~~in large areas of industry, such as rotating machines, flow around helicopters, or with moving grids as encountered in fluid–structure interactions with vibrating surfaces.~~

~~We have also added a short section, which is a straightforward extension of the general integral form of the momentum equation, in presence of solid bodies, providing the formulation to post-process CFD data in order to extract the forces exerted on a body by the flow, such as lift and drag.~~

1.1 GENERAL FORM OF A CONSERVATION LAW

As mentioned in the introduction, the conservation law is the fundamental concept behind the laws of fluid mechanics.

But what is a conservation law?
It is altogether very simple in its basic logic, but can become complicated by its internal content. Conservation means that the variation of a conserved (intensive) flow quantity within a given volume is due to the net effect of some internal sources and of the amount of that quantity which is crossing the boundary surface. This amount is called the ***flux*** and its expression results from the mechanical and thermodynamic properties of the fluid. It will be defined more precisely in the next section. Similarly, the sources attached to a given flow quantity are also assumed to be known from basic studies. The fluxes and the sources are in general dependent on the space–time coordinates, as well as on the fluid motion. The associated fluxes are vectors for a scalar quantity and tensors for a vector quantity like momentum.

We can state the conservation law for a quantity U as the following logical consistency rule:

> ***The variation of the total amount of a quantity U inside a given domain is equal to the balance between the amount of that quantity entering and leaving the considered domain, plus the contributions from eventual sources generating that quantity.***

Hence, we are looking at the rate of change of the quantity U during the flow evolution, as a flow is a moving and continuously changing system.

Although we will write the conservation law for an undefined quantity U, it should be mentioned at this stage that not all flow quantities obey a conservation law. The identification of the quantities that obey a conservation law is defined by the study of the physical properties of a fluid flow system. It is known today that the laws describing the evolution of fluid flows (this is what we call fluid dynamics) are totally defined by the conservation of the following three quantities:

1. Mass
2. Momentum
3. Energy.

This represents in total five equations, as the momentum, defined as the product of density and velocity, is a vector with three components in space.

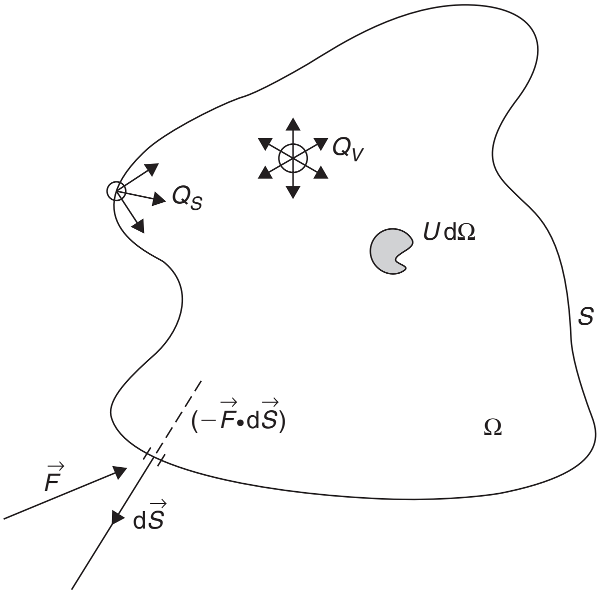

Figure 1.1.1 *General form of a conservation law for a scalar quantity.*

On the other hand, it is essential to keep in mind that other quantities, such as pressure, temperature, entropy, for instance, do ***not*** satisfy a conservation law. This does not mean that we cannot write an equation for these quantities, it just means that this equation will not be in the form of a conservation law.

1.1.1 Scalar Conservation Law

Let us consider a scalar quantity per unit volume U, defined as a flow related property.

We now consider an arbitrary volume Ω, *fixed in space*, bounded by a closed surface S (see Figure 1.1.1) crossed by the fluid flow.

The surface S is *arbitrary* and is called a *control surface*, while the volume Ω is called a *control volume*.

Our goal here is to write the fundamental law in its most general form, by expressing the balance of the variation of U, for a totally arbitrary domain Ω. *This control volume can be anywhere in the flow domain and can be of arbitrary shape and size.*

To apply the conservation law as defined above, we have to translate mathematically the quantities involved. The first one is the '*total amount of a quantity U inside a given domain*'. If we consider the domain of volume Ω, the total amount of U in Ω is given by

$$\int_\Omega U\,\mathrm{d}\Omega$$

and the variation per unit time of the quantity U within the volume Ω is given by

$$\frac{\partial}{\partial t}\int_\Omega U\,\mathrm{d}\Omega$$

Remark

I wish here to draw your attention to the interpretation of this mathematical expression. The above relation would be read by a mathematician as 'the partial derivative with respect to time of the volume integral of U over Ω'. However, I would like you to 'translate' this mathematical language in its physical meaning, by reading this relation instead as: 'the variation (∂) per unit of time (./∂t) of the total amount of U in Ω'. Try therefore, whenever appropriate, to always 'read' a mathematical expression by its translation of a physical property.

Coming back to the conservation law, we have now to translate mathematically '*the amount of that quantity U entering and leaving the considered domain*'.

This is where the physics comes in: we know from the study of the laws of physics that the local intensity of U will vary through the effect of quantities called ***fluxes***, which express the contribution from the surrounding points to the local value of U, describing how the quantity U is transported by the flow.

The ***flux*** is a fundamental quantity associated to a conserved flow variable U, and is defined as ***the amount of U crossing the unit of surface per unit of time***. It is therefore a directional quantity, with a direction and an amplitude, so that it can be represented as a vector. If this vector is locally parallel to the surface, then nothing will enter the domain. Consequently, only the component of the flux in the direction of the normal to the surface will enter the domain and contribute to the rate of change of U. So, *the amount of U crossing the surface element* $\mathrm{d}\vec{S}$ *per unit of time* is defined by the scalar product of the flux and the local surface element (see Figure 1.1.1),

$$F_n \, \mathrm{d}S = \vec{F} \cdot \mathrm{d}\vec{S}$$

with the surface element vector $\mathrm{d}\vec{S}$ pointing along the ***outward normal***.

The net total contribution from the incoming fluxes is the sum over all surface elements $\mathrm{d}\vec{S}$ of the closed surface S, and is given by

$$-\oint_S \vec{F} \cdot \mathrm{d}\vec{S}$$

The minus sign is introduced because we consider the flux contribution as positive when it enters the domain. With the outward normal as positive, the scalar product will be negative for an entering flux, as seen from Figure 1.1.1. Hence the need to add the minus sign. If we had defined the inward normal as positive, we would not have added the minus sign. However, the generally accepted convention is to define as positive the outward normal, so that the minus sign is of current acceptance.

To finalize the balance accounts, we have to add contributions from the sources of the quantity U.

These sources can be divided into volume and surface sources, Q_V and $\vec{Q}_S$ and the total contribution is

$$\int_\Omega Q_V \, \mathrm{d}\Omega + \oint_S \vec{Q}_S \cdot \mathrm{d}\vec{S}$$

Hence, the general form of the conservation law for the quantity U is

$$\frac{\partial}{\partial t}\int_{\Omega} U\,\mathrm{d}\Omega = -\oint_{S} \vec{F}\cdot \mathrm{d}\vec{S} + \int_{\Omega} Q_V\,\mathrm{d}\Omega + \oint_{S} \vec{Q}_S \cdot \mathrm{d}\vec{S}$$

which is generally written as

$$\frac{\partial}{\partial t}\int_{\Omega} U\,\mathrm{d}\Omega + \oint_{S} \vec{F}\cdot \mathrm{d}\vec{S} = \int_{\Omega} Q_V\,\mathrm{d}\Omega + \oint_{S} \vec{Q}_S \cdot \mathrm{d}\vec{S} \tag{1.1.1}$$

This is called the integral conservation form and is the most general expression of a conservation law.

This form has some remarkable properties:

- Equation (1.1.1) is valid for any fixed surface S and volume Ω.
- The internal variation of U, in absence of volume sources, depends only on the flux contributions *through* the surface S and *not on the flux values inside the volume* Ω.
- The fluxes do not appear under a derivative or gradient operator and may therefore be discontinuous, as will be the case in the presence of shock waves.

Why are these properties so important, in particular the second one? The importance arises from the fact that we will require this property to remain valid also *after* discretization, to ensure hereby that we satisfy the conservation law at the discrete level. When this is the case, we will speak of a '***conservative numerical scheme***'.

For instance, in an internal flow calculation it is essential to ensure mass conservation, that is constancy of the mass flow in all sections, for any grid resolution. Basically, we see from equation (1.1.1) that if the discretization leads to values of fluxes inside the domain, they will not be distinguishable from the volume sources and will therefore act as such. These 'numerical' sources will then destroy the conservation property of the relevant quantity. For mass conservation, eventual numerical sources will create or destroy mass and hence the mass flow rate will not remain constant. As we will see in Chapter 5, this property can easily be satisfied on arbitrary grids, in particular through application of the finite volume method.

Differential form of a conservation law

An alternative, local differential form of the conservation law can be derived by applying Gauss' theorem to the surface integral term of the fluxes and the surface sources, assuming that these fluxes and surface sources are continuous.

Gauss' theorem states that the surface integral of the flux is equal to the volume integral of the divergence of this flux:

$$\oint_{S} \vec{F}\cdot \mathrm{d}\vec{S} = \int_{\Omega} \vec{\nabla}\cdot \vec{F}\,\mathrm{d}\Omega$$

for any volume Ω, enclosed by the surface S, where the gradient or divergence operator $\vec{\nabla}$ is introduced. The explicit expression of this gradient operator is defined later in Cartesian coordinates, see equation (1.2.7).

Introducing this relation in the integral conservation law (1.1.1), we obtain

$$\int_\Omega \frac{\partial U}{\partial t}\,\mathrm{d}\Omega + \int_\Omega \vec{\nabla}\cdot\vec{F}\,\mathrm{d}\Omega = \int_\Omega Q_V\,\mathrm{d}\Omega + \int_\Omega \vec{\nabla}\cdot\vec{Q}_S\,\mathrm{d}\Omega \tag{1.1.2}$$

Since equation (1.1.2) is written for an arbitrary volume Ω, it must be valid locally in any point of the flow domain. This leads to the ***differential form of the conservation law***,

$$\frac{\partial U}{\partial t} + \vec{\nabla}\cdot\vec{F} = Q_V + \vec{\nabla}.\vec{Q}_S \tag{1.1.3}$$

or

$$\frac{\partial U}{\partial t} + \vec{\nabla}\cdot(\vec{F} - \vec{Q}_S) = Q_V \tag{1.1.4}$$

It is seen from these equations that surface sources have the same effect on the system as a flux term and therefore we might as well consider them from the start as an additional flux. However, we favor the present classification in fluxes and sources, since it allows a clear physical interpretation of all the contributions to the evolution of the quantity U. In any case, the term $(\vec{F} - \vec{Q}_S)$ can be considered as an ***effective flux***. This will be considered for the momentum conservation law, Section 1.3, where the pressure and shear stresses are indeed acting as surface sources, but they are currently added to the other flux terms to form one 'effective' flux for momentum conservation.

Note that:

- The fluxes (and surface sources) appear *exclusively* under the gradient operator, which is the only space derivative term. This is the direct translation of the surface integral of the fluxes in the integral form (1.1.1).
- **This indicates the way to recognize a conservation law in differential form. Look at all the space derivative terms: if they can be grouped as a divergence operator, then the equation is in conservation form**. If not, the equation is said to be in '**non-conservative**' **form**, or in '**quasi-linear**' form.
- This differential form is more restrictive than the integral form, as it requires the fluxes to be differentiable, i.e. having at least C1 continuity, which is not the case in presence of shock waves, for instance.
- For any quantity U, physical assumptions must provide definitions for the fluxes and the source terms, in function of other computed variables.

1.1.2 Convection–Diffusion Form of a Conservation Law

In Section 1.1.1, we have not provided any specific information concerning the fluxes, except for the fact that they do exist for any conserved quantity U. However, we can now be more specific and look closer to the physics of transport of a quantity U in a fluid flow.

The fluxes are generated from two contributions: a contribution due to the convective transport of the fluid and a contribution due to the molecular agitation, which can be present even when the fluid is at rest.

The first component, *which is always present*, is the ***convective*** flux $\vec{F}_C$, attached to the quantity U in a flow of velocity $\vec{v}$. ***It represents the amount of U that is carried away or transported by the flow*** and is defined as

$$\vec{F}_C = U\,\vec{v} \tag{1.1.5}$$

The local contribution of the convective flux through a surface element $\mathrm{d}\vec{S}$, $(\vec{F}_C.\mathrm{d}\vec{S})$ has an important physical significance.

For $U = \rho$ the fluid density, the corresponding convective flux through the surface $\mathrm{d}\vec{S}$ is equal to the local ***mass flow rate***, where we designate the mass flow rate by $\dot{m}$

$$\rho\vec{v}\cdot \mathrm{d}\vec{S} = \mathrm{d}\dot{m} \tag{1.1.6}$$

This quantity represents the amount of mass flowing through the surface dS, per unit of time, and is expressed in kg/s.

For a different conserved quantity $U = \rho u$, ***where u is the quantity per unit mass***, the contribution of the convective flux is equal to

$$\vec{F}_C \cdot \mathrm{d}\vec{S} = \rho u\vec{v}\cdot \mathrm{d}\vec{S} = u\,\mathrm{d}\dot{m} \tag{1.1.7}$$

clearly showing the physical meaning of the convective flux as defined by the quantity u entrained by the local mass flow rate.

The second component is a ***diffusive*** flux $\vec{F}_D$, defined as the contribution present in fluids at rest, due to the macroscopic effect of the molecular thermal agitation. The effect of the molecular motion translates in the tendency of a fluid toward equilibrium and uniformity, since differences in the intensity of the considered quantity create a transfer in space such as to reduce the non-homogeneity. This contribution to the total flux is proportional to the gradient of the corresponding quantity, since it has to vanish for a homogeneous distribution.

Diffusive fluxes do not always exist; for instance, from an analysis of the physical properties of fluid, it is known that in a single-phase fluid at rest, no diffusion of specific mass is possible since any displacement of specific mass implies a macroscopic displacement of fluid particles. Therefore, there will be no diffusive flux contribution to the mass conservation equation.

The phenomenon of diffusion is indeed totally different from convection. We can best understand the physics of diffusion by the following experiment, which establishes the basics of diffusion.

Consider a reservoir of water, at rest, and inject a drop of a colored (black) dye, supposed having the same density as water.

Look at Figure 1.1.2. What is going to happen? Will the drop stay in its position? As you probably know from basics physics, we observe that after a certain time the whole of the reservoir will become colored. What has happened?

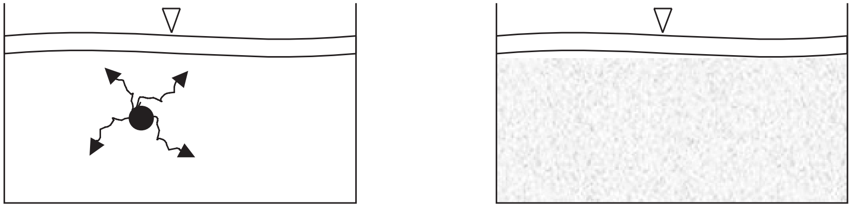

Figure 1.1.2 *A colored dye diffusing in a water reservoir.*

Due to the molecular agitation, the dye molecules are constantly in collision with the water molecules and will be 'hit' many times in all directions to wind up in arbitrary positions. As a result, after a certain time, we will find dye molecules everywhere and the whole reservoir will be colored. For us, as observer, we do not see the molecules, but we see the macroscopic results of these collisions and we notice the following ***empirical*** facts:

- The process appears as a diffusion, since a local concentration peak diffuses from a high local value to a lower concentration, in all directions.
- The process stops when there is no dye concentration differences anymore between two points, that is when uniformity is reached, which corresponds to a statistically homogenous distribution of the dye molecules between the water molecules.
- The diffusion process between two points is proportional to the concentration difference between these points and will tend to reduce these differences.
- An evolution whereby the concentration difference between two points increases (called anti-diffusion) has never been observed in this experiment.

The 'transport' of the dye molecules can therefore be described, from the point of view of continuum mechanics (since we view the fluid as a continuous media, instead of seen as constituted by molecules), by expressing the macroscopic observations by the existence of a diffusive flux, with the following properties:

- The diffusive flux is proportional to the gradient of the concentration, the gradient being the mathematical expression for the concentration difference between neighboring points, in their direction.
- It has to be opposite to the gradient, to express the tendency toward uniformity.
- It will be proportional to a diffusivity factor, which expresses its 'intensity', depending on the nature of the considered quantity and its environment.

This is summarized by the mathematical gradient ***law of Fick***, where κ is the diffusivity coefficient:

$$\vec{F}_{\mathrm{D}} = -\kappa\rho\vec{\nabla}u \tag{1.1.8}$$

Observe that the diffusivity constant κ has units of m^2/s for any quantity U.

Equation (1.1.3) then becomes

$$\frac{\partial \rho u}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}u) = \vec{\nabla}\cdot(\kappa\rho\vec{\nabla}u) + Q_V + \vec{\nabla}\cdot\vec{Q}_S \tag{1.1.9}$$

This equation is the general conservative form of a ***transport equation*** for the quantity $U = \rho u$ and is also referred to as a ***convection–diffusion equation***.

The structure of this equation is of utmost importance, both from physical as well as mathematical point of view and you should study this very carefully, as it forms the backbone of all mathematical modeling of fluid flow phenomena.

The convection–diffusion equation takes its name from the physical properties of the two flux contributions and from their specific mathematical expressions, which reflect very different physical properties. *Therefore, the following properties will provide significant and fundamental guidelines when setting up a CFD discretization.*

Convective and diffusive fluxes have indeed totally different physical properties:

- Convective fluxes describe the 'passive' transport of the conserved variable by the flow, which you can visualize as a piece of wood carried away by a river flow.
- Consequently the convective flux describes a phenomenon that has directional properties, as it is proportional to the velocity. A convective flux cannot provide a contribution in a direction transverse or opposite to the flow direction. It has therefore properties very similar to wave propagation phenomena, which are also essentially directional, for a selected propagation direction. *We will see in Chapter 3 that the relation between convective transport and wave propagation is indeed very close.*
- Observe that the convective flux appears in the conservation law (1.1.9) as a ***first order partial derivative term***, through the gradient term on the left-hand side.
- Another very important property of the convective flux, is that it is mostly ***nonlinear*** as the velocity field will generally depend on the transported variable. This nonlinearity is an essential property of fluid dynamics, the most notorious being turbulence, which is a direct consequence of the nonlinearity of the momentum conservation equation (see Section 1.3).
- The diffusion effects appear in the conservation law (1.1.9) as a ***second order partial derivative term***. In particular, for constant values of the product $(\kappa\rho)$, the diffusion term is the Laplace operator. This gives us the physical interpretation of the Laplace operator, as describing an isotropic diffusion, in all directions x, y, z, of the three-dimensional space

$$\Delta u \triangleq \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

- *Remember therefore, that each time you come across a Laplace equation or a Laplace operator, it describes a physical phenomenon corresponding to an isotropic diffusion.*

We can summarize now the essential differences between convection and diffusion in Table 1.1.1.

These differences are crucial to the understanding of the physics of flows, but also to the rules for discretization and to essential properties of CFD numerical schemes.

We can already mention here a most fundamental rule of numerical discretizations, which will be elaborated further in the following chapters, namely:

> ***The properties of a numerical discretization scheme may NEVER be in contradiction with the physics it aims to describe.***

It is therefore of uttermost importance to clearly understand the physical properties of the equations to be discretized and the mathematical translation of these properties. This particular issue, namely the one-to-one relation between physical interpretation and mathematical properties of the equations will be treated in Chapter 3.

Table 1.1.1 *Differences between convection and diffusion.*

Convection	*Diffusion*
Expresses the transport of the considered quantity by the flow	Translates the effects of molecular collisions
Does not exist in a fluid at rest	Does exist in a fluid at rest
All quantities are convected by the flow	Not all quantities are subjected to diffusion
Directional behavior	Isotropic behavior
Leads to first order space derivatives in the conservation law	Leads to second order space derivatives in the conservation law
Is generally nonlinear, when the flow velocity depends on the transported variable	Is generally linear for constant fluid properties

For instance, a numerical scheme tuned to handle a diffusion equation, such as a Laplace equation ($\Delta u = 0$) or a Poisson equation ($\Delta u = q$), will not work when applied to a pure convection dominated equation. See Section 11.3.2.2 in Chapter 11 for an example of great historical significance, related to the first attempts to treat transonic potential flows numerically, during the 1960s, in the early years of CFD development.

The Peclet number

The solution of convection–diffusion equations will strongly depend on the relative strength of the two conflicting phenomena, which can range from pure convection to pure diffusion.

It is therefore important in many applications to be able to judge this relative strength by an appropriate indicator, which should be a non-dimensional number. If we compare the convective and diffusive fluxes, given respectively by equations (1.1.5) and (1.1.8), we can define a measure of their ratio, as follows:

$$\frac{|\vec{F}_{\mathrm{C}}|}{|\vec{F}_{\mathrm{D}}|} \approx \frac{\rho u V}{\rho \kappa u / L} = \frac{VL}{\kappa} \tag{1.1.10}$$

where V is a reference velocity and L a reference length, such that V/L is a measure of the gradient of u. The ratio in the right-hand side is the non-dimensional ***Peclet number***, measuring the relative strength between convection and diffusion:

$$\mathrm{Pe} \equiv \frac{VL}{\kappa} \tag{1.1.11}$$

Hence, if this ratio is much larger than one, the evolution of the quantity U will be dominated by convection, while it will be dominated by diffusion when the Peclet number is lower than 1. For values in the intermediate range, the solution U will have a mixed behavior, influenced both by convection and diffusion.

We will come back to these important properties in several chapters of this Volume.