

Environmental Transport and Fate

Chapter 1

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Definitions

Advection, Diffusion

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Concentration

The concentration of a substance, such as sulfur dioxide NO_2 in the air or dissolved oxygen in the water, is defined as the amount of the substance per unit volume of the fluid containing it:

$$c = \frac{\text{amount of substance}}{\text{volume of fluid}} = \frac{m}{V}$$

The amount of the substance is usually taken as its mass.
In that case, the dimensions of c is mass per volume (such kg/m^3 or mg/L).

Sometimes, the amount may be expressed in mass of one of the components (such as sulfur alone, because it may occur in various forms incl. SO_2 and SO_3).

When water is the ambient fluid and chemical reactions occur, it is convenient to express concentrations in moles per volume. The unit is then moles/L, called molarity. [1 mole = 6.02×10^{23} molecules, such that the mass of a mole is exactly the molecular weight followed by the gram unit. *Example:* One mole of SO_2 has a mass of $32 + 2 \times 16 = 64$ g.]



In **air**, which is compressible, concentrations may change not because the mass of the contaminant varies but because the volume of air containing it is modified by a pressure change. To avoid possible ambiguities (in reporting observations or in setting maximum permissible values, for instance), it is good practice to express atmospheric concentrations in

moles of substance per mole of air, or	← most common
in partial pressure, or	← occasional
in mass of substance per mass of air.	← almost never used

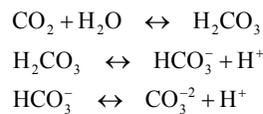
Similarly, in dealing with **soils**, which are subject to compaction, it is preferable to express concentrations in mass of substance per mass of soil. In this context, a further distinction is commonly made between dry and wet soil.

The evaluation of the ratio quantity-per-volume requires the choice of some volume, over which the count is performed. This automatically translates into **averaging** over this volume. If the volume is chosen too small, irrelevant statistical variations arise in the count, which lead to unnecessary and undesirable noise, while if the volume is chosen too large, information is lost by excessive smoothing over space. Therefore, the volume chosen should be neither too small nor too large. In practice, it should be substantially smaller than the domain under consideration but larger than the small-scale turbulent fluctuations chosen to be left unresolved.

If there are several constituents, we introduce one concentration for each:

$$\text{constituent } i \rightarrow c_i = \frac{m_i}{V} \text{ for } i=1, 2, 3, \dots$$

An example is the dissociation of carbon dioxide in water:



while we always have:



This leads to considering the concentrations of the following substances:

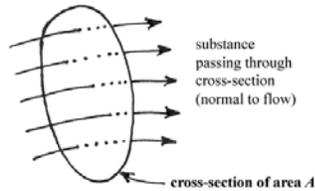


Flux

It is not enough to have a concentration at one place, we also need to know how much of it is being moved from place to place. For this, we define a second quantity, the flux.



A water cascade on the road towards Soda in National Park Stelvio / Sillerspich (Italy).



The flux of a substance in a particular direction is defined as the quantity of that substance passing through a section perpendicular to that direction per unit area and per unit time:

$$\text{flux} = q = \frac{\text{amount that passes through cross - section}}{\text{cross - sectional area} \times \text{time duration}} = \frac{m}{A \Delta t}$$

If the amount is a mass, then the flux q is a rate of mass per area per time, and its units are $\text{kg}/\text{m}^2\text{s}$.

The amount of substance traversing the cross-section over which the count is performed depends on the nature of the transporting process.

If this process is the passive entrainment of the substance by the carrying fluid, then the flux can be easily related to the substance concentration and the fluid velocity, as follows:

$$q = \frac{\text{amount}}{\text{volume of fluid}} \times \frac{\text{volume of fluid}}{\text{area} \times \text{time}} = c u$$

where u is the entraining fluid velocity.

This process is called **ADVECTION**, a term that simply means passive transport by the moving fluid that contains the substance.

Advection is but one process by which a substance can be carried from place to place. Another, important process is **DIFFUSION**, whereby molecular agitation and/or small-scale turbulent motions act to move the substance randomly with respect to the mean motion of fluid.

Denoting this flux by j , we then write:

$$q = \text{advection} + \text{diffusion}$$

$$q = c u + j$$

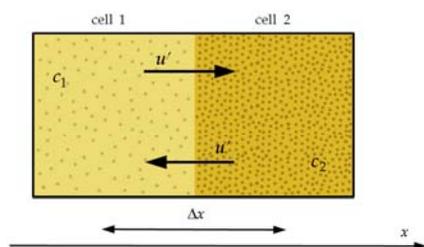
A possible other transport process is **SETTLING**, caused by the vertical motion of particles of the substance through the fluid under the action of gravity.

In this case, the relative velocity of the particles is simply added to the vertical component of the fluid velocity.

Diffusion

Diffusion is the process by which a substance is moved from one place to another under the action of random fluctuations. At the molecular level, the cause is the perpetual agitation of molecules; at the turbulence level, it is advection by the turbulent eddies of the carrying fluid.

Although, we can distinguish molecular diffusion from turbulent diffusion, it remains that in either case the impossibility to describe the details of the motions calls for a statistical approach.



Consider the two-box system on the left and assume that there is no net flow from one box to the other. Thus, the fluctuating flow u' in one direction is compensated by another flow of same magnitude in the opposite direction. The length Δx is taken as the distance between box centers.

A simple budget yields: Net flux from 1 to 2 = flux from 1 to 2 – flux from 2 to 1:

$$j = c_1 u' - c_2 u'$$

$$= -u' (c_2 - c_1) = -u' \Delta c$$

$$j = c_1 u' - c_2 u'$$

$$= -u'(c_2 - c_1) = -u' \Delta c$$

Multiplying and dividing by Δx and taking the limit toward an infinitely small distance, we obtain

$$j = -(u' \Delta x) \frac{\Delta c}{\Delta x} \rightarrow j = -D \frac{dc}{dx}$$

where D is called the diffusion coefficient, or **DIFFUSIVITY**. Its units are m^2/s .

The diffusive flux of substance is thus proportional to the gradient of the concentration. In retrospect, this makes sense; if there were no difference in concentrations between the boxes, the flux from one into the other would be exactly compensated by the flux in the opposite direction yielding no visible transfer; it is the concentration difference (the gradient) that matters. Further, the greater the concentration difference, the larger the imbalance of fluxes, and thus the net flux increases with the gradient.

The above expression is called Fick's law of diffusion and is analogous to Fourier's law of heat conduction. (Heat flows from hot to cold with a flux equal to a conductivity coefficient times the temperature gradient.) The expression 'Fickian diffusion' is sometimes used to imply the above relation.



Adolf Eugen Fick (1829-1901)
 German physiologist
 inventor of contact lenses
 after whom Fick's Law of diffusion is named.

