DERIVATION OF BASIC TRANSPORT EQUATION
Definitions

Basic dimensions

\[ [M] \rightarrow \text{Mass} \]
\[ [L] \rightarrow \text{Length} \]
\[ [T] \rightarrow \text{Time} \]

Concentration

\[ \text{Mass per unit volume} \]
\[ [M \cdot L^{-3}] \]

Mass Flow Rate

\[ \text{Mass per unit time} \]
\[ [M \cdot T^{-1}] \]

Flux

\[ \text{Mass flow rate through unit area} \]
\[ [M \cdot L^{-2} \cdot T^{-1}] \]
The Transport Equation

Mass balance for a control volume where the transport occurs only in one direction (say x-direction)

*Mass entering the control volume* \rightarrow \text{Control Volume} \rightarrow \text{Mass leaving the control volume}

\[ \Delta x \]

Positive x direction
The mass balance for this case can be written in the following form

\[ V \frac{\partial C}{\partial t} = A \cdot J_1 - A \cdot J_2 \]  

Equation 1
The Transport Equation

A closer look to Equation 1

\[ V \cdot \frac{\partial C}{\partial t} = A \cdot J_1 - A \cdot J_2 \]

Volume [L^3] \quad Concentration over time [M \cdot L^{-3} \cdot T^{-1}]

Area [L^2] \quad Flux [M \cdot L^{-2} \cdot T^{-1}]

Area [L^2] \quad Flux [M \cdot L^{-2} \cdot T^{-1}]

\[ [L^3] \cdot [M \cdot L^{-3} \cdot T^{-1}] = [M \cdot T^{-1}] \]

Mass over time

\[ [L^2] \cdot [M \cdot L^{-2} \cdot T^{-1}] = [M \cdot T^{-1}] \]

Mass over time
The Transport Equation

Change of mass in unit volume (divide all sides of Equation 1 by the volume)

$$\frac{\partial C}{\partial t} = \frac{A}{V} \cdot J_1 - \frac{A}{V} \cdot J_2$$  \hspace{1cm} \text{Equation 2}

Rearrangements

$$\frac{\partial C}{\partial t} = \frac{A}{V} \cdot (J_1 - J_2)$$  \hspace{1cm} \text{Equation 3}
The Transport Equation

The flux is changing in x direction with gradient of $\frac{\partial J}{\partial x}$

Therefore

$$J_2 = J_1 + \frac{\partial J}{\partial x} \cdot \Delta x$$

Equation 4
The Transport Equation

\[ \frac{\partial C}{\partial t} = \frac{A}{V} \cdot \left( J_1 - J_2 \right) \]  
\[ \text{Equation 3} \]

\[ J_2 = J_1 + \frac{\partial J}{\partial x} \cdot \Delta x \]  
\[ \text{Equation 4} \]

\[ \frac{\partial C}{\partial t} = \frac{A}{V} \cdot \left( J_1 - \left( J_1 + \frac{\partial J}{\partial x} \cdot \Delta x \right) \right) \]  
\[ \text{Equation 5} \]
The Transport Equation

Rearrangements

\[
\frac{\partial C}{\partial t} = \frac{A}{V} \cdot \left( J_1 - \left( J_1 + \frac{\partial J}{\partial x} \cdot \Delta x \right) \right)
\]

Equation 5

\[
\frac{V}{A} = \Delta x \implies \frac{A}{V} = \frac{1}{\Delta x}
\]

Equation 6

\[
\frac{\partial C}{\partial t} = \frac{1}{\Delta x} \cdot \left( J_1 - J_1 - \frac{\partial J}{\partial x} \cdot \Delta x \right)
\]

Equation 7
The Transport Equation

Rearrangements

\[ \frac{\partial C}{\partial t} = \frac{1}{\Delta x} \cdot \left( J_1 - J_1 - \frac{\partial J}{\partial x} \cdot \Delta x \right) \]

Equation 7

Finally, the most general transport equation in x direction is:

\[ \frac{\partial C}{\partial t} = - \frac{\partial J}{\partial x} \]

Equation 8
The Transport Equation

We are living in a 3 dimensional space, where the same rules for the general mass balance and transport are valid in all dimensions. Therefore

\[
\frac{\partial C}{\partial t} = - \sum_{i=1}^{3} \frac{\partial}{\partial x_i} J_i \\
\begin{align*}
x_1 &= x \\
x_2 &= y \\
x_3 &= z
\end{align*}
\]

Equation 9

\[
\frac{\partial C}{\partial t} = - \left( \frac{\partial}{\partial x} J_x + \frac{\partial}{\partial y} J_y + \frac{\partial}{\partial z} J_z \right)
\]

Equation 10
The Transport Equation

• The transport equation is derived for a conservative tracer (material)
• The control volume is constant as the time progresses
• The flux (J) can be anything (flows, dispersion, etc.)
The Advective Flux
The advective flux can be analyzed with the simple conceptual model, which includes two control volumes. **Advection occurs only towards one direction in a time interval.**
$\Delta x$ is defined as the distance, which a particle can pass in a time interval of $\Delta t$. The assumption is that the particles move on the direction of positive x only.
The number of particles (analogous to mass) moving from control volume I to control volume II in the time interval $\Delta t$ can be calculated using the Equation below, where

$$Q = C \cdot \Delta x \cdot A$$

Equation 11

where $Q$ is the number of particles (analogous to mass) passing from volume I to control volume II in the time interval $\Delta t$ [M], $C$ is the concentration of any material dissolved in water in control volume I [M·L$^{-3}$], $\Delta x$ is the distance [L] and $A$ is the cross section area between the control volumes [L$^2$].
Number of particles passing from I to II in $\Delta t$

$$Q = C \cdot \Delta x \cdot A$$

Division by time:

$$\frac{Q}{\Delta t} = \frac{C \cdot \Delta x \cdot A}{\Delta t}$$

Number of particles passing from I to II in unit time

Division by cross-section area:

$$\frac{Q}{A \cdot \Delta t} = J_{ADV} = \frac{\Delta x}{\Delta t} \cdot C$$

Number of particles passing from I to II in unit time per unit area = FLUX

$$J_{ADV} = \lim_{\Delta t \to 0} \left( \frac{\Delta x}{\Delta t} \cdot C \right) = \frac{\partial x}{\partial t} \cdot C$$

Advective flux

Equation 12
The Advection Flux

\[ J_{\text{ADV}} = \frac{\partial X}{\partial t} \cdot C \]  

Equation 12
The Dispersive Flux
The dispersive flux can be analyzed with the simple conceptual model too. This conceptual model also includes two control volumes. **Dispersion occurs towards both directions in a time interval.**
$\Delta x$ is defined as the distance, which a particle can pass in a time interval of $\Delta t$. The assumption is that the particles move on positive and negative $x$ directions. In this case there are two directions, which particles can move in the time interval of $\Delta t$. 

![Diagram showing two regions I and II with particles moving in both directions](image)
Another assumption is that a particle does not change its direction during the time interval of $\Delta t$ and that the probability to move to positive and negative $x$ directions are equal (50%) for all particles.

Therefore, there are two components of the dispersive mass transfer, one from the control volume I to control volume II and the second from the control volume II to control volume I.
\begin{align*}
q_1 &= 0.5 \cdot C_1 \cdot \Delta x \cdot A \quad \text{Equation 13} \\
q_2 &= 0.5 \cdot C_2 \cdot \Delta x \cdot A \quad \text{Equation 14} \\
Q &= q_1 - q_2 \quad \text{Equation 15} \\
Q &= 0.5 \cdot \Delta x \cdot A \left( C_1 - C_2 \right) \quad \text{Equation 16}
\end{align*}
Number of particles passing from I to II in $\Delta t$

$$Q = 0.5 \cdot \Delta x \cdot A \cdot (C_1 - C_2)$$

Equation 16

$$\frac{Q}{\Delta t} = \frac{0.5 \cdot \Delta x \cdot A \cdot (C_1 - C_2)}{\Delta t}$$

Equation 17

$$C_2 = C_1 + \frac{\partial C}{\partial x} \cdot \Delta x$$

Equation 18

$$\frac{Q}{A \cdot \Delta t} = J_{DISP} = \frac{-0.5 \cdot \Delta x \cdot \frac{\partial C}{\partial x} \cdot \Delta x}{\Delta t}$$

Equation 22

Number of particles passing from I to II in unit time per unit area = FLUX

Divide by time

Number of particles passing from I to II in unit time

$$\frac{Q}{\Delta t} = 0.5 \cdot \Delta x \cdot A \cdot \left( C_1 - \left( C_1 + \frac{\partial C}{\partial x} \cdot \Delta x \right) \right)$$

Equation 19

Divide by Area

$$\frac{Q}{\Delta t} = \frac{0.5 \cdot \Delta x \cdot A \cdot \left( C_1 - C_1 - \frac{\partial C}{\partial x} \cdot \Delta x \right)}{\Delta t}$$

Equation 20

$$\frac{Q}{\Delta t} = -0.5 \cdot \Delta x \cdot A \frac{\partial C}{\partial x} \cdot \Delta x$$

Equation 21
\[
\frac{Q}{A \cdot \Delta t} = J_{\text{DISP}} = \frac{-0.5 \cdot \Delta x \cdot \frac{\partial C}{\partial x} \cdot \Delta x}{\Delta t}
\]

Equation 22

\[
J_{\text{DISP}} = -\frac{0.5 \cdot (\Delta x)^2}{\Delta t} \cdot \frac{\partial C}{\partial x}
\]

Equation 23

\[
D = \frac{0.5 \cdot (\Delta x)^2}{\Delta t}
\]

Equation 24

\[
J_{\text{DISP}} = -D \cdot \frac{\partial C}{\partial x}
\]

Equation 25
Dispersion

Generally:
Molecular diffusion $\ll$ Turbulent diffusion $\ll$ Longitudinal dispersion
Ranges of the Dispersion Coefficient ($D$)
The Dispersive Flux

\[ J_{\text{DISP}} = -D \cdot \frac{\partial C}{\partial x} \]

Equation 25
THE ADVECTION-DISPERSION EQUATION FOR A CONSERVATIVE MATERIAL
The Advection-Dispersion Equation

\[ \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} J \]
Equation 8

\[ J_{\text{advection}} = \frac{\partial x}{\partial t} \cdot C \]
Equation 12

\[ J_{\text{dispersion}} = -D \cdot \frac{\partial C}{\partial x} \]
Equation 25

\[ J = J_{\text{advection}} + J_{\text{dispersion}} \]
Equation 26

\[ \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left( J_{\text{advection}} + J_{\text{dispersion}} \right) \]
Equation 27
The Advection-Dispersion Equation

\[
\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left( J_{\text{advection}} + J_{\text{dispersion}} \right) \tag{Equation 27}
\]

\[
\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} J_{\text{advection}} - \frac{\partial}{\partial x} J_{\text{dispersion}} \tag{Equation 28}
\]

\[
J_{\text{advection}} = \frac{\partial x}{\partial t} \cdot C
\]

\[
J_{\text{dispersion}} = -D \cdot \frac{\partial C}{\partial x}
\]

\[
\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left( \frac{\partial x}{\partial t} \cdot C \right) - \frac{\partial}{\partial x} \left( -D \cdot \frac{\partial C}{\partial x} \right) \tag{Equation 29}
\]
The Advection-Dispersion Equation

\[ \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left( \frac{\partial x}{\partial t} \cdot C \right) - \frac{\partial}{\partial x} \left( -D \cdot \frac{\partial C}{\partial x} \right) \]

Equation 29

Velocity \( u \) in \( x \) direction

\[ u \cdot \frac{\partial C}{\partial x} \]

\[ -D \cdot \frac{\partial^2 C}{\partial x^2} \]

\[ \frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D \cdot \frac{\partial^2 C}{\partial x^2} \]

Equation 30
Dimensional Analysis of the Advection-Dispersion Equation

\[
\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D \cdot \frac{\partial^2 C}{\partial x^2}
\]

Equation 30

Concentration over time

Velocity times concentration over space

\[ [L^2 \cdot T^{-1}] \cdot [M \cdot L^{-3} \cdot L^{-2}] \]

\[ = [M \cdot L^{-3} \cdot T^{-1}] \]
The Advection-Dispersion Equation

We are living in a 3 dimensional space, where the same rules for the general mass balance and transport are valid in all dimensions. Therefore

$$\frac{\partial C}{\partial t} = \sum_{i=1}^{3} \left( -u_i \cdot \frac{\partial C}{\partial x_i} + D_i \cdot \frac{\partial^2 C}{\partial x_i^2} \right) \quad x_1 = x, \ u_1 = u, \ D_1 = D_x$$

$$x_2 = y, \ u_2 = v, \ D_2 = D_y$$

$$x_3 = z, \ u_3 = w, \ D_3 = D_z$$

Equation 31

$$\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} + D_y \cdot \frac{\partial^2 C}{\partial y^2} - w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2}$$

Equation 32
THE ADVECTION-DISPERSION EQUATION FOR A NON CONSERVATIVE MATERIAL
The Advection-Dispersion Equation for non conservative materials

\[
\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} + D_y \cdot \frac{\partial^2 C}{\partial y^2} - w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2}
\]

Equation 32

\[
\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} + D_y \cdot \frac{\partial^2 C}{\partial y^2}
\]

\[
- w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2} + \sum k \cdot C
\]

Equation 33
The Transport Equation for non-conservative materials with sedimentation

\[ \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + D_x \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial y} + D_y \frac{\partial^2 C}{\partial y^2} + w \frac{\partial C}{\partial z} + D_z \frac{\partial^2 C}{\partial z^2} + \sum k \cdot C \]

Equation 33

\[ \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + D_x \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial y} + D_y \frac{\partial^2 C}{\partial y^2} - w \frac{\partial C}{\partial z} + D_z \frac{\partial^2 C}{\partial z^2} + \sum k \cdot C - \nu_{\text{sedimentation}} \frac{\partial C}{\partial z} \]

Equation 34
Transport Equation with all Components

\[
\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} + D_y \cdot \frac{\partial^2 C}{\partial y^2} + \sum k \cdot C - \psi_{\text{sedimentation}} \cdot \frac{\partial C}{\partial z}
\]

- External loads
- Interaction with bottom
- Other sources and sinks
Dimensional Analysis of Components

\[
\left( \frac{\partial C}{\partial t} \right)_{\text{reaction kinetics}} = \sum C \cdot k
\]

\([M \cdot L^{-3}] \cdot [T^{-1}] = [M \cdot L^{-3} \cdot T^{-1}]\)

\[
\left( \frac{\partial C}{\partial t} \right)_{\text{sedimentation}} = -\nu_{\text{sedimentation}} \cdot \frac{\partial C}{\partial z}
\]

\([L \cdot T^{-1}] \cdot [M \cdot L^{-3} \cdot L^{-1}] = [M \cdot L^{-3} \cdot T^{-1}]\)

\[
\left( \frac{\partial C}{\partial t} \right)_{\text{external}} = \pm \text{ external sources and sinks}
\]

Must be given in \([M \cdot L^{-3} \cdot T^{-1}]\)
Advection-Dispersion Equation with all components

\[
\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial y} + D_y \cdot \frac{\partial^2 C}{\partial y^2} \\
- w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2} \\
+ \sum k \cdot C - \nu_{\text{sedimentation}} \cdot \frac{\partial C}{\partial z} \\
\pm \text{external sources and sinks}
\]

Equation 35