3 Evolution Equation

3.1 Introduction to transport phenomena

Transport phenomena study the evolution of properties in a fluid with motion (advection) and/or to molecular dynamics (diffusion). In fluids, transport is much more effective than in solids, because the molecules can have relative movement, transporting heat (associated to their kinetic energy) but also their own matter and thus in fluids we can also study mass transport.

Mathematic description of transport phenomena has been done long time ago, however, the resolution of the transport equations in practical situations has been made possible only by numerical methods and computers. Before the advent of computers transport processes had to be studied using empirical formulations (derived from experiments) or analytical solutions in simple geometries.

The impossibility of resolving the general equations conducted to specific solutions for different application, e.g. meteorology, oceanography or engineering making these disciplines apparently very different from each other. Even inside engineering, hydraulics, hydrology and fluid mechanics use to be treated as very different disciplines although they are in fact quite similar. The text of this chapter has in mind the numerical resolution of the equations and follows a global approach based on the concept of conservation principle, which is valid in any application.

A conservation principle can be stated as:

{The rate of accumulation of a property inside a control volume} = {what flows in minus what flows out}+{Production minus Consumption}

Using this conservation principle, evolution equations for any property inside a control volume can be derived adding production and consumption processes – specific of each property – to transport across its surface, common to every property.

3.1.1 The continuum matter hypotheses

The hypothesis of "continuum matter" is a basic assumption of Fluid Mechanics. According to this hypothesis the smallest amount of fluid that we can consider is much larger than a molecule and thus we will never be able to individualise molecules. Therefore, when one tells about velocity, we are referring to the average velocity of an ensemble of molecules.

However, when the velocity is zero, although there is no advection, there is still movement of individual molecules due to Brownian movement and thus there is transport. The transport associated to the average velocity is designated by advection. The transport that in fact exists but cannot be accounted by advection is called diffusion.

So, the need for two transport processes: advection and diffusion is a consequence of the continuum matter hypotheses.

3.2 Velocity and advective transport

What is velocity? Mathematically velocity is the displacement per unit of time. It is defined instantaneously and at each point:

$$v_i = \frac{dx_i}{dt}$$

If represented by a function of space and time, one can know it at every point, e.g.

$$v_x = ky$$

If it is not represented by a function, a list of values measured in a finite number of points has to be used and one has to make hypotheses for the distribution between those points (e.g. interpolation). The difference between the effective velocity and the approach assumed must be accounted again by diffusion.

In transport phenomena velocity is used to compute the advective flux, that is the flux across a surface. Thus, the best definition of velocity is not the one based on the displacement per unit of time, but the flux of volume per unit of area:

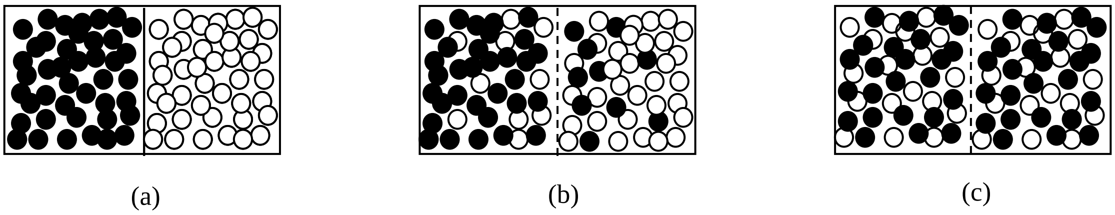
$$v_i = \frac{d\phi}{dA} n_i$$

Where $n_i$is the normal to the surface dA and v_i is the velocity perpendicular to the surface. So, in practical terms, the velocity in transport phenomena is always the average velocity across a surface, and thus the advective transport computed depends on the surface. Diffusion is the difference between the real transport and that accounted using the selected surface. If the surface is infinitesimal, then the velocity is defined at every point. Even though, a diffusion flux must be computed because the Brownian movement is not being considered. In this case the diffusivity necessary to balance the transport is the molecular diffusivity. If the surface is larger, then a larger diffusivity is necessary (turbulent diffusivity in turbulent flows and sub-grid diffusivity in numerical models).

3.3 Diffusivity and Diffusive Transport

Diffusion in laminar flows results from movements at molecular scale not represented by the velocity (Brownian movement). The concept of diffusion and diffusivity can be put into evidence considering the case represented in Figura 1. The Figure represents a box with two compartments. The left compartment is filled with black molecules and the right compartment is filled with white molecules. The fluids are at rest, i.e. the macroscopic velocity is null and in the initial situation

(Figure a, on the left) the two fluids are kept apart by a diaphragm. Although the macroscopic velocity is null, molecules still move randomly, with individual velocities (Brownian velocity) dependent of the temperature. If the diaphragm is removed, particles from each side will keep moving mixing the two side of the box (stage "b" in the Figure). After enough time the percentage of white and dark fluid molecules will become the same in both box half's. At this stage, the probability of a white molecule to move from the right side of the box into its left side is equal to the probability of another white molecule to move the way around and there is no net exchange.



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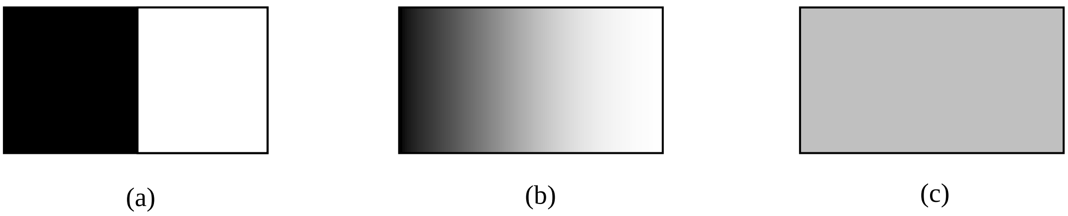
A macroscopic view of the microscopic process described above is represented in Figura 2. In the initial condition (a) one would see black fluid on the left side of the box and white fluid on the right side. After removing the diaphragm one would see a grey area between the two fluids to form and moving along the box (Figure b) corresponding to the mixing zone and after complete mixing, a homogeneous grey fluid would be observed (Figure c).



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Let us consider a surface inside the box (Figura 3). The molecules are moving with a typical v_b. Designating by Δl the free path between two collisions and by $(c_l - c_{l+\Delta l})$ the difference of concentration between the starting point and the collision point, one can say that the net diffusive flux per unit of area is:

$$\phi_{dif} = v_b(c_l - c_{l+\Delta l})$$

But,

$$(c_l - c_{l+\Delta l}) = \Delta l \frac{\partial c}{\partial l}$$

That replace above gives:

$$\phi_{dif} = v_b \Delta l \frac{\partial c}{\partial l}$$

But, according to the Fick law, the diffusive flux is:

$$\phi_{dif} = -\vartheta \frac{\partial c}{\partial l}$$

And thus, one can say that diffusivity is:

$$\vartheta = v_b \Delta l$$

i.e. the diffusivity is the product of the difference between the real velocity of elementary particles in the flow (molecules in molecular diffusivity) by the length of the free movement of those particles. In turbulent flow the elementary particle is the largest eddy and the free length is the mixing length, proportional to the size of that eddy.

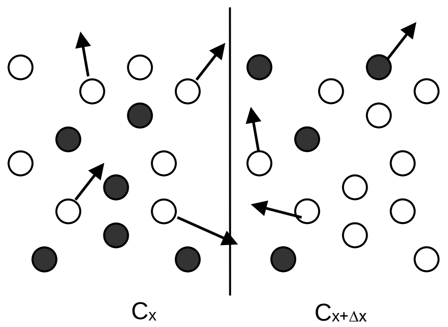

Figura 3: Control section within the box. The concentration of black molecules is space variable. Molecules are assumed to have an individual velocity v_b.

In case of a numerical model, we will see that the length to be used is the size of the grid and the velocity to be considered is the variability of the velocity, proportional to the average velocity.

3.3.1 The Advective flux

The advective flux accounts for the amount of property transported per unit of time by fluid velocity across a surface. If the property is designated by "B", its dimensions are [B] T^{-1} and can be expressed as[1]:

$$\Phi_{adv} = \frac{B}{t} = \frac{B}{Vol} * \frac{Vol}{t}$$

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where Vol is the volume $\frac{B}{Vol}$. has the dimensions of a specific quantity [amount per unit of volume, concentration in case of mass]. The ratio between the volume and the time [L^3T^{-1}] is the flow rate that can be calculated as the product of the velocity [LT^{-1}] by the area [L^2] of the surface. The discharge per unit of area is the velocity and thus, the transport produced by the velocity per unit of area is:

$$\phi_{adv_i} = \beta v_i$$

Where β is the concentration and v_i is the velocity relative to the surface. This flux is a vector parallel to the velocity. The flux across an elementary area, *dA*, not perpendicular to the velocity is given by:

$$d(\Phi_{adv}) = \beta(\vec{v}.\vec{n})dA = v_i n_i \mathrm{dA}$$

where $\vec{n}$ is the external normal to the elementary surface *dA*. In case of a finite surface *A*, the total flux is the summation of the elementary fluxes across the elementary areas composing it. This summation can be represented by the integral over that surface:

$$\Phi_{adv} = \iint_A d\Phi_{adv} = \iint_A \beta(\vec{v}.\vec{n})dA$$

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This is the generic definition of the advective flux of a property *B*, across a surface *A*.

3.3.2 Diffusive flux

Diffusive flux is the net transport associated to the Brownian movement of molecules in case of a laminar flow and to the turbulent velocity in case of turbulent flow and generically to the velocity not described by the velocity definition used to compute the advective flow. Diffusion transports

[1] [*B*] means "dimensions of *B*" and T means time

isolines perpendicularly to themselves, i.e. in the direction of the gradient and opposite sense, as found out by Fick, who stated that the diffusive flux per unit of area is given by[2]:

$$\phi_{dif_i} = -\vartheta \frac{\partial \beta}{\partial x_i}$$

Where ϑ is the diffusivity.

Both β gradient and diffusivity can vary spatially, implying the calculation of the flux on elementary surfaces:

$$d(\Phi_{dif}) = -\vartheta(\vec{\nabla}\beta.\vec{n})dA = \left(-\vartheta \frac{\partial \beta}{\partial x_i}.n_i\right)dA$$

Where again n is the normal to the elementary surface. Its integration along the overall surface gives:

$$\Phi_{dif} = \iint_A d\Phi_{dif} = \iint_A -\vartheta(\vec{\nabla}\beta.\vec{n})dA$$

Where $\vec{n}$ is the normal to the elementary surface.

3.4 Rate of change of the property contained inside a control volume

The total amount contained inside a control volume is given by:

$$B = \iiint_{Vol} \beta dVol$$

The rate of change of the matter inside the volume is given by:

$$\frac{\partial B}{\partial t} = \frac{\partial}{\partial t}\left(\iiint_{Vol} \beta dVol\right)$$

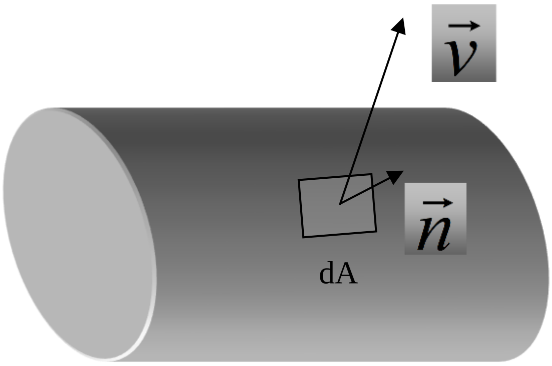
3.5 The evolution Equation

Applying the conservation principle of conservation one can write:

$$\frac{\partial}{\partial t}\left(\iiint_{Vol} \beta dVol\right) = -\iint_A \beta(\vec{v}.\vec{n})dA - \iint_A -\vartheta(\vec{\nabla}\beta.\vec{n})dA + Sources - Sinks$$

The minus signs on the second member of the equation account for the fact that the convention to compute the flux across a closed surface is to use the external normal to compute the internal product. This means that when the internal product is negative, the flux is entering into the volume. The integral equation:

[2] In the previous paragraph we have seen that it could not be other way around and we have even seen how diffusivity appears.



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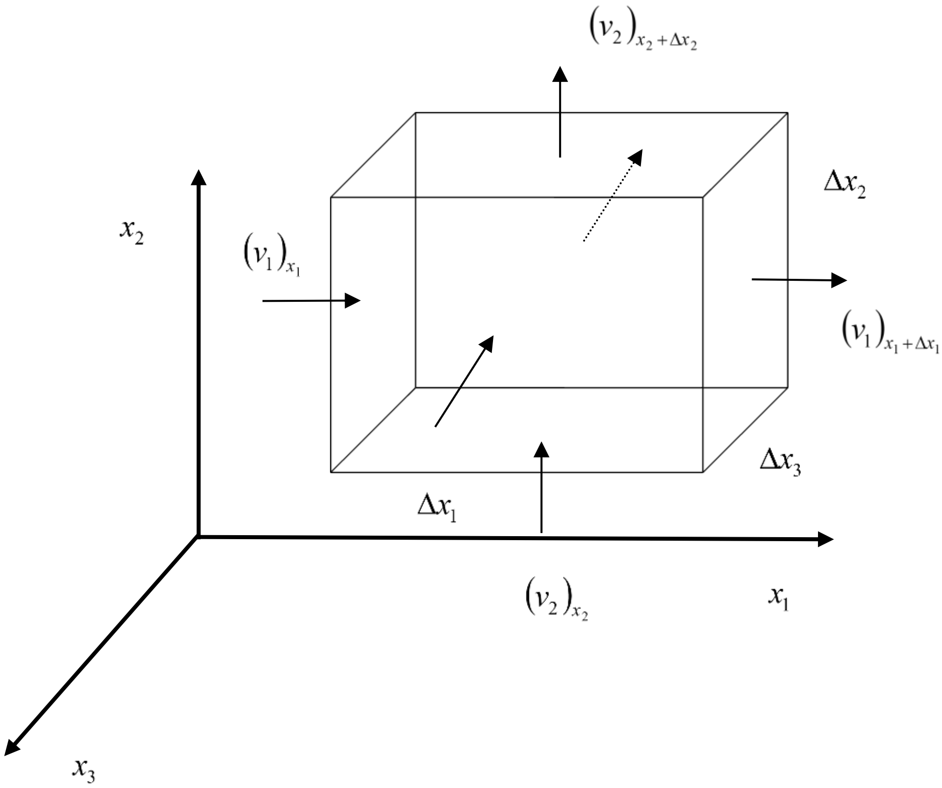
The evolution (or conservation) equation written in the integral form is quite intuitive and holds for any generic volume, as represented in the figure above, but it is difficult to handle in real conditions, because integrals are difficult to compute, except into very simple geometries and very simple functions. The differential form permits to get solutions in some more conditions, but still quite academic. For generic conditions, numerical methods must be used. This will be addressed in the next paragraphs.

3.5.1 Elementary area and elementary volume

The transport across a finite surface *A* is the integral of the transport across infinitesimal areas. Mathematically infinitesimal areas are infinitesimal. However, if we divide our surface into smaller surfaces (that we will call here elementary areas) small enough to allow the assumption of uniform property distribution over them, then we can replace integrals by summations. Fluxes across an elementary surface are the product of the fluxes per unit of area by the area of the elementary surface. This is a basic assumption on modelling.

An elementary volume is a volume limited by elementary surfaces, inside which properties can be considered as being uniformly distributed, i.e. they can be represented by the average values. The total amount of a property inside an elementary volume is given by the product of its average specific value by the elementary volume.

Applying these concepts, one can transform the integral equation into an algebraic equation. One can also remove the internal products considering a volume with elementary surfaces perpendicular to the coordinated axis. Doing so for cartesian coordinates one has to consider a geometry of the type:



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In this geometry, the volume is given by:

$$Vol = \Delta x_1 \Delta x_2 \Delta x_3$$

And the area of a face perpendicular to the axis k is given by:

$$A_k = \Delta x_i \Delta x_j$$

Assuming the particular case of a constant volume, i.e. a volume that does not vary in time one can simplify the integrals to obtain an algebraic equation.

3.6 Algebraic Evolution Equation

Assuming the geometric restrictions described in the previous paragraph one can start transforming the integral evolution equation:

$$\frac{\partial}{\partial t}\left(\iiint_{Vol} \beta dVol\right) = -\iint_A \beta(\vec{v}.\vec{n})dA - \iint_A -\vartheta\left(\vec{\nabla}\beta.\vec{n}\right)dA + Sources - Sinks$$

The rate of accumulation becomes:

$$\frac{\partial B}{\partial t} = \frac{\partial}{\partial t}\left(\iiint_{Vol} \beta dVol\right) = \frac{B^{t+\Delta t} - B^{t}}{\Delta t} = \Delta x_1 \Delta x_2 \Delta x_3 \frac{(\beta^{t+\Delta t} - \beta^{t})}{\Delta t}$$

The advective fluxes becomes:

$$\Phi_{adv} = -\iint_A \beta(\vec{v}.\vec{n})dA = \Delta x_2 \Delta x_3 \left[(\beta v_1)_{x_1} - (\beta v_1)_{x_1+\Delta x_1}\right]$$
$$+\Delta x_1 \Delta x_3 \left[(\beta v_2)_{x_2} - (\beta v_2)_{x_2+\Delta x_2}\right]$$
$$+\Delta x_1 \Delta x_2 \left[(\beta v_3)_{x_3} - (\beta v_3)_{x_3+\Delta x_3}\right]$$

And the diffusive flux becomes:

$$\Phi_{dif} = \iint_A -\vartheta(\vec{\nabla}\beta.\vec{n})dA = \Delta x_2 \Delta x_3 \left[\vartheta \frac{\beta_{x_1+\Delta x_1} - \beta_{x_1}}{\Delta x_1} - \vartheta \frac{\beta_{x_1} - \beta_{x_1-\Delta x_1}}{\Delta x_1}\right]$$
$$+\Delta x_1 \Delta x_3 \left[\vartheta \frac{\beta_{x_2+\Delta x_2} - \beta_{x_2}}{\Delta x_2} - \vartheta \frac{\beta_{x_2} - \beta_{x_2-\Delta x_2}}{\Delta x_2}\right]$$
$$+\Delta x_1 \Delta x_2 \left[\vartheta \frac{\beta_{x_3+\Delta x_3} - \beta_{x_3}}{\Delta x_3} - \vartheta \frac{\beta_{x_3} - \beta_{x_3-\Delta x_3}}{\Delta x_3}\right]$$

Summing up and dividing by the volume, i.e. calculating per unit of volume, one gets:

$$\frac{(\beta^{t+\Delta t} - \beta^{t})}{\Delta t} = \frac{1}{\Delta x_1}\left[(\beta v_1)_{x_1} - (\beta v_1)_{x_1+\Delta x_1}\right] + \frac{1}{\Delta x_2}\left[(\beta v_2)_{x_2} - (\beta v_2)_{x_2+\Delta x_2}\right] + \frac{1}{\Delta x_3}\left[(\beta v_3)_{x_3} - (\beta v_3)_{x_3+\Delta x_3}\right]$$

That is an algebraic equation quantifying the rate of change of a property inside a cartesian elementary volume constant in time and with properties uniformly distributed inside the volume and over every face. If we shrink the volume to zero, one gets a partial differential equation.

3.7 Differential form of the evolution equation

The algebraic equation of the last paragraph becomes a partial differential equation if the time step and the spatial step are shrink to zero:

$$lim\left(\frac{(\beta^{t+\Delta t} - \beta^{t})}{\Delta t}\right)_{\Delta t -> 0} = \frac{\partial \beta}{\partial t}$$

And identically for space

$$lim\left(\frac{(\beta v_i)_{x_i} - (\beta v_1)_{x_i+\Delta x_i}}{\Delta x_i}\right)_{\Delta x_i -> 0} = -\frac{\partial \beta v_i}{\partial x_i}$$

$$lim\left(\frac{\vartheta \frac{\beta_{x_i+\Delta x_i} - \beta_{x_i}}{\Delta x_i} - \vartheta \frac{\beta_{x_i} - \beta_{x_i-\Delta x_i}}{\Delta x_i}}{\Delta x_i}\right)_{\Delta x_i -> 0} = \vartheta \frac{\partial^2 \beta}{\partial x_i^2}$$

And we get:

$$\frac{\partial \beta}{\partial t} + \frac{\partial \beta v_i}{\partial x_i} = \vartheta \frac{\partial^2 \beta}{\partial x_i^2} + sources - sinks$$

Considering only incompressible flows (divergence of the velocity null) this equation can be rearranged to get:

$$\frac{\partial \beta}{\partial t} + v_i \frac{\partial \beta}{\partial x_i} = \vartheta \frac{\partial^2 \beta}{\partial x_i^2} + sources - sinks$$

This equation is the advection-diffusion equation written in its the most usual form. Analysing the equation together with the initial integral equation it is easy to understand the physical meaning of the terms. The time derivative is the rate of accumulation in one point. It is null if the problem is stationary. The advective term accounts for the difference between what is arriving at a point and leaving. If the spatial derivative is null what is arriving is equal to what is leaving and this term is null. It is also null if the velocity relative to the point velocity is null, i.e. if there is no movement relative to our reference. The diffusive term is null is the gradient is constant, i.e. if the second derivative is null.

This equation can be written in different forms:

$$\frac{\partial \beta}{\partial t} = -\frac{\partial}{\partial x_i}\left(\beta v_i - \vartheta \frac{\partial \beta}{\partial x_i}\right) + sources - sinks$$

In this form it states that the rate of accumulation at a point is the symmetric of the divergence of the advective plus the diffusive fluxes plus sources-sinks, that put into evidence that the divergence is the difference between what is leaving a point and what is being brought to the point.

Or, using the definition of total derivative:

$$\frac{d\beta}{dt} = \frac{\partial \beta}{\partial t} + v_i \frac{\partial \beta}{\partial x_i}$$

As,

$$\frac{d\beta}{dt} = \frac{\partial}{\partial x_i}\left(\vartheta \frac{\partial \beta}{\partial x_i}\right) + sources - sinks$$

The total derivative is equal to the partial time derivative is the velocity relative to the refence is null. This happens if the reference is moving at the same speed as the flow. In that case there would be no flow entering of leaving our control volume, or saying in a different way, we would be watching always the same fluid (or the same material). This is why the total derivative is also called the “material derivative”

3.8 Lagrangian vs Eulerian reference

The way how we watch the fluid is the difference between the Lagrangian and the Eulerian formulations. In the lagrangian formulation we are observing always the same material, i.e. our reference is moving with the fluid. In the atmosphere this is the case of a balloon and in the water would be the case of a boat with a broken engine. When we describe a flow on a map we are on the Eulerian Formulation. This is the most common, since we do not move with the flow.

In a laboratory, when a biologist studies fish or phytoplankton inside an aquarium (usually called mesocosmos) he is using a Lagrangian system. The walls of the mesocosm use to be in a solid material and consequently there is no diffusive flux across them and thus biologists usually write their equations as:

$$\frac{d\beta}{dt} = sources - sinks$$

And in general they write a system of equation, since the source of a property (e.g. Phytoplankton) is a sink of another property (Nutrients) and the sink of phytoplankton is a source of other variables (e.g. zooplankton detritus, CO2, etc.).

In natural systems nothing is lost. The so called "circular economy" aims to mimetic this feature of the nature, to be sustainable as the natural cycles are.

3.8.1 Boundary and Initial conditions

Partial differential equations relate values of properties to their time and space derivatives. Spatial derivatives relate values of the property in neighbouring points and consequently their evaluation at boundaries require the knowledge of information from outside the studying area: boundary conditions.

From the deduction of our equation it is clear that boundary conditions can be imposed as fluxes (Neumann type) or as imposed values (Dirichlet type). If we know the fluxes we can compute the rate of change of the variable. If we impose the value of the variable we do not need to compute the fluxes. To compute the time derivative, we need initial conditions too. Initial conditions must be specified in terms of property values. On contrary spatial boundary conditions can be specified in terms of values or in terms of their derivatives.

Comparing differential and integral forms of evolution equations shows that imposing boundary conditions in terms of spatial derivatives in differential equations is in fact equivalent to impose fluxes across the boundary in integral equations.

Physically boundaries can be divided into two main groups: solid boundaries and open boundaries. Solid boundaries are impermeable and consequently there is no water flux and no advective transport across them. Diffusive flux across solid boundaries can be neglected for most dissolved substances, but not for momentum, where it is represented by bottom shear stress. In a water body or in the atmosphere, solid matter can be deposited or be eroded from the bottom, resulting into apparent fluxes across that solid boundary.

In tidal flows some regions cover and uncover according to the level of the water. The boundary between covered and uncovered regions is a moving solid boundary and its location must be calculated by the model at each time step.

Open boundaries are artificial boundaries and usually require elaborated formulations. At open boundaries, conditions must be specified using measurements or a larger model. In some cases, they can be estimated using the solution calculated inside the domain (radiative boundaries).