

# Chapter 1

## Introductory remarks and starting assumptions

### Solids, liquids and gases

At macroscopic level, the most noticeable difference between solids and fluids lies in their different deformation capability. Under the action of a small external force, solids respond with a small deformation. Such behavior arises because in solids the internal force counteracting the external force is proportional to the deformation. Fluids, on the other hand, are easily deformed under the action of external forces. The internal resistive force turns out to be proportional to the rate of deformation, rather than to the deformation itself. As a direct consequence, fluids adapt their shape to that of the containers limiting them.

The differences between liquids and gases are much less fundamental. A first difference concerns their density: the density of liquids is much larger than that of gases (for given conditions of temperature and pressure), which in turn causes the force required to accelerate liquids to be much larger than that involved in the motion of gases. Concerning the mechanical properties of liquids and gases, perhaps the most fundamental difference lies in their compressibility. The increment of density associated with the application of a given overpressure is much less pronounced in liquids than it is in gases, which is expressed by the inequality

$$\left(\frac{\partial\rho}{\partial p}\right)_{T,l} \ll \left(\frac{\partial\rho}{\partial p}\right)_{T,g}, \quad (1.1)$$

where  $\rho$ ,  $p$  and  $T$  represent the density, pressure and temperature, respectively. As an illustrative example, consider a balloon full of air. We all know that it is relatively simple to reduce the volume of the balloon by appropriately pressing with our hands, that is, we can easily increase the gas density by applying an overpressure. Things are quite different when the balloon is full of water instead: the balloon deforms under the action of an overpressure, but its volume- and therefore the liquid density- remains virtually unaltered<sup>1</sup>. Similarly, by varying the temperature while maintaining the pressure constant one may change the density of a gas appreciably, whereas the same temperature variation would only slightly modify the density of a given liquid. Because of their low compressibility, under most conditions one may study the motion of liquids as if they had constant density. When we introduce that assumption, we shall say that the liquid behaves as a “perfect liquid”.

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<sup>1</sup>In fact, the overpressure needed to halve the specific volume of water is on the order of  $10^6$  atmospheres.

All of the macroscopic properties mentioned above are the result of the different microscopic structure exhibited by solids, liquids and gases. The force exerted between two molecules is known to be a function of the distance between their centers  $d$ , with a variation that is schematically represented in Fig. 1.1.

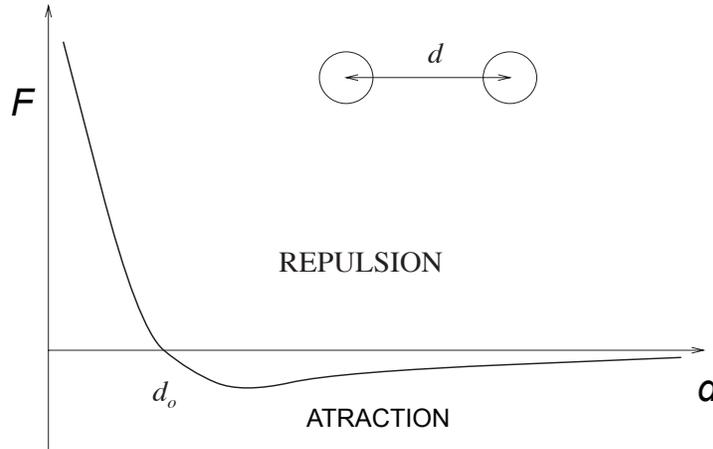


Figure 1.1: Schematic representation of the force between two molecules as a function of the distance between their centers.

When the distance becomes very small, the two molecules tend to repel each other, whereas an attraction force appears for values of  $d$  larger than a critical value  $d_o$ , on the order of the characteristic molecular size  $d_o \simeq 3 \times 10^{-10}$  m, for which the system of two molecules would remain in stable equilibrium.

For known values of the density  $\rho$  and molar mass  $W$ , it is straightforward to compute the average distance between two molecules according to  $d = (\rho N_A / W)^{-1/3}$ , where  $N_A = 6.023 \times 10^{23}$  molecules/mol is the so-called Avogadro's number. The computation reveals that for gases at normal ambient temperature and pressure  $d \simeq 3 \times 10^{-9}$  m  $\simeq 10d_o$ , while the molecules of liquids and solids are much more closely packed, with characteristic inter-molecular distances  $d \simeq d_o$ . Gas molecules can be expected to experience very weak attraction forces and, in the first approximation, one may assume that they move freely, interacting with the surrounding molecules only when collisions take place. This microscopic view explains the high compressibility of gases, as well as their deformation capability and their ability to fill up all of the available space in the container. In solids and liquids the intermolecular forces can be expected to be much more important. The repulsion force keeps molecules from getting closer, which explains the low compressibility of liquids and solids. Their different deformation capability emerges because, although the intermolecular distance is similar, the liquid molecules are in continuous relative motion with respect to their neighboring counterparts, whereas the molecules in a solid occupy fixed relative positions. It is worth mentioning that, although water is clearly a liquid, other substances exhibit a dual behavior and are not easily classified as solid or liquid. Paint is one such example: if we let it sit for long enough it will end up behaving as a highly elastic solid, readily recovering the liquid state when stirred at a sufficiently fast rate.

## The fluid as a continuum: fluid particles.

The matter in a given fluid is discretely distributed: molecules in gases are separated by large distances, and, even for liquids, whose molecules are closely packed together, the mass is concentrated in the nuclei. The large number of molecules involved appears as a key complicating feature of the fluid motion (at normal ambient conditions, there exist of the order of  $3 \times 10^{16}$  molecules in a cubic millimeter of air and about one thousand times more in a cubic millimeter of water). Clearly, it is hopeless to try to describe the overall dynamics by accounting for the fate of each individual molecule, a computation that would require in principle integration of Newton's second law for each single molecule to determine its location and velocity, with account taken of intermolecular forces and collisions. This is a phenomenal computation that is out of reach of present and foreseeable future computational capabilities. A different perspective, based on the so-called continuum hypotheses, is to be adopted instead.

In previous years we have studied systems with uniform properties that had only a few degrees of freedom. For instance, in classical equilibrium thermodynamics the state of a gas within a given container was described by giving its density and temperature, both assumed to be uniform, while in mechanics the motion of a rigid body was determined in terms of its velocity and angular velocity, that is, a total of six degrees of freedom. In fluids, our experience tells us that things are not quite so simple. We have all seen the motion of suspended dust particles as they are made visible by a beam of sun light crossing a window, which allows us to visualize the complex air motion driven by buoyancy in a room. Clearly, a single velocity vector is not sufficient to describe this system, characterized by large spatial and temporal variations.

In the following discussion, we will use the concept of macroscopic distance,  $L$ , defined for a given flow field as the characteristic distance that needs to be traveled to observe *significant* variations of the different flow properties. For instance, for the buoyancy dominated air flow in your bedroom one could tentatively say that significant velocity variations occur over distances on the order of  $L = 10$  cm. This macroscopic distance is of interest when describing the flow field because it tells you how detailed your description must be to give a realistic picture of the flow. For the bedroom example, with velocity variations occurring over distances of the order of  $L = 10$  cm, to describe the velocity field at a given instant of time it would be enough to provide the velocity vector at points separated 1 cm apart (or perhaps 1 mm apart, if one wants the description to be very accurate). Based on this observation, it is natural to approach the study of fluid motion by dividing the fluid in small parcels called *fluid particles* with respect to which we shall define the concepts of velocity, density, etc. Each particle is centered at a location  $\bar{x}$  at a time  $t$ . Their size must be much smaller than the characteristic macroscopic distance  $L$  of the fluid system under study, so that the velocity, density, etc of the system can be described accurately as continuous functions of  $\bar{x}$  and  $t$  in terms of the properties of each fluid particle. The assumption that the different fluid properties can be described as continuous functions (although they are not, as mentioned above in connection with the mass distribution) is the so-called *continuum hypotheses*, also used in other branches of mechanics, such as elasticity.

To investigate the conditions of validity of the continuum hypotheses it is of interest to consider as an example the case of a gas and the concept of density. For a fluid particle of volume  $\delta V$  centered at  $\bar{x}$  at time  $t$  the density is defined according to  $\rho = \sum m_i / \delta V$ , where  $\sum m_i$  is the sum of the masses of all molecules contained in the fluid particle. For the proposed continuum description to make sense, the value of  $\rho$  should be independent of  $\delta V$ , so that the value of the density at time  $t$  and position  $\bar{x}$  can be defined uniquely as  $\rho(\bar{x}, t)$ . To see whether that

independence is verified, we plot in Fig. 1.2 the variation of  $\sum m_i/\delta V$  as a function of the fluid particle size  $(\delta V)^{1/3}$ .

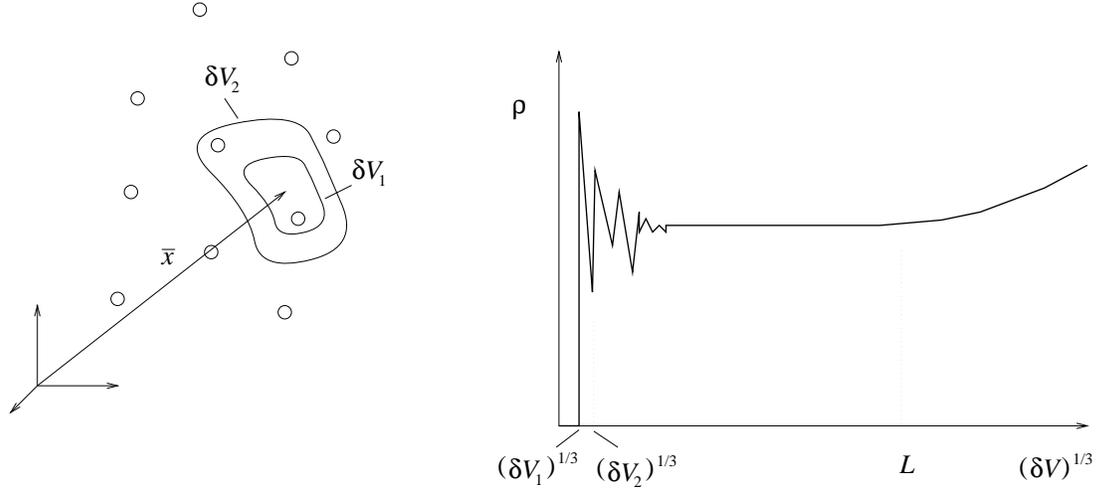


Figure 1.2: The concept of fluid particle.

When the size of the fluid particle is much smaller than the characteristic intermolecular distance  $d$ , it is very likely that the fluid particle be empty, and the associated density defined as  $\sum m_i/\delta V$  be identically zero. As the size increases, a critical value is reached for which the first molecule enters the particle, leading to an abrupt change in the density. A decrease in density would follow for increasing values of  $(\delta V)^{1/3}$ , until the second molecule enters the fluid particle, leading to a new jump in the density. Subsequent jumps would be progressively smaller for increasing values of  $\delta V$ , and would become almost inappreciable when the fluid-particle size  $(\delta V)^{1/3}$  reaches values much larger than  $d$ , when the particle contains a large number of molecules  $\delta V/d^3 \gg 1$ . The plateau value, defining uniquely the density at time  $t$  and position  $\bar{x}$ , remains independent of  $\delta V$  for increasing values of the particle size, until the particle is so large that it begins to embody fluid parcels with truly different properties, i.e., for  $(\delta V)^{1/3} \sim L$ . According to the figure, uniquely defined flow properties based on the fluid particle concept can be defined if and only if the fluid-particle size falls in the intermediate range

$$d \ll (\delta V)^{1/3} \ll L. \quad (1.2)$$

The development therefore depends critically on the condition  $L \gg d$ , which enables the introduction of fluid particles with well defined properties. Since for air at normal ambient density  $d \simeq 3.4 \times 10^{-9}$  m, most flows of engineering interest easily satisfy the required condition and are therefore amenable to a continuum description. Note that, in liquid flow, with characteristic intermolecular distances  $d \simeq d_o \simeq 3 \times 10^{-10}$  m, the condition  $L \gg d$  can be satisfied even more easily than it is for gases. Extreme examples for which the continuum description is not applicable because  $L \sim d$  include rarefied flows over re-entering vehicles in the upper atmosphere, for which the average distance between neighboring molecules become very large, and the tiny flows appearing in micro and nanotechnology applications.

## Density, velocity and internal energy

The concept of fluid particle allows us to define the density of the fluid according to

$$\rho(\bar{x}, t) = \lim_{\delta V \rightarrow 0} \frac{\sum m_i}{\delta V}, \quad (1.3)$$

subject to the additional condition  $(\delta V)^{1/3} \gg d$  needed to avoid the discrete character of the fluid at microscopic level. Similarly, the fluid velocity can be defined as the mass averaged value of the velocity of the molecules contained within the fluid particle

$$\bar{v} = \lim_{\delta V \rightarrow 0} \frac{\sum m_i \bar{v}_i}{\sum m_i}, \quad (1.4)$$

which is the velocity of the center of mass for the given set of molecules. On the other hand, the energy per unit mass contained inside  $\delta V$  is given by  $\sum E_i / \sum m_i$ , where  $E_i = m_i |\bar{v}_i|^2 / 2 + E_{v_i} + E_{r_i} + \dots$  represents the energy of each individual molecule, obtained as the sum of the kinetic energy associated with translation  $m_i |\bar{v}_i|^2 / 2$ , those corresponding to rotation  $E_{r_i}$  and vibration  $E_{v_i}$  (for non-monoatomic molecules), etc. It is customary to write the energy per unit mass by accounting separately for the kinetic energy associated with the flow velocity  $|\bar{v}|^2 / 2$ , thereby giving

$$\lim_{\delta V \rightarrow 0} \frac{\sum E_i}{\sum m_i} = e + |\bar{v}|^2 / 2, \quad (1.5)$$

where

$$e = \lim_{\delta V \rightarrow 0} \frac{\sum m_i |\bar{v}_i - \bar{v}|^2 / 2 + E_{v_i} + E_{r_i} + \dots}{\sum m_i} \quad (1.6)$$

is the so-called internal energy (the derivation of (1.6) is left as an exercise for the reader). The first term above,  $|\bar{v}_i - \bar{v}|^2 / 2$ , corresponds to the kinetic energy of the random molecular motion, a quantity directly associated with the definition of temperature.

## Local thermodynamic equilibrium

Classical thermodynamics deals with systems that are in mechanical and thermal equilibrium, for which all thermodynamic properties are spatially uniform and constant in time. When the evolution of a given system is studied with the laws of classical thermodynamics, it is assumed that the process is so slow that the system at each instant can be considered to be in equilibrium. A very useful result for homogeneous systems in equilibrium is that their thermodynamic state is completely determined by giving the values of any two independent state variables, while the corresponding values of the other state variables can be computed through the equations of state. Fluid mechanics deals with systems that are not in thermodynamic equilibrium, with fluid properties changing both spatially and temporally. It is however found that the results of equilibrium thermodynamics are approximately valid for most of the non-equilibrium states found in fluid mechanics, in that an observer moving with the local fluid velocity can describe the fluid state in terms of thermodynamic variables that are inter-related by the same equations of state that apply for systems in strict equilibrium. This hypothesis of *local thermodynamic equilibrium* can be rigorously justified through the kinetic energy for gases, whereas for liquids it is substantiated by ample experimental evidence.

In the case of gases, molecules exchange momentum and energy through collisions, adjusting in that way their state to the local state of molecular motion. Molecular collisions constitute therefore the mechanism that enables thermodynamic equilibrium to be attained in a gas. The average distance travelled by a molecule between two subsequent collisions, called the mean free path  $\lambda$ , can be estimated by equating the volume swept by the molecule in its displacement between collisions,  $d_o^2\lambda$ , to the volume per molecule that exists in the gas,  $d^3$ , to give  $\lambda/d \simeq (d/d_o)^2$ , yielding for instance  $\lambda \simeq 4 \times 10^{-7}$  m for air in normal ambient conditions. The corresponding time between collisions  $\tau$  can be estimated by anticipating that molecules move with an average velocity  $a$  close to that of sound, giving for example  $\tau = \lambda/a \simeq 10^{-9}$  s for normal ambient conditions.

For gas systems in which the mean free path  $\lambda$  is much smaller than the macroscopic length  $L$  each molecule will undergo a large number of collisions before reaching regions with different macroscopic properties. As a result, the fluid state remains at all times very close to the equilibrium conditions corresponding to the local values of density and internal energy. Hence, the criterion to be satisfied in a gas for the local thermodynamic equilibrium approximation to apply is

$$\frac{\lambda}{L} \ll 1 \tag{1.7}$$

where  $\lambda/L$  is the so-called Knudsen number. Likewise, for unsteady gas flow, if  $\mathcal{T}$  denotes the characteristic time for variation of the macroscopic gas properties, the condition to be satisfied for local thermodynamic equilibrium is that  $\mathcal{T} \gg \tau$ . Note that the criterion given in (1.7) is more restrictive than that associated with the continuum hypothesis (Eq. 1.2).

## Thermodynamic variables and useful relationships

From the continuum hypothesis, we have been able to define the flow velocity  $\bar{v}(\bar{x}, t)$  together with the density  $\rho(\bar{x}, t)$  and internal energy  $e(\bar{x}, t)$ . By incorporating now the assumption of local thermodynamic equilibrium, the remaining thermodynamic variables are determined through the equations of state. For instance, the local value of the entropy per unit mass  $s(\bar{x}, t)$  can be obtained through an equation of state  $s = s(e, \rho)$ , which can be alternatively written in the form  $e = e(s, \rho)$ . Since

$$de = Tds - pd(1/\rho) \tag{1.8}$$

the corresponding temperature and pressure follow from

$$T = \left( \frac{\partial e}{\partial s} \right)_\rho \tag{1.9}$$

and

$$p = - \left( \frac{\partial e}{\partial \rho^{-1}} \right)_s \tag{1.10}$$

Analogously, the enthalpy per unit mass can be defined as  $h = e + p/\rho$ .

Since a complete account of thermodynamic variables and equations of state can be found in any basic book of classical thermodynamics, we shall limit the presentation here to a brief summary of the equations of state that are most useful for the analysis of problems of fluid motion. The treatment is restricted to two idealized fluid states, the so-called perfect liquids and perfect gases.

### Perfect liquids

A perfect liquid satisfies that its density  $\rho$  and specific heat  $c$  are constants, so that one can write

$$\rho = \rho_o \tag{1.11}$$

and

$$e = cT + e_o, \tag{1.12}$$

where  $e_o$  is the internal energy associated with the absolute zero temperature. From the definition of enthalpy, it follows that

$$h = cT + e_o + p/\rho_o, \tag{1.13}$$

whereas by integration of 1.8 one obtains

$$s = c \ln(T) + s_o, \tag{1.14}$$

where  $s_o$  is an integration constant defining an arbitrary reference state. Many liquids behave as perfect over relatively large intervals of pressure and temperature. For instance, in most applications water can be assumed to be a perfect liquid with density  $\rho_o = 10^3 \text{ kg/m}^3$  and specific heat  $c = 4180 \text{ J/(kg K)}$ .

### Perfect gases

The equation of state for a perfect gas is

$$p/\rho = R_g T, \tag{1.15}$$

where the gas constant  $R_g = R^o/W$  is obtained as the ratio of the universal gas constant  $R^o = 8.314 \text{ J/(mol K)}$  and the mean molar mass of the gas  $W$ . The thermal equations of state for the internal energy, enthalpy, and entropy are given by

$$e = c_v T + e_o, \tag{1.16}$$

$$h = c_p T + e_o, \tag{1.17}$$

$$s = c_v \ln(p/\rho^\gamma) + s_o, \tag{1.18}$$

where  $c_v$  and  $c_p = c_v + R_g$  are, respectively, the specific heats at constant volume and at constant pressure. The ratio of specific heats  $\gamma = c_p/c_v$  equals  $\gamma = 7/5$  for diatomic gases. Treating air as a perfect gas with  $R_g = 287 \text{ J/(kg K)}$  and  $c_v = 717 \text{ J/(kg K)}$  is an excellent approximation under most conditions of practical interest. At extremely high pressures or extremely low temperatures, however, the equation of state (1.15) must be replaced by a more complex expression (e.g., Van der Waals equation). Also, the assumption of constant specific heats must be relaxed in systems where the temperature changes appreciably, as occurs for instance in combustion processes.