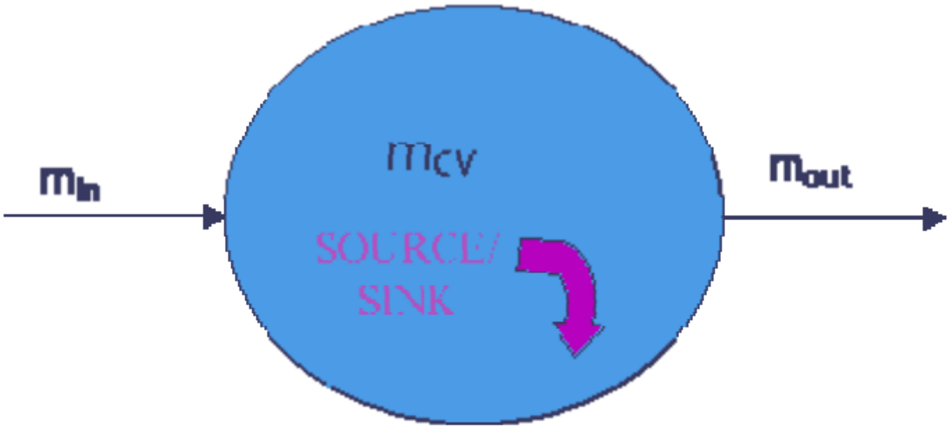
2. Conservation of Mass



This section discusses the law of conservation of mass within a control volume, expressed in both integral and differential forms. Mathematical descriptions of advective and diffusive fluxes into/out of a control volume are shown, the end result being the all-important mass transport equation. The concept of the total derivative is also introduced, allowing us to relate Eulerian (fixed position) and Lagrangian (moving with the flow) perspectives. Two animations further explain the total derivative, showing the temporal temperature change of a probe moving through a spatial temperature gradient. The example problems require application of both forms of the law of conservation of mass to solve transport problems in both industrial and environmental contexts.

2. Conservation of Mass

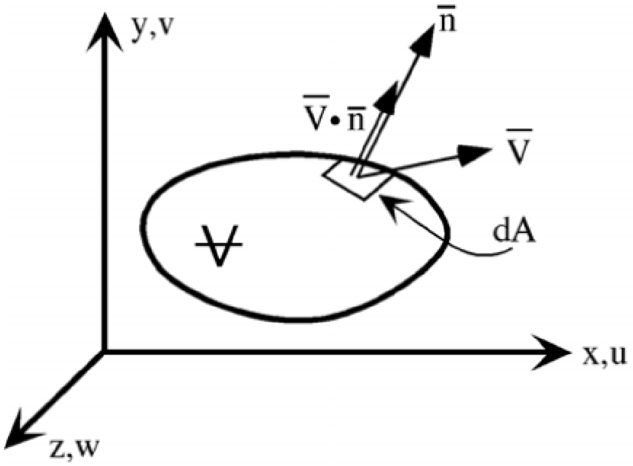
The equation of mass conservation expresses a budget for the addition and removal of mass from a defined region of fluid. Consider a fixed, non-deforming volume of fluid, $\forall$, called the control volume (cv), which has a defined surface boundary, called the control surface (cs). Conservation of mass requires that the time rate of change of mass within the control volume equals the rate at which mass enters the control volume plus the rate at which mass is gained or lost within the control volume due to sources and sinks. A mathematical expression of this law is described below.

Within the control volume there is a distribution of some species defined by the concentration field, C(x,y,z). The total mass within the control volume is

(1) $M = \int_{cv} C \, d\forall$.

M can change over time due to sources and sinks located within the volume, or due to fluxes of mass across the control volume boundaries. In a fluid system there are two forms of mass flux, advection and diffusion. The net flux of mass out of the control volume due to advection is described by the integral,

$$(2) \qquad \int_{cs} C\,\vec{V}\cdot\vec{n}\,dA.$$



Here, $\vec{V} = (u,v,w)$ is the velocity vector and $\vec{n}$ is the outward pointing normal for surface segment dA. $\vec{V}\cdot\vec{n}$ represents the velocity component perpendicular to the area segment dA. The definition of $\vec{n}$ as the outward facing normal makes (2) the net flux out of $\forall$. That is, flow out of $\forall$ (same direction as $\vec{n}$) contributes positively to the integral, and flows into $\forall$ (opposite to $\vec{n}$) contribute negatively. The net flux out of the control volume due to diffusion is defined using Fick's Law.

$$(3) \qquad -\int_{cs} D_n \frac{\partial C}{\partial n} dA,$$

Note that the concentration gradients are defined along the axis $\vec{n}$, *i.e.* everywhere perpendicular to the surface, and position outward. Denoting D_n as the diffusion coefficients along the axis $\vec{n}$ allows for anisotropy in D. For molecular diffusion and/or isotropic turbulence D is not a function of direction and the subscript may be dropped. The final mathematical expression for conservation of mass combines (1), (2), and (3).

Conservation of Mass in Integral (Control Volume) Form

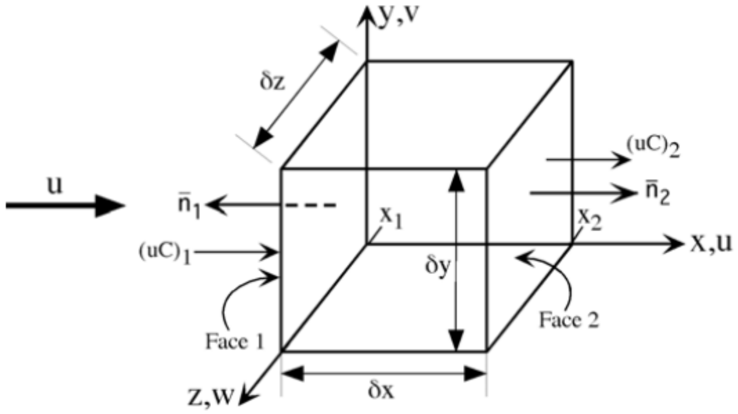
(4) $$\underbrace{\frac{\partial}{\partial t}\int_{cv} C\, d\forall}_{\text{time rate of change of mass within cv}} = \underbrace{-\int_{cs} C\,\vec{V}\cdot\vec{n}\,dA}_{\text{advective flux into control volume}} + \underbrace{\int_{cs} D_n \frac{\partial C}{\partial n} dA}_{\text{diffusive flux into control volume}} \quad \underbrace{\pm S}_{\text{source sink}}$$

Differential Form of Conservation of Mass

The differential form of conservation of mass is derived by evaluating (4) for an infinitely small, cubic volume. The volume is sufficient small that we assume the concentration within the volume is essential uniform. The volume is rigid, so that the dimensions ∂x, ∂y, and ∂z are constant. The two surface integrals (terms 2 and 3 in (4)) reduce to a sum of fluxes across each of the six cube faces.

(5) $$\frac{\partial C}{\partial t}\partial\forall = \sum_{i=1}^{6}\left[-C\vec{V}\cdot\vec{n}dA + D_n\frac{\partial C}{\partial n}dA\right]_i \pm S$$

As an example, consider fluxes in the x-direction across the faces numbered 1 and 2, and located at $x = x_1$ and x_2, respectively.



On face 1 $\vec{n}$ points in the negative x direction, such that $\vec{V}\cdot\vec{n} = -u$, and $\partial C/\partial n = -\partial C/\partial x$. The evaluation of the surface integral for face 1 is then,

(6) Flux across 1 = $(uC)_1\,\partial y\partial z - (D_x\,\partial C/\partial x)_1\,\partial y\partial z$.

Similarly for face 2, but noting that $\vec{n}$ points in the positive x direction,

(7) Flux across 2 = $-(uC)_2\,\partial y\partial z + (D_x\,\partial C/\partial x)_2\,\partial y\partial z$

The net x-direction flux into the control volume is the sum of (6) and (7).

(8) Net flux in x = $(\,(uC)_1 - (uC)_2 - (D_x\,\partial C/\partial x)_1 + (D_x\,\partial C/\partial x)_2\,)\partial y\partial z$.

If we assume that C, u, $\partial C/\partial x$, and D_x are continuous functions of x, a Taylor expansion may be used to express each parameter at x_2 as a function of the same parameter at x_1.

(9) $$(uC)_2 = (uC)_1 + \frac{\partial}{\partial x}(uC)\,\partial x + \text{higher order terms}$$

(10) $$(D_x\frac{\partial C}{\partial x})_2 = (D_x\frac{\partial C}{\partial x})_1 + \frac{\partial}{\partial x}(D_x\frac{\partial C}{\partial x})\,\partial x + \text{higher order terms.}$$

If we drop the higher order terms and replace $(uC)_2$ and $(D_x\partial C/\partial x)_2$ in (8) with the expressions in (9) and (10), then (8) becomes,

(11) $$\text{Net flux in x} = \left[-\frac{\partial uC}{\partial x} + \frac{\partial}{\partial x}D_x\frac{\partial C}{\partial x}\right]\partial x\partial y\partial z.$$

Similar expressions can be found for flux across the remaining four faces. Combining these in (5) and noting $\partial \text{V} = \partial x\partial y\partial z$,

Conservation of Mass in Differential Form

(12) $$\frac{\partial C}{\partial t} = -\frac{\partial uC}{\partial x} - \frac{\partial vC}{\partial y} - \frac{\partial wC}{\partial z} + \frac{\partial}{\partial x}D_x\frac{\partial C}{\partial x} + \frac{\partial}{\partial y}D_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial z}D_z\frac{\partial C}{\partial z} \pm S.$$

This expression can be simplified under the following conditions.
First, consider the expansion of the advective fluxes in (12),

(13) $$\frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial wC}{\partial z} = \left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right]C + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}$$

If the flow field is incompressible, then from continuity

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0.$$

This eliminates the bracketed term in (13). Thus, conservation of mass for incompressible flow may be expressed as follows. By convention, advective terms are brought to the left.

Conservation of Mass for Incompressible Flow

(14) $$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}D_x\frac{\partial C}{\partial x}+\frac{\partial}{\partial y}D_y\frac{\partial C}{\partial y}+\frac{\partial}{\partial z}D_z\frac{\partial C}{\partial z}\pm S$$

Furthermore, when the coefficients of diffusion are homogeneous, $D_i \neq f(x, y, \text{or } z)$,

(14a) $$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=+D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}+D_z\frac{\partial^2 C}{\partial z^2}\pm S.$$

If the diffusion coefficients are additionally isotropic, $D_x = D_y = D_z$, then

(14b) $$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=D\left[\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}+\frac{\partial^2 C}{\partial z^2}\right]\pm S.$$

For laminar flow molecular diffusion controls the diffusive flux. In general, molecular diffusion is both homogeneous and isotropic, such that (14b) is appropriate for laminar flow. For turbulent flow turbulent transport dominates the diffusive flux. Commonly the turbulence field is both heterogeneous and anisotropic and the diffusion coefficients will be as well.

2.1. Material Derivative

Fluid motion and any constituent (temperature, concentration) transported by fluid motion can be described from two frames of reference, one which is stationary or one which is moving along with the flow. In the *Eulerian* perspective, the flow and its scalar constituents are described with respect to fixed spatial positions, $\vec{X}$=(x,y,z) and with respect to time (t), and are written, e.g. $\vec{V}(\vec{X},t)$ and $C(\vec{X},t)$. In the *Lagrangian* perspective moves with the flow, and traces the history of individual fluid particles. Unlike the Eulerian description, in which spatial position is a fixed reference, in the

Lagrangian perspective, the spatial position is another variable of the particle. The flow variables are written with respect to time (t) and to a single, initial reference position, *e.g.* $\vec{X}_0$ the particle position at t = 0, such that the variables are recorded as $\vec{X}(\vec{X}_0, t)$ and $C\,(\vec{X}_0, t)$.

The Eulerian perspective is generally easier to represent, and therefore is more common in analysis and flow description. However, the physics and transport of flow are more fundamentally related to the Lagrangian perspective. For example, the Navier-Stokes equations essentially represent Newton's Second Law ($\vec{F} = m\vec{a}$) applied to fluid particles. For transport problems, *e.g.*, tracking the evolution of a phytoplankton patch as is grows (source), is preyed upon (sink) and diffuses, one again sees the conceptual advantage of a Lagrangian perspective - predicting concentration following the patch. Because both perspectives are important, it is important to understand how they are related.

Consider F(x,y,z,t) to be any variable of the flow described in terms of fixed Eulerian coordinates, (x, y, z). We wish to relate this description to a Lagrangian perspective, specifically to describe the rate of change in F observed while following an individual particle through the flow. First, we can describe a change in F, namely dF, due to a small change in spatial position ($d\vec{X}$) and/or time (dt), as

$$(15) \qquad dF = \frac{\partial F}{\partial t}dt + \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy + \frac{\partial F}{\partial z}dz.$$

Next, we constrain the increments dt and $d\vec{X}$ such that they follow the trajectory of an individual particle, specifically, dx = u dt, dy=v dt, and dz=w dt. Then (15) becomes,

$$(16) \qquad dF = \frac{\partial F}{\partial t}dt + u\frac{\partial F}{\partial x}dt + v\frac{\partial F}{\partial y}dt + w\frac{\partial F}{\partial z}dt.$$

Dividing by dt produces a derivative that represents the rate of change in F observed when following the trajectory of a fluid particle. To emphasize this special definition the derivative is given the notation DF/Dt, i.e.

$$(17) \qquad \frac{DF}{Dt} = \frac{\partial F}{\partial t} + u\frac{\partial F}{\partial x} + v\frac{\partial F}{\partial y} + w\frac{\partial F}{\partial z}.$$

The notation DF/Dt is called the material derivative (also the particle derivative, the substantial derivative, and the total derivative) to emphasize that it is taken following a fluid particle. The material derivative has two parts. First, $\partial F/\partial t$, called the local derivative, represents the rate of change at any fixed point. For steady flow, $\partial/\partial t = 0$. The remaining terms, $u\partial F/\partial x + v\partial F/\partial y + w\partial F/\partial z$, are called the advective derivative, because they record changes in F which arise as the fluid element advects through a spatial gradients in F. The following animations help to demonstrate the material derivative.

Steady Temperature Field: This animation shows a one-dimensional system with a spatial gradient of temperature, T(x). A temperature probe (white dot) moves with the flow, making a Lagrangian observation. The probe records the material (total) derivative, which in one dimension is,

$$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x}. \tag{18}$$

Probes located at the fixed positions A, B, and C make Eulerian observations. They show a steady temperature field, *i.e.* $\partial T/\partial t = 0$, such that the material derivative is equal to the advective derivative, $DT/Dt = u\, \partial T/\partial x$. This is quantified in the lower right corner of the animation. The temperature field shown here could result from a steady, uniform flow through a heating element. The temperature of the fluid rises steadily as heat is added along the flow path.

Unsteady Temperature Field: This animation shows a one-dimensional system with an unsteady temperature field, T(x, t). One temperature probe is moving with the flow (white dot) at velocity u, and it records the material derivative given in (18). Three additional probes are located at the fixed positions A, B, and C. These probes record the local derivative, $\partial T/\partial t$, which is non-zero (unsteady), but is the same at each position. The value of each derivative is given in the lower right hand corner.

Steady, Spatially Accelerating Flow in a Pipe: In this animation, flow through a pipe accelerates downstream as the pipe cross-section decreases, *i.e.* $\partial u/\partial x > 0$. Three probes measuring the flow at fixed positions, A, B, and C, show that the flow is steady, $\partial u/\partial t = 0$ at every position. Another velocity probe is moving with the flow (blue dot) and records the material (total) derivative, Du/Dt. Within each section of the pipe, $Du/Dt = 0$, as shown by the blue trace in the Velocity vs. Time graph. At the step changes in cross-sectional area, the fluid locally accelerates, $\partial u/\partial x > 0$, and at these positions $Du/Dt = u\, \partial u/\partial x$.

What is the mean velocity in this system? From the perspective of transport, the best definition of mean velocity is a Lagrangian definition, *i.e.* the mean velocity experienced by a probe moving with the flow. The probe takes 109 seconds to traverse the pipe which is 90-m in length. This gives a velocity of $90/109 = 0.83\ \mathrm{ms}^{-1}$. One is tempted to define a mean Eulerian velocity based on the spatial average of the velocity within the three sections. As the segment lengths are equal within this one-dimensional system, the average is straightforward, $(0.50 + 0.89 + 2.0)/3 = 1.13$ m/s. This value is meaningless, however, from the perspective of transport, because it does not predict the travel time through the system, *i.e.* $90\text{-m}/1.13\text{-ms}^{-1} = 80\ \mathrm{s} \neq 109\ \mathrm{s}$.

CLASS EXERCISE (WITH SOLUTION)

Problem 1

Many water bodies have problems with anoxia, low levels of dissolved oxygen (DO) in the water column due to phytoplankton respiration. Lake Monger in Western Australia is one such water body. A colleague asks you to predict DO profiles in the lake to determine whether anoxia will occur. Prelimary investigations reveal that there are negligible horizontal gradients of DO across the lake. However, the competing effects of oxygen consumption by phytoplankton and reaeration from the surface cause significant vertical gradients of DO.

(a) Assuming steady-state conditions, derive the governing equation for the vertical (z) profile of dissolved oxygen from equation 14b in the theory. Also assume that the phytoplankton represent a first-order oxygen sink (i.e. the rate of consumption of dissolved oxygen is proportional to its concentration in the water, with constant of proportionality = k). Vertical flows in the lake can also be assumed to be insignificant.

(b) Find the solution to this equation, subject to the following boundary conditions:

- reaeration at the surface ($z = 0$) keeps the water at the surface saturated with dissolved oxygen at a concentration of 8 mg/L.
- the sediments ($z = -10\,m$) are sufficiently impermeable and abiotic to represent a no-flux boundary for dissolved oxygen.

Use typical values of $D = 0.1\,cm^2/s$ and $k = 0.05\,day^{-1}$ (which corresponds to high phytoplankton levels).

(c) Where in the water column would you expect the lowest concentration of DO?

(d) Your colleague tells you that DO concentrations below 1 mg/L are considered dangerous. Determine whether Lake Monger will have dangerously low levels of dissolved oxygen. What if eutrophication increase the phytoplankton population, such that $k = 0.1\,day^{-1}$?

CLASS EXERCISE – SOLUTION

(a) The general equation (14b) is

$$\underset{(1)}{\frac{\partial C}{\partial t}} + \underset{(2)}{u\frac{\partial C}{\partial x}} + \underset{(3)}{v\frac{\partial C}{\partial y}} + \underset{(4)}{w\frac{\partial C}{\partial z}} = D[\underset{(5)}{\frac{\partial^2 C}{\partial x^2}} + \underset{(6)}{\frac{\partial^2 C}{\partial y^2}} + \underset{(7)}{\frac{\partial^2 C}{\partial z^2}}] \quad \underset{(8)}{\pm S}$$

We can eliminate several terms in this equation:

(1) because we are looking at steady-state conditions,

(2), (3), (5) and (6) due to the negligible horizontal gradients of DO concentration and

(4) due to the insignificant vertical flows.

Thus, the equation reduces to

$$0 = D\left[\frac{\partial^2 C}{\partial z^2}\right] - S$$

noting that phytoplankton are a sink of dissolved oxygen. For first-order removal, $S = kC$, so our governing equation is:

$$D\left[\frac{\partial^2 C}{\partial z^2}\right] - kC = 0$$

(b) The general solution to this governing equation is:

$$C(z) = Aexp\left(z\sqrt{\frac{k}{D}}\right) + Bexp\left(-z\sqrt{\frac{k}{D}}\right)$$

where A and B are constants. We use our boundary conditions to determine A and B.

- $C|_{z=0} = 8 \Rightarrow A + B = 8$
- No flux at $z = -10\,m \Rightarrow \left.\frac{\partial C}{\partial z}\right|_{z=-10} = 0.$

Therefore,

$$A\sqrt{\frac{k}{D}}exp\left((-10\,m)\sqrt{\frac{k}{D}}\right) - B\sqrt{\frac{k}{D}}exp\left(-(-10\,m)\sqrt{\frac{k}{D}}\right) = 0$$

$$\Rightarrow Aexp\left((-10\,m)\sqrt{\frac{k}{D}}\right) = Bexp\left((10\,m)\sqrt{\frac{k}{D}}\right).$$

Using our values for k and D,

$$\sqrt{\frac{k}{D}} = \sqrt{\frac{0.05\,day^{-1}}{0.1\,cm^2s^{-1}}} = \sqrt{\frac{5.787\times10^{-7}\,s^{-1}}{10^{-5}\,m^2s^{-1}}} = 0.240/m$$

Therefore, from our second boundary condition,

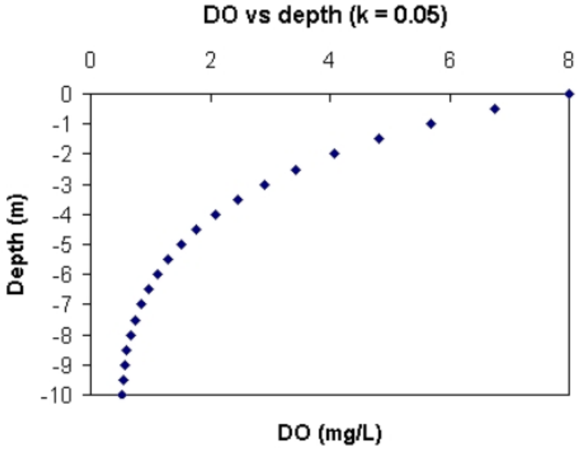
$$Aexp\,(-2.4) = Bexp(2.4) \Rightarrow 0.091A = 11.0B \Rightarrow A = 121.5B$$

Solving the boundary condition equations simultaneously gives A = 7.935, B = 0.065.

Therefore,

$$C(z) = 7.935exp(0.240z) + 0.065exp(-0.240z) \quad \text{[for z in meters]}$$

(c) As we have only a DO sink in the water column, the lowest concentration of DO will be found at the point furthest from the surface, which is maintained at a constant concentration. Thus, we expect the DO concentration to be lowest at z = -10 m. This is confirmed by looking at the plot of the vertical profile of DO in the water column (note that we have satisfied both boundary conditions).



(d) As we can see from the above plot, $C_{min} = 1.4\,mg/L$. However, if $k = 0.1\,day^{-1}$, repetition of the above calculation yields a minimum concentration of approximately $0.5\,mg/L$, meaning the the health of Lake Monger is under threat.