4 The mass balance

4.1 Macroscopic mass balance

Intuitively, the principle of mass conservation is before our eyes in daily practice: if we draw biscuits from a bag, sooner or later, we will end up with an empty bag; if we drive our car without refilling the tank, at some point we will run out of fuel; if we pour more water in the kitchen sink than it can flow away, water will eventually overflow. In these and many other common situations, we know that the mass entering or exiting a system cannot disappear or be created, but it must end up somewhere. From a scientific perspective, it was the french chemist Antoine-Laurent de Lavoisier, in 1789, the first to establish the principle of mass conservation. His experiments led to the conclusion that the number of atoms of the single elements is preserved during chemical reactions. In other words, mass cannot be created nor destroyed (unless we consider nuclear reactions, which is beyond the scope of this course).

The mass conservation in transport phenomena is expressed in terms of general macroscopic and microscopic mass balance equations. Transport phenomena generally involve pipes, reactors, heat exchangers, or other instrumentation with well defined geometries and specific inlet and outlet sections. However, the mass balance equations are derived for the most general case, namely considering a control volume such as in Figure 4.1. The orientation of the surface S, defined by the normal unit vector $\mathbf{n}$, is different in each point of S (by convention, the orientation of $\mathbf{n}$ is towards the outside of V). In addition, all infinitesimal elements of the surface S are permeable to mass (for simplicity, you can think of the surface as a net). Let the control volume V be fixed in space and subjected to an arbitrary mass flow field $\mathbf{v}$. In other words, each point $P = (x, y, z)$ of V corresponds to a specific density value $\rho = \rho(x, y, z)$ and velocity vector $\mathbf{v} = \mathbf{v}(x, y, z)$. Note that, in general, density and velocity are also functions of time t, hence the balance is referred to a generic interval time

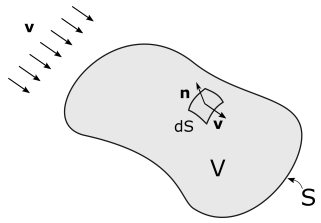


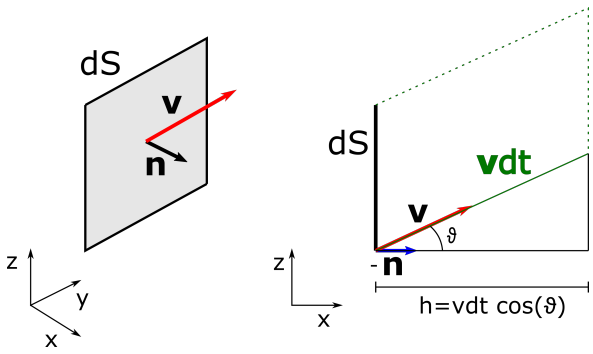
Figure 4.1: A generic control volume

dt. Since mass cannot be generated or consumed, the general equation of the mass balance is the following:

$$IN - OUT = ACC \tag{4.1}$$

In order to apply Equation 4.1 to the control volume of Figure 4.1, we need to divide the surface S in an infinite number of infinitesimal elements dS, small enough that they can be considered flat. In other words, dS must be small enough to be characterized by a single normal unit vector $\mathbf{n}$, by a single density value ρ, and by a single velocity vector $\mathbf{v}$. Let us assume that the single element dS is a square, as depicted in figure 4.2.

Figure 4.2: Evaluation of the flow rate through the infinitesimal surface element dS.



Let us consider an infinitesimal interval time dt. During dt, the fluid crossing dS travels the distance $\mathbf{v}dt$. Therefore, the volume of fluid dV, crossing dS in the interval time dt, corresponds to the parallelepiped having base dS and lateral side $\mathbf{v}dt$. In general, such parallelepiped is oblique, as $\mathbf{n}$ and $\mathbf{v}$ do not have the same direction. Hence, the volume dV is obtained from the product of dS by the height of the parallelepiped h, which is given by the projection of $\mathbf{v}dt$ along the direction of $\mathbf{n}$. By using vector operations, we can express h through a scalar product: $h = \mathbf{v}dt \cdot \mathbf{n}$. The volume dV is then obtained as follows:

$$dV = \mathbf{v}dt \cdot \mathbf{n}dS \tag{4.2}$$

The infinitesimal volumetric flow rate dQ, namely the volume of fluid crossing the surface dS per unit time, is given by:

$$dQ = \frac{dV}{dt} = \mathbf{v} \cdot \mathbf{n}dS \tag{4.3}$$

The infinitesimal mass flow rate $d\dot{m}$ is obtained multiplying the volumetric flow rate by density:

$$d\dot{m} = \rho \mathbf{v} \cdot \mathbf{n}dS \tag{4.4}$$

It is now important to note that, since the unit vector $\mathbf{n}$ points towards the outside of the control volume, any infintesimal mass flow rate entering the control volume is negative. In fact, the mass flow rate $d\dot{m}$ enters the control volume if the angle θ between the velocity vector $\mathbf{v}$ and the unit vector $\mathbf{n}$ is comprised between $90°$ and $180°$. In such an angle interval, $\cos(\theta)$ is negative. On the other hand, $d\dot{m}$ exits the control volume if the angle θ is comprised between $0°$ and $90°$. In such a range $\cos(\theta)$ is positive. Therefore, according to our convention, the mass flow rate contributions entering the control volume are negative whereas the ones exiting the control volume are positive. However, based on the signs in equation 4.1, it is more convenient to have the entering mass positive and the exiting mass negative. Hence, we add a minus on the left term of equation 4.4, and we write:

$$d\dot{m} = -\rho \mathbf{v} \cdot \mathbf{n} dS \tag{4.5}$$

The term $d\dot{m}$ refers to the infinitesimal surface dS. The global mass flow rate crossing the system per unit time is obtained by summing the contributions of all infinitesimal elements dS of the surface S. This is done through a surface integral:

$$IN - OUT = \left(- \int_S \rho \mathbf{v} \cdot \mathbf{n} dS \right) dt \tag{4.6}$$

From Equation 4.6, we get a mathematical expression for the $IN - OUT$ term of Equation 4.1. In order to obtain the mass balance equation, there remains to find a mathematical formulation of the accumulation term.
The total mass contained in the control volume V at a time instant t can be calculated as:

$$m_V = \int_V \rho dV \tag{4.7}$$

Going through a volume integration in Equation 4.7 is necessary, as the density is generally not constant in each point of the volume V. Hence, we divide the volume V in an infinite number of infinitesimal elements dV, small enough that the density can be considered constant in each of them. Then, the mass dm contained in each element dV is given by the product ρdV. The total mass is the sum of all contributions coming from the elements dV, that is, the volume integral of Equation 4.7.
Based on equation 4.7, the mass accumulated inside the control volume in the generic interval time dt is given by:

$$ACC = \int_V \rho dV \Big|_{t+dt} - \int_V \rho dV \Big|_t \tag{4.8}$$

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Now we have found a mathematical expression for all terms of equation 4.1. Substituting Equation 4.6 and Equation 4.8 into Equation 4.1, we obtain:

$$\left(-\int_S \rho \mathbf{v}\cdot\mathbf{n}dS\right)dt = \int_V \rho dV\Big|_{t+dt} - \int_V \rho dV\Big|_t \tag{4.9}$$

Dividing equation 4.9 by dt and bringing it to the limit as dt approaches zero we have:

$$-\int_S \rho\mathbf{v}\cdot\mathbf{n}\,dS = \frac{d}{dt}\int_V \rho\,dV \tag{4.10}$$

Equation 4.10 is the general equation for the *macroscopic mass balance*.
The term $\rho\mathbf{v}$ is the mass flux (mass crossing a surface per unit time and unit surface). As mentioned in the previous chapter, the mass flux is obtained by the product of velocity into mass concentration.

4.2 Microscopic mass balance

Equation 4.10 represents the macroscopic mass balance. In this section, we are going to derive a local expression of the mass balance, which is particularly useful for implementing computational fluid dynamics. In order to obtain the microscopic mass balance from Equation 4.10, we are going to use the divergence theorem (also known as Gauss' theorem), in order to transform the surface integral into a volume integral.

Theorem 4.1: Divergence Theorem

Let V be a volume bounded by a piecewise smooth closed surface S with positive orientation pointing out of V, and let $\mathbf{a} = \mathbf{a}(x, y, z)$ be a vector field with continuous first order partial derivatives, Then

$$\int_S \mathbf{a}\cdot\mathbf{n}dS = \int_V \boldsymbol{\nabla}\cdot\mathbf{a}dV \tag{4.11}$$

Applying the theorem 4.11 to the left term of equation 4.10, we have:

$$-\int_S \rho\mathbf{v}\cdot\mathbf{n}dS = -\int_V \boldsymbol{\nabla}\cdot\rho\mathbf{v}dV \tag{4.12}$$

Substituting equation 4.12 into equation 4.10 we have:

$$-\int_V \boldsymbol{\nabla}\cdot\rho\mathbf{v}dV = \frac{d}{dt}\int_V \rho dV \tag{4.13}$$

Since the control volume V is fixed in space, the time derivative on the right term of Equation 4.13 can be swapped with the integral over the volume V, yielding:

$$-\int_V \boldsymbol{\nabla} \cdot \rho \mathbf{v} dV = \int_V \frac{\partial}{\partial t} \rho dV \tag{4.14}$$

Using the linearity rules of integration, we can bring the left term of Equation 4.14 to the right side, and write:

$$\int_V \left(\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{v} \right) dV = 0 \tag{4.15}$$

Since the choice of the control volume is arbitrary, there is only one way to verify Equation 4.15: the integrand function must be identically zero in each point of the control volume. Hence, from Equation 4.15, it results that:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{v} = 0 \tag{4.16}$$

Equation 4.16 is the equation of the *microscopic mass balance*, also referred to as *continuity equation*.
Let us consider some particular cases of Equation 4.16. If we assume steady conditions, the time derivative of density is null, hence Equation 4.16 becomes the following:

$$\boldsymbol{\nabla} \cdot \rho \mathbf{v} = 0 \tag{4.17}$$

If we consider an incompressible fluid (constant density), Equation 4.17 becomes:

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{4.18}$$

namely, in a Cartesian coordinate system, we have:

$$\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} = 0 \tag{4.19}$$

Equation 4.19 states that, if the fluid velocity is decreasing in one direction, then it must increase in the others, in order to keep the sum of all velocity derivatives equal to zero.

4.3 Lagrangian and Eulerian approach to mass balance

Equation 4.16 was derived considering a control volume fixed in space. Such an approach is called *Eulerian*. On the other hand, the microscopic mass balance can be reformulated considering a local reference system moving with the fluid particle. Such an approach is called *Lagrangian*, and uses the concept of *substantial derivative*. In general, density depends on time

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and position. However, in a moving reference system we have to consider that position also depends on time. In such a case, the time dependence of density is expressed in the following way:

$$\rho = \rho(t; x_1(t), x_2(t), x_3(t)) \tag{4.20}$$

Based on Equation 4.20, the time derivative of density is obtained through the chain rule of derivatives, as follows:

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial \rho}{\partial x_2}\frac{\partial x_2}{\partial t} + \frac{\partial \rho}{\partial x_3}\frac{\partial x_3}{\partial t} = \\ &= \frac{\partial \rho}{\partial t} + v_1\frac{\partial \rho}{\partial x_1} + v_2\frac{\partial \rho}{\partial x_2} + v_3\frac{\partial \rho}{\partial x_3} = \\ &= \frac{\partial \rho}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}\rho = \frac{D\rho}{Dt} \end{aligned} \tag{4.21}$$

In Equation 4.21 we have used the definitions of velocity $v_i = \frac{dx_i}{dt}$ and substantial derivative.
The Substantial derivative of a function $\alpha(t, x_1(t), x_2(t), x_3(t))$ is defined as:

$$\frac{D\alpha}{Dt} = \frac{\partial \alpha}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}\alpha = \frac{\partial \alpha}{\partial t} + v_1\frac{\partial \alpha}{\partial x_1} + v_2\frac{\partial \alpha}{\partial x_2} + v_3\frac{\partial \alpha}{\partial x_3} \tag{4.22}$$

Therefore, with the Lagrangian approach, Equation 4.16 can be re-written as[1]:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot\rho\mathbf{v} = \frac{\partial \rho}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}\rho + \rho\boldsymbol{\nabla}\cdot\mathbf{v} = \frac{D\rho}{Dt} + \rho\boldsymbol{\nabla}\cdot\mathbf{v} = 0 \tag{4.23}$$

The two forms of the mass balance corresponding to the two different approaches are listed in Table 4.1.

Eulerian approach:	$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla}\cdot\rho\mathbf{v}$
Lagrangian approach:	$\frac{D\rho}{Dt} = -\rho\boldsymbol{\nabla}\cdot\mathbf{v}$

Table 4.1: mass balance in Eulerian and Lagrangian approach.

For an incompressible fluid, the density is constant in both time and space, then:

$$\frac{D\rho}{Dt} = 0 \tag{4.24}$$

Hence, from equation 4.23, equation 4.18 is again obtained.

[1] note that:

$$\begin{aligned} \boldsymbol{\nabla}\cdot\rho\mathbf{v} &= \frac{\partial}{\partial x_i}\mathbf{e}_i\cdot\rho v_j\mathbf{e}_j = \\ &= \frac{\partial}{\partial x_i}(\rho v_j)\boldsymbol{\delta}_{ij} = \frac{\partial}{\partial x_i}(\rho v_i) = \\ &= \rho\frac{\partial v_i}{\partial x_i} + v_i\frac{\partial \rho}{\partial x_i} \\ &= \rho\boldsymbol{\nabla}\cdot\mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\rho \end{aligned}$$