}(t,x)\cdot\nabla_x\varphi(t,x)\Big)\,\mathrm{d}x$$

which is well defined for any $\varphi \in C_c^1([0,T)\times\overline{\Omega})$. Moreover, it follows from (1.13), that

$$\langle\sigma;\varphi\rangle \ \geq 0 \text{ for any } \varphi \in C_c^\infty([0,T)\times\overline{\Omega}),\ \varphi \geq 0. \tag{1.15}$$

Next, for any compact set $K \subset [0,T)\times\overline{\Omega}$ we can find a function χ_K such that

$$\chi_K = \chi_K(t) \in C_c^\infty[0,T),\ 0\leq \chi_K \leq 1,\ \partial_t\chi_K \leq 0,\ \chi_K = 1 \text{ on } K. \tag{1.16}$$

In particular, as a direct consequence of (1.15), we get

$$\langle \sigma;\chi_K\rangle \leq \operatorname*{ess\,sup}_{t\in(0,T)} \|d(t,\cdot)\|_{L^1(\Omega)} \text{ for any } K. \tag{1.17}$$

We claim that σ can be extended in a unique way as a bounded non-negative linear form on the vector space $C_c([0,T)\times\overline{\Omega})$. Indeed for any sequence $\{\varphi_n\}_{n=1}^\infty$ of (smooth) functions supported by a fixed compact set $K\subset[0,T)\times\overline{\Omega}$, we have

$$|\,\langle\sigma;\varphi_n\rangle - \langle\sigma;\varphi_m\rangle\,| \leq \ \langle\sigma;\chi_K\rangle\,\|\varphi_n-\varphi_m\|_{C(K)},$$

with χ_K constructed in (1.16).

By virtue of Riesz's representation theorem (Theorem 0.9), the linear form σ can be identified with a non-negative Borel measure on the set $[0,T)\times\overline{\Omega}$. Finally, because of the uniform estimate (1.17) on the value of $\sigma[K]$ for any compact set $K\subset[0,T)\times\overline{\Omega}$, the measure $\sigma[[0,T)\times\overline{\Omega}]$ of the full domain is finite, in particular σ can be trivially extended (by zero) to the set $[0,T]\times\overline{\Omega}$. Let us point out, however, that such an extension represents only a suitable convention (the measure σ is defined on a *compact* set $[0,T]\times\overline{\Omega}$) without any real impact on formula (1.14).

To conclude, we recall that the *weak formulation* of a balance law introduced in (1.10) is deliberately expressed in the space-fixed, Eulerian form rather than a "body-fixed" material description. This convention avoids the ambiguous notion of trajectory in the situation where $\mathbf{F}$, typically proportional to the velocity of the fluid, is not regular enough to give rise to a unique system of streamlines.

1.3 Field equations

In accordance with the general approach delineated in Section 1.2, the basic physical principles formulated in terms of balance laws will be understood in the sense of integral identities similar to (1.10) rather than systems of partial differential equations set forth in classical textbooks on fluid mechanics. Nonetheless, in the course of formal discussion, we stick to the standard terminology "equation" or "field equation" even if these mathematical objects are represented by an infinite system of integral identities to be satisfied for a suitable class of test functions rather than a single equation. Accordingly, the macroscopic quantities characterizing the state of a material in continuum mechanics are called *fields*, the balance laws they obey are termed *field equations.*

1.3.1 Conservation of mass

The fluid *density* $\varrho = \varrho(t, x)$ is a fundamental state variable describing the distribution of mass. The integral

$$M(B) = \int_B \varrho(t, x) \ \mathrm{d}x$$

represents the total amount of mass of the fluid contained in a set $B \subset \Omega$ at an instant t. In a broader sense, the density could be a non-negative measure defined on a suitable system of subsets of the ambient space Ω. However, for the purposes of this study, we content ourselves with $\varrho(t, \cdot)$ that is absolutely continuous with respect to the standard Lebesgue measure on $\mathbb{R}^3$, therefore representable by a non-negative measurable function.

Motivated by the general approach described in the previous part, we write the physical principle of *mass conservation* in the form

$$\int_B \varrho(t_2, x) \ \mathrm{d}x - \int_B \varrho(t_1, x) \ \mathrm{d}x + \int_{t_1}^{t_2} \int_{\partial B} \varrho(t, x)\mathbf{u}(t, x) \cdot \mathbf{n} \ \mathrm{dS}_x \ \mathrm{d}t = 0$$

for any (smooth) subset $B \subset \Omega$, where $\mathbf{u} = \mathbf{u}(t, x)$ is the velocity field determining the motion of the fluid. Thus assuming, for a moment, that all quantities are smooth, we deduce the *equation of continuity* in the differential form

$$\partial_t \varrho(t, x) + \mathrm{div}_x(\varrho(t, x)\mathbf{u}(t, x)) = 0 \text{ in } (0, T) \times \Omega. \tag{1.18}$$

In addition, we impose *impermeability* of the boundary $\partial\Omega$, meaning,

$$\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{1.19}$$

Multiplying (1.18) on $B(\varrho) + \varrho B'(\varrho)$, where B is a continuously differentiable function, we easily deduce that

$$\partial_t(\varrho B(\varrho)) + \mathrm{div}_x(\varrho B(\varrho)\mathbf{u}) + b(\varrho)\mathrm{div}_x\mathbf{u} = 0 \tag{1.20}$$

for any $b \in BC[0,\infty)$ (bounded and continuous functions), where

$$B(\varrho) = B(1) + \int_1^{\varrho} \frac{b(z)}{z^2}\,\mathrm{d}z. \tag{1.21}$$

Equation (1.20) can be viewed as a *renormalized variant* of (1.18).

Summing up the previous discussion and returning to the weak formulation, we introduce

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■ RENORMALIZED EQUATION OF CONTINUITY:

$$\int_0^T \int_\Omega \Big(\varrho B(\varrho)\partial_t\varphi + \varrho B(\varrho)\mathbf{u}\cdot\nabla_x\varphi - b(\varrho)\mathrm{div}_x\mathbf{u}\ \varphi \Big)\,\mathrm{d}x\,\mathrm{d}t = -\int_\Omega \varrho_0 B(\varrho_0)\varphi(0,\cdot)\,\mathrm{d}x \tag{1.22}$$

to be satisfied for any test function $\varphi \in C_c^\infty([0,T)\times\overline{\Omega})$, and any B, b interrelated through (1.21), where b is continuous and uniformly bounded function on $\mathbb{R}$.

The family of integral identities (1.22) represents a mathematical formulation of the physical principle of *mass conservation.* Formally, relation (1.22) reduces to (1.20) provided all quantities are smooth, and, furthermore, to (1.18) if we take $b \equiv 0$, $B(1) = 1$. The initial distribution of the density is determined by a given function $\varrho_0 = \varrho(0,\cdot)$, while the boundary conditions (1.19) are satisfied implicitly through the choice of test functions in (1.22) in the spirit of (1.10).

In a certain sense, the renormalized equation (1.22) can be viewed as a very weak formulation of (1.18) since, at least for $B(1) = 0$, the density ϱ need not be integrable. On the other hand, relation (1.22) requires integrability of the velocity field $\mathbf{u}$ at the level of first derivatives, specifically, $\mathrm{div}_x\mathbf{u}$ must be integrable on the set $[0,T)\times\overline{\Omega}$.

In contrast to (1.18), relation (1.22) provides a useful piece of information on the mass transport and possible density oscillations in terms of the initial data. It is important to note that (1.22) can be deduced from (1.18) even at the level of the weak formulation as soon as the density is a bounded measurable function (see Section 10.18 in Appendix).

1.3.2 Balance of linear momentum

In accordance with *Newton's second law*, the flux associated to the momentum $\varrho\mathbf{u}$ in the Eulerian coordinate system can be written in the form $(\varrho\mathbf{u}\otimes\mathbf{u} - \mathbb{T})$, where the symbol $\mathbb{T}$ stands for the stress tensor introduced in Section 1.1. In accordance with Stokes' law (1.1), the *balance of linear momentum* reads

$$\partial_t(\varrho\mathbf{u}) + \mathrm{div}_x(\varrho\mathbf{u}\otimes\mathbf{u}) + \nabla_x p = \mathrm{div}_x\mathbb{S} + \varrho\mathbf{f} \ \text{in}\ \mathcal{D}'((0,T)\times\Omega;\mathbb{R}^3), \tag{1.23}$$

or,

$$\int_0^T \int_\Omega \Big((\varrho \mathbf{u}) \cdot \partial_t \varphi + \varrho (\mathbf{u} \otimes \mathbf{u}) : \nabla_x \varphi + p \mathrm{div}_x \varphi \Big) \ \mathrm{d}x \ \mathrm{d}t$$
$$= \int_0^T \int_\Omega \Big(\mathbb{S} : \nabla_x \varphi - \varrho \mathbf{f} \cdot \varphi \Big) \ \mathrm{d}x - \int_\Omega (\varrho \mathbf{u})_0 \cdot \varphi(0, \cdot) \ \mathrm{d}x, \tag{1.24}$$

to be satisfied by any test function $\varphi \in C_c^\infty([0,T) \times \Omega; \mathbb{R}^3)$. Note that relation (1.24) already includes the initial condition

$$\varrho \mathbf{u}(0, \cdot) = (\varrho \mathbf{u})_0 \text{ in } \Omega. \tag{1.25}$$

Analogously, as in the previous sections, the variational formulation (1.24) may include implicit satisfaction of boundary conditions provided the class of admissible test functions is extended "up to the boundary". Roughly speaking, the test functions should belong to the same regularity class as the velocity field $\mathbf{u}$. Accordingly, in order to enforce the impermeability condition (1.19), we take

$$\varphi \in C_c^\infty([0,T) \times \overline{\Omega}; \mathbb{R}^3), \ \ \varphi \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{1.26}$$

Postulating relation (1.24) for any test function satisfying (1.26), we deduce formally that

$$(\mathbb{S}\mathbf{n}) \times \mathbf{n}|_{\partial\Omega} = 0, \tag{1.27}$$

which means, the tangential component of the normal stress forces vanishes on the boundary. This behavior of the stress characterizes *complete slip* of the fluid against the boundary.

In the theory of *viscous fluids*, however, it is more customary to impose the *no-slip boundary condition*

$$\mathbf{u}|_{\partial\Omega} = 0, \tag{1.28}$$

together with the associated class of test functions

$$\varphi \in C_c^\infty([0,T) \times \Omega; \mathbb{R}^3). \tag{1.29}$$

The no-slip boundary condition (1.28) and even the impermeability condition (1.19) require a concept of *trace* of the field $\mathbf{u}$ on the boundary $\partial\Omega$. Therefore the velocity field $\mathbf{u}$ must belong to a "better" space than just $L^p(\Omega; \mathbb{R}^3)$. As for the impermeability hypothesis (1.19), we recall the Gauss-Green theorem yielding

$$\int_{\partial\Omega} \varphi \mathbf{u} \cdot \mathbf{n} \ \mathrm{dS}_x = \int_\Omega \nabla_x \varphi \cdot \mathbf{u} \ \mathrm{d}x + \int_\Omega \varphi \ \mathrm{div}_x \mathbf{u} \ \mathrm{d}x. \tag{1.30}$$

Consequently, we need both $\mathbf{u}$ and $\mathrm{div}_x \mathbf{u}$ to be at least integrable on Ω for (1.19) to make sense. The no-slip boundary condition (1.28) requires the partial derivatives of $\mathbf{u}$ to be at least (locally) integrable in Ω (cf. Theorem 0.6).

Before leaving this section, we give a concise formulation of *Newton's second law* in terms of

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■ BALANCE OF MOMENTUM:

$$\int_0^T \int_\Omega \Big((\varrho \mathbf{u}) \cdot \partial_t \varphi + \varrho (\mathbf{u} \otimes \mathbf{u}) : \nabla_x \varphi + p \mathrm{div}_x \varphi \Big) \ \mathrm{d}x \ \mathrm{d}t$$
$$= \int_0^T \int_\Omega \Big(\mathbb{S} : \nabla_x \varphi - \varrho \mathbf{f} \cdot \varphi \Big) \ \mathrm{d}x - \int_\Omega (\varrho \mathbf{u})_0 \cdot \varphi(0, \cdot) \ \mathrm{d}x \tag{1.31}$$

must be satisfied by any test function φ belonging to the class $C_c^\infty([0,T) \times \Omega; \mathbb{R}^3)$ if the no-slip boundary conditions (1.28) are imposed, or

$$\varphi \in C_c^\infty([0,T) \times \overline{\Omega}; \mathbb{R}^3), \ \ \varphi \cdot \mathbf{n}|_{\partial\Omega} = 0,$$

in the case of complete slip boundary conditions (1.19), (1.27).

1.3.3 Total energy

The *energy density* $\mathcal{E}$ can be written in the form

$$\mathcal{E} = \frac{1}{2} \varrho |\mathbf{u}|^2 + \varrho e(\varrho, \vartheta), \tag{1.32}$$

where the symbol e denotes the specific internal energy introduced in Section 1.1.

Multiplying equation (1.23) on $\mathbf{u}$ we deduce the kinetic energy balance

$$\partial_t \Big(\frac{1}{2} \varrho |\mathbf{u}|^2 \Big) + \mathrm{div}_x \Big(\frac{1}{2} \varrho |\mathbf{u}|^2 \mathbf{u} \Big) = \mathrm{div}_x (\mathbb{T} \mathbf{u}) - \mathbb{T} : \nabla_x \mathbf{u} + \varrho \mathbf{f} \cdot \mathbf{u}, \tag{1.33}$$

where the stress tensor $\mathbb{T}$ is related to $\mathbb{S}$ and p by means of Stokes' law (1.1). On the other hand, by virtue of the *First law of thermodynamics*, the changes of the energy of the system are caused only by external sources, in particular, the internal energy balance reads

$$\partial_t (\varrho e) + \mathrm{div}_x (\varrho e \mathbf{u}) + \mathrm{div}_x \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{u} - p \mathrm{div}_x \mathbf{u} + \varrho \mathcal{Q}, \tag{1.34}$$

where the term $\varrho \mathcal{Q}$ represent the volumetric rate of the internal energy production, and $\mathbf{q}$ is the internal energy flux.

Consequently, the *energy balance* equation may be written in the form

$$\partial_t \mathcal{E} + \mathrm{div}_x (\mathcal{E} \mathbf{u}) + \mathrm{div}_x \Big(\mathbf{q} - \mathbb{S} \mathbf{u} + p \mathbf{u} \Big) = \varrho \mathbf{f} \cdot \mathbf{u} + \varrho \mathcal{Q}. \tag{1.35}$$

Relation (1.35) can be integrated over the whole domain Ω in order to obtain the balance of total energy. Performing by parts integration of the resulting expression we finally arrive at

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■ TOTAL ENERGY BALANCE:

$$\int_\Omega \mathcal{E}(t_2,\cdot)\ \mathrm{d}x - \int_\Omega \mathcal{E}(t_1,\cdot)\ \mathrm{d}x = \int_{t_1}^{t_2}\int_\Omega \Big(\varrho\mathbf{f}\cdot\mathbf{u} + \varrho\mathcal{Q}\Big)\ \mathrm{d}x\ \mathrm{d}t \tag{1.36}$$

for any $0 \leq t_1 \leq t_2 \leq T$ provided

$$\mathbf{q}\cdot\mathbf{n}|_{\partial\Omega} = 0, \tag{1.37}$$

and either the no-slip boundary condition (1.28) or the complete slip boundary conditions (1.19), (1.27) hold.

In the previous considerations, the internal energy e has been introduced to balance the dissipative terms in (1.33). Its specific form required by Gibbs' equation (1.2) is a consequence of the *Second law of thermodynamics* discussed in the next section.

1.3.4 Entropy

The *Second law of thermodynamics* is the central principle around which we intend to build up the mathematical theory used in this study. As a matter of fact, Gibbs' equation (1.2) should be viewed as a constraint imposed on p and e by the principles of statistical physics, namely $\frac{1}{\vartheta}(De + pD\frac{1}{\varrho})$ must be a perfect gradient. Accordingly, the internal energy balance equation (1.34) can be rewritten in the form of *entropy balance*

$$\partial_t(\varrho s) + \mathrm{div}_x(\varrho s\mathbf{u}) + \mathrm{div}_x\Big(\frac{\mathbf{q}}{\vartheta}\Big) = \sigma + \frac{\varrho}{\vartheta}\mathcal{Q}, \tag{1.38}$$

with the *entropy production rate*

$$\sigma = \frac{1}{\vartheta}\Big(\mathbb{S} : \nabla_x\mathbf{u} - \frac{\mathbf{q}\cdot\nabla_x\vartheta}{\vartheta}\Big). \tag{1.39}$$

The *Second law of thermodynamics* postulates that the entropy production rate σ must be nonnegative for any admissible thermodynamic process. As we will see below, this can be viewed as a restriction imposed on the constitutive relations for $\mathbb{S}$ and $\mathbf{q}$.

A weak formulation of equation (1.38) reads

■ ENTROPY BALANCE EQUATION:

$$\int_0^T \int_\Omega \Big(\varrho s \partial_t \varphi + \varrho s \mathbf{u} \cdot \nabla_x \varphi + \Big(\frac{\mathbf{q}}{\vartheta} \Big) \cdot \nabla_x \varphi \ \mathrm{d}x \Big) \ \mathrm{d}t \tag{1.40}$$
$$= - \int_\Omega (\varrho s)_0 \varphi \ \mathrm{d}x - \int_0^T \int_\Omega \sigma \varphi \ \mathrm{d}x \ \mathrm{d}t - \int_0^T \int_\Omega \frac{\varrho}{\vartheta} \mathcal{Q} \varphi \ \mathrm{d}x \ \mathrm{d}t$$

must be satisfied for any test function $\varphi \in C_c^\infty([0,T) \times \overline{\Omega})$. Note that (1.40) already includes the no-flux boundary condition (1.37) as well as the initial condition $\varrho s(0,\cdot) = (\varrho s)_0$.

In the framework of the weak solutions considered in this book, the entropy production rate σ will be a non-negative measure satisfying

$$\sigma \geq \frac{1}{\vartheta} \Big(\mathbb{S} : \nabla_x \mathbf{u} - \frac{\mathbf{q} \cdot \nabla_x \vartheta}{\vartheta} \Big)$$

in place of (1.39). Such a stipulation reflects one of the expected features of the weak solutions, namely they produce maximal dissipation rate of the kinetic energy enhanced by the presence of singularities that are not captured by the "classical" formula (1.39). As we will see in Chapter 2, this approach still leads to a (formally) well-posed problem.

1.4 Constitutive relations

The field equations derived in Section 1.3 must be supplemented with a set of *constitutive relations* characterizing the material properties of a concrete fluid. In particular, the viscous stress tensor $\mathbb{S}$, the internal energy flux $\mathbf{q}$ as well as the thermodynamic functions p, e, and s must be determined in terms of the independent state variables $\{\varrho, \mathbf{u}, \vartheta\}$.

1.4.1 Molecular energy and transport terms

The *Second law of thermodynamics*, together with its implications on the sign of the entropy production rate discussed in Section 1.3.4, gives rise to further restrictions that must be imposed on the transport terms $\mathbb{S}$, $\mathbf{q}$. In particular, as the entropy production is non-negative for any admissible physical process, we deduce from (1.39) that

$$\mathbb{S} : \nabla_x \mathbf{u} \geq 0, \ \ -\mathbf{q} \cdot \nabla_x \vartheta \geq 0. \tag{1.41}$$

A fundamental hypothesis of the mathematical theory developed in this book asserts that the constitutive equations relating $\mathbb{S}$, $\mathbf{q}$ to the affinities $\nabla_x \mathbf{u}$, $\nabla_x \vartheta$ are *linear*. Such a stipulation gives rise to

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■ NEWTON'S RHEOLOGICAL LAW:

$$\mathbb{S} = \mu \Big(\nabla_x \mathbf{u} + \nabla_x^T \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \ \mathbb{I} \Big) + \eta \mathrm{div}_x \mathbf{u} \ \mathbb{I}; \tag{1.42}$$

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and

■ FOURIER'S LAW:

$$\mathbf{q} = -\kappa \nabla_x \vartheta. \tag{1.43}$$

The specific form of $\mathbb{S}$ can be deduced from the physical principle of the material frame indifference, see Chorin and Marsden [47] for details.

Writing

$$\mathbb{S} : \nabla_x \mathbf{u} = \frac{\mu}{2} \Big| \nabla_x \mathbf{u} + \nabla_x^T \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \mathbb{I} \Big|^2 + \eta |\mathrm{div}_x \mathbf{u}|^2,$$

we conclude, by virtue of (1.41), that the *shear viscosity coefficient* μ, the *bulk viscosity coefficient* η, as well as the *heat conductivity coefficient* κ must be non-negative. As our theory is primarily concerned with viscous and heat conducting fluids, we shall always assume that the shear viscosity coefficient μ as well as the heat conductivity coefficient κ are strictly positive. On the other hand, it is customary, at least for certain gases, to neglect the second term in (1.42) setting the bulk viscosity coefficient $\eta = 0$.

1.4.2 State equations

Gibbs' equation (1.2) relates the *thermal equation of state*

$$p = p(\varrho, \vartheta)$$

to the *caloric equation of state*

$$e = e(\varrho, \vartheta),$$

in particular, p and e must obey Maxwell's relation (1.3).

The mathematical theory of singular limits developed in this book leans essentially on

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■ HYPOTHESIS OF THERMODYNAMIC STABILITY:

$$\frac{\partial e(\varrho, \vartheta)}{\partial \vartheta} > 0, \ \frac{\partial p(\varrho, \vartheta)}{\partial \varrho} > 0. \tag{1.44}$$

The meaning of (1.44) is that both the *specific heat at constant volume* $c_v = \partial e/\partial\vartheta$ and the *compressibility* of the fluid $\partial p/\partial\varrho$ are positive although the latter condition is apparently violated by the standard Van der Waals equation of state.

In order to fix ideas, we focus on the simplest possible situation supposing the fluid is a monoatomic gas. In this case, it can be deduced by the methods of statistical physics that the molecular pressure $p = p_M$ and the associated internal energy $e = e_M$ are interrelated through

$$p_M(\varrho,\vartheta) = \frac{2}{3}\varrho e_M(\varrho,\vartheta) \tag{1.45}$$

(see Eliezer et al. [71]). It is a routine matter to check that (1.45) is compatible with (1.3) only if there is a function P such that

$$p_M(\varrho,\vartheta) = \vartheta^{5/2} P\Big(\frac{\varrho}{\vartheta^{3/2}}\Big). \tag{1.46}$$

Indeed inserting (1.45) into (1.3) gives rise to a first-order partial differential equation that can be solved by means of the change of variables $q(Z,\vartheta) = p(Z\vartheta^{3/2},\vartheta)$.

If P is linear, we recover the standard *Boyle-Marriot state equation* of perfect gas,

$$p_M(\varrho,\vartheta) = \mathrm{R}\varrho\vartheta \quad \text{with a positive gas constant } R. \tag{1.47}$$

As a matter of fact, formula (1.46) applies to any real gas, monoatomic or not, at least in the following two domains of the (ϱ,ϑ)-plane:

- NON-DEGENERATE REGION, where the density is low and/or the temperature is sufficiently large, specifically,

$$\frac{\varrho}{\vartheta^{\frac{3}{2}}} < \underline{Z} \tag{1.48}$$

  for a certain positive constant $\underline{Z}$. Here the fluid can be considered as a mixture of classical gases that obeys Dalton's law, hence the pressure p is given by the state equation (1.47) (see Galavotti [93]);
- DEGENERATE AREA

$$\frac{\varrho}{\vartheta^{\frac{3}{2}}} > \overline{Z}, \ \text{with } \overline{Z} \gg \underline{Z}, \tag{1.49}$$

  where the gas is completely ionized, and the nuclei as well as the free electrons behave like a monoatomic gas satisfying (1.46). If, in addition, we assume that in the degenerate area at least one of the gas constituents, for instance the cloud of free electrons, behaves as a Fermi gas, we obtain

$$\lim_{\vartheta\to 0} e_M(\varrho,\vartheta) > 0 \text{ for any fixed } \varrho > 0 \tag{1.50}$$

  (see Müller and Ruggeri [160]).

Finally, we suppose that the specific heat at constant volume is uniformly bounded, meaning

$$c_v = \frac{\partial e_M(\varrho,\vartheta)}{\partial \vartheta} \leq c \text{ for all } \varrho,\ \vartheta > 0, \tag{1.51}$$

with obvious implications on the specific form of the function P in (1.46) discussed in detail in Chapter 2.

It is worth noting that, unlike (1.47), the previous assumptions are in perfect agreement with the *Third law of thermodynamics* requiring the entropy to vanish when the absolute temperature approaches zero (see Callen [40]).

1.4.3 Effect of thermal radiation

Before starting our discussion, let us point out that the interaction of matter and *radiation* (photon gas) occurring in the high temperature regime is a complex problem, a complete discussion of which goes beyond the scope of the present study. Here we restrict ourselves to the very special but still physically relevant situation, where the emitted photons are in thermal equilibrium with the other constituents of the fluid, in particular, the whole system admits a single temperature ϑ (see the monograph by Oxenius [169]).

Under these circumstances, it is well known that the heat conductivity is substantially enhanced by the radiation effect, in particular, the *heat conductivity coefficient* κ takes the form

$$\kappa = \kappa_M + \kappa_R,\ \kappa_R = k\vartheta^3,\ k > 0, \tag{1.52}$$

where κ_M denotes the standard "molecular" transport coefficient and κ_R represents the contribution due to radiation. The influence of the radiative transport is particularly relevant in some astrophysical models studied in the asymptotic limit of small Péclet (Prandtl) number in Chapter 6.

Similarly, the standard molecular pressure p_M is augmented by its radiation counterpart p_R so that, finally,

$$p(\varrho,\vartheta) = p_M(\varrho,\vartheta) + p_R(\vartheta),\ \text{where } p_R(\vartheta) = \frac{a}{3}\vartheta^4,\ a > 0; \tag{1.53}$$

whence, in accordance with Gibbs' equation (1.2),

$$e(\varrho,\vartheta) = e_M(\varrho,\vartheta) + e_R(\varrho,\vartheta),\ \text{where } \varrho e_R(\varrho,\vartheta) = a\vartheta^4, \tag{1.54}$$

and

$$s(\varrho,\vartheta) = s_M(\varrho,\vartheta) + s_R(\varrho,\vartheta),\ \text{with } \varrho s_R(\varrho,\vartheta) = \frac{4}{3}a\vartheta^3. \tag{1.55}$$

1.4.4 Typical values of some physical coefficients

In order to get better insight concerning the magnitude and proportionality of the different material forces acting on a fluid, we conclude this introductory part by reviewing the typical values of several physical constants introduced in the preceding text.

The quantity R appearing in formula (1.47) is the specific gas constant, the value of which for a gas (or a mixture of gases) equals $\overline{R}/M$, where $\overline{R}$ is the universal gas constant ($\overline{R} = 8.314JK^{-1}\mathrm{mol}^{-1}$), and M is the molar mass (or a weighted average of molar masses of the mixture components). For dry air, we get $R = 2.87J\mathrm{kg}^{-1}K^{-1}$.

In formulas (1.53–1.55), the symbol a stands for the Stefan-Boltzmann constant ($a = 5.67 \cdot 10^{-8}JK^{-4}m^{-2}s^{-1}$), while the coefficient k in formula (1.52) is related to a by $k = \frac{4}{3}alc$, where l denotes the mean free path of photons (typically $l \approx 10^{-7} - 10^{-8}m$), and c is the speed of light ($c = 3 \cdot 10^{8}ms^{-1}$).

The specific heat at constant volume c_v takes the value $c_v = 2.87J\mathrm{kg}^{-1}K^{-1}$ for the dry air, in particular, $e_R \approx 1J\mathrm{kg}^{-1}$, $e_M \approx 10^2 - 10^3J\mathrm{kg}^{-1}$ at the atmospheric temperature, while at the temperature of order 10^3K attained, for instance, in the solar radiative zone, $e_R \approx 10^3 - 10^4J\mathrm{kg}^{-1}$ and $e_M \approx 10^3 - 10^4J\mathrm{kg}^{-1}$. Accordingly, the effect of radiation is often negligible under the “normal” laboratory conditions on the Earth ($e_M/e_R \approx 10^2 - 10^3$) but becomes highly significant in the models of hot stars studied in astrophysics ($e_M/e_R \approx 10^{-1} - 10$). However, radiation plays an important role in certain meteorological models under specific circumstances.

The kinetic theory predicts the viscosity of gases to be proportional to $\sqrt{\vartheta}$ or a certain power of ϑ varying with the specific model and characteristic temperatures. This prediction is confirmed by experimental observations; a generally accepted formula is the so-called Shutherlang correlation yielding

$$\mu = \frac{A\sqrt{\vartheta}}{1 + B/\vartheta} \text{ for } \vartheta \text{ “large”},$$

where A and B are experimentally determined constants. For the air in the range of pressures between $1 - 10$atm, we have $A = 1.46\mathrm{kgm}^{-1}\mathrm{s}^{-1}\mathrm{K}^{-1/2}$, $B = 100.4\mathrm{K}$. The dependence of the transport coefficients on the temperature plays a significant role in the mathematical theory developed in this book.

The specific values of physical constants presented in this part are taken over from Bolz and Tuve [26].