Environmental Transport and Fate

# Chapter 2 – Diffusion – Part 4: Generalization to 3D

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Although the analysis of one-dimensional problems can find applications to spatially elongated systems that, in first approximation, may be modeled as one-dimensional (such as a pipe or a river), it remains that most engineering problems are two- or three-dimensional. We therefore need to extend our previous analysis to higher dimensions.

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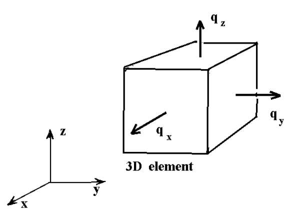
For the time being, let us continue to assume that there is no mean fluid velocity, namely there is no advective component and the flux of substance is purely diffusive. The difference from the previous sections is that diffusion is now regarded as proceeding in all three directions of space. The flux quantity has three components (east-west, north-south and up-down) and is a vector. Thus,

$$\vec{q} = (q_x, q_y, q_z)$$

Similar arguments as those outlined previously can be replayed here to obtain:

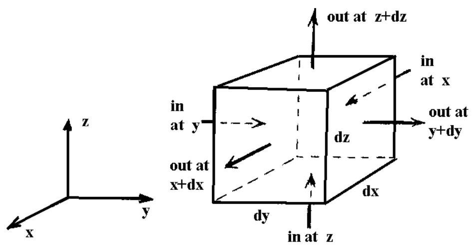



$$q_x = -D\frac{\partial c}{\partial x}, \quad q_y = -D\frac{\partial c}{\partial y}, \quad q_z = -D\frac{\partial c}{\partial z}$$

$$\vec{q} = -D\left(\frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}, \frac{\partial c}{\partial z}\right)$$

$$\vec{q} = -D\vec{\nabla} c$$

Budget in three dimensions




Rate of accumulation =
Σ imports + Σ exports

$$\frac{\partial}{\partial t}(c\ dxdydz) = \left(q_x \text{ at } x\right) dydz - \left(q_x \text{ at } x+dx\right) dydz$$
$$+\left(q_y \text{ at } y\right) dxdz - \left(q_y \text{ at } y+dy\right) dxdz$$
$$+\left(q_z \text{ at } z\right) dxdy - \left(q_z \text{ at } z+dz\right) dxdy$$

$$dxdydz \frac{\partial c}{\partial t} = -\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right) dxdydz \longrightarrow \frac{\partial c}{\partial t} = -\vec{\nabla}\cdot\vec{q}$$

With $q_x = -D\dfrac{\partial c}{\partial x}, \quad q_y = -D\dfrac{\partial c}{\partial y}, \quad q_z = -D\dfrac{\partial c}{\partial z}$

$\vec{q} = -D\vec{\nabla}c$

the preceding budget yields the following equation governing the 3D concentration:

$$\boxed{\begin{aligned} \frac{\partial c}{\partial t} &= D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right) \\ \frac{\partial c}{\partial t} &= D\vec{\nabla}\cdot(\vec{\nabla}c) = D\nabla^2 c \end{aligned}}$$

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Nomenclature:

$$\vec{\nabla}* = \left(\frac{\partial *}{\partial x}, \frac{\partial *}{\partial y}, \frac{\partial *}{\partial z}\right) = \text{gradient of scalar } *$$

$$\vec{\nabla}\cdot\vec{*} = \frac{\partial *_x}{\partial x} + \frac{\partial *_y}{\partial y} + \frac{\partial *_z}{\partial z} = \text{divergence of vector } \vec{*}$$

$$\nabla^2 * = \frac{\partial^2 *}{\partial x^2} + \frac{\partial^2 *}{\partial y^2} + \frac{\partial^2 *}{\partial z^2} = \text{Laplacian of } *$$

## Prototypical solution at 3D

It is straightforward to verify that the product of three prototypical solutions at 1D forms the 3D solution for the case of an instantaneous (at $t = 0$) and localized (at $x = y = z = 0$) release:

$$c(x,y,z,t) = \frac{M}{\left(\sqrt{4\pi\, Dt}\right)^3} \exp\left( -\frac{x^2+y^2+z^2}{4Dt} \right)$$

in which $M$ is the mass released.

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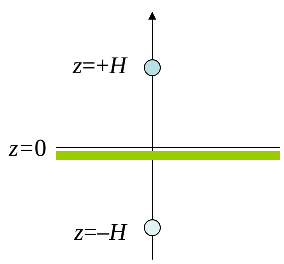
<u>Note</u>: Solution at 2D is

$$c(x,y,t) = \frac{M}{\left(\sqrt{4\pi\, Dt}\right)^2} \exp\left( -\frac{x^2+y^2}{4Dt} \right)$$

in which $M$ is the mass released per length of missing dimension $z$.

## Presence of an impermeable boundary

Such as a horizontal boundary




If the boundary is at z = 0 and the release at z = +H, an image is necessary at z = –H, to render the flux at the boundary equal to zero.

The solution is thus:

$$c(x,y,z,t) = \frac{M}{\left(\sqrt{4\pi\, Dt}\right)^3} \exp\left( -\frac{x^2+y^2}{4Dt} \right) \left[ \exp\left( -\frac{(z-H)^2}{4Dt} \right) + \exp\left( -\frac{(z+H)^2}{4Dt} \right) \right]$$

Some algebra leads to:

Maximum concentration at ground $c_{\text{max center ground}} = 0.1472 \dfrac{M}{H^3}$

which occurs at $t_{\max} = \dfrac{H^2}{6D}$