DERIVATION OF BASIC TRANSPORT EQUATION

Definitions

Basic dimensions

[M] → Mass

[L] → Length

[T] → Time

Concentration

Mass per unit volume

$[\mathbf{M \cdot L^{-3}}]$

Mass Flow Rate

Mass per unit time

$[\mathbf{M \cdot T^{-1}}]$

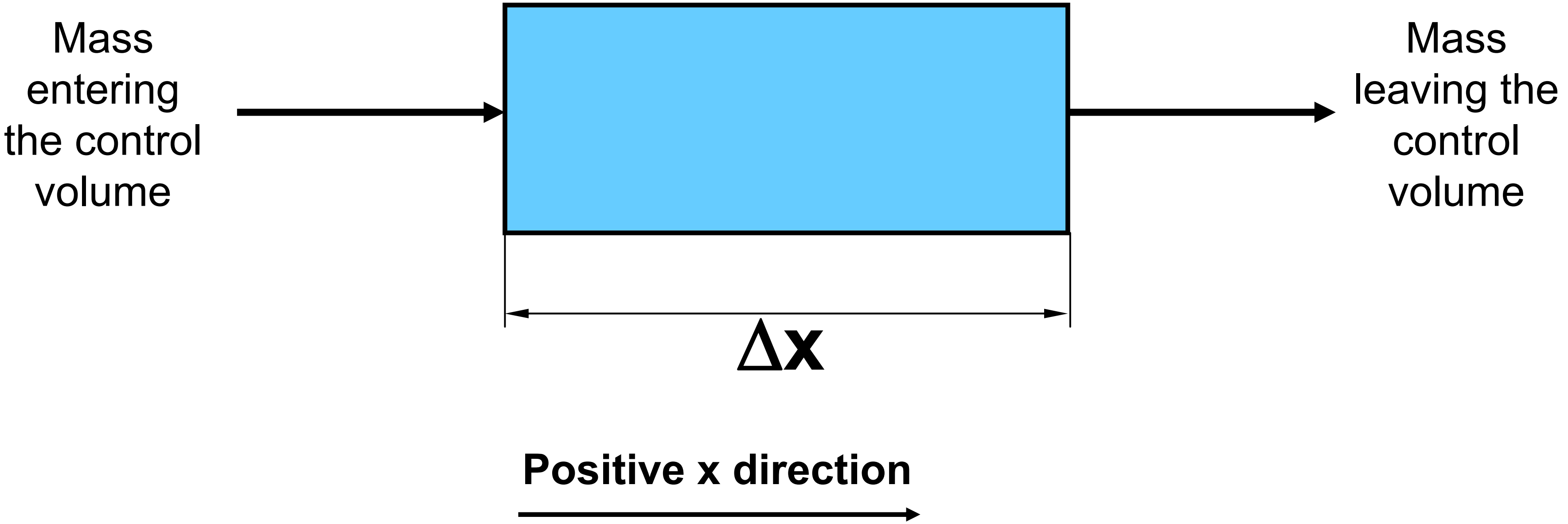
Flux

Mass flow rate through unit area

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

The Transport Equation

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



The Transport Equation

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

$$\begin{bmatrix} \text{Change of} \\ \text{mass in the} \\ \text{control volume} \\ \text{in a time} \\ \text{interval } \Delta t \end{bmatrix} = \begin{bmatrix} \text{Mass entering} \\ \text{the control} \\ \text{volume in } \Delta t \end{bmatrix} - \begin{bmatrix} \text{Mass leaving} \\ \text{the control} \\ \text{volume in } \Delta t \end{bmatrix}$$

$$\underbrace{V \frac{\partial C}{\partial t}} = \underbrace{A \cdot J_1} - \underbrace{A \cdot J_2}$$

Equation 1

The Transport Equation

A closer look to Equation 1

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

- V: **Volume [L^3]**
- $\frac{\partial C}{\partial t}$: **Concentration over time [$M \cdot L^{-3} \cdot T^{-1}$]**
- A: **Area [L^2]**
- J_1: **Flux [$M \cdot L^{-2} \cdot T^{-1}$]**
- A: **Area [L^2]**
- J_2: **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)

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

Equation 2

Rearrangements

$$\frac{\partial C}{\partial t} = \frac{A}{V} \cdot \left(J_1 - J_2\right)$$

Equation 3

The Transport Equation

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

Therefore

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

The Transport Equation

$$\frac{\partial C}{\partial t} = \frac{A}{V} \cdot (J_1 - J_2)$$ Equation 3

$$J_2 = J_1 + \frac{\partial J}{\partial x} \cdot \Delta x$$ Equation 4

$$\frac{\partial C}{\partial t} = \frac{A}{V} \cdot \left(J_1 - \left(J_1 + \frac{\partial J}{\partial x} \cdot \Delta x \right) \right)$$ Equation 5

The Transport Equation

Rearrangements

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

$$\frac{V}{A} = \Delta x \Rightarrow \frac{A}{V} = \frac{1}{\Delta x} \quad \text{Equation 6}$$

$$\frac{\partial C}{\partial t} = \frac{1}{\Delta x} \cdot \left(J_1 - J_1 - \frac{\partial J}{\partial x} \cdot \Delta x \right) \quad \text{Equation 7}$$

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

$$\frac{\partial C}{\partial t} = -\sum_{i=1}^{3} \frac{\partial}{\partial x_i} J_i$$

$x_1 = x$

$x_2 = y$

$x_3 = z$

Equation 9

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

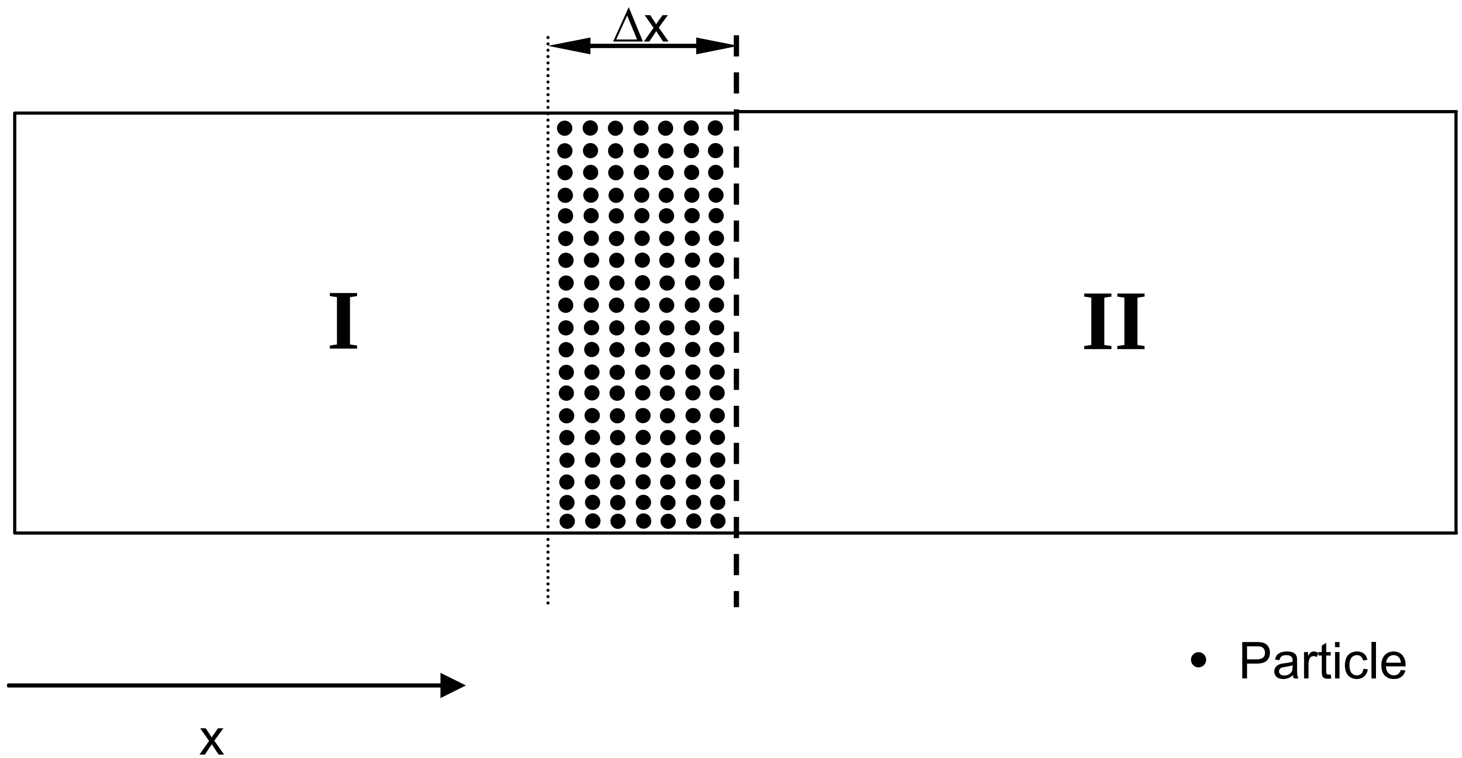
Equation 10

The Transport Equation

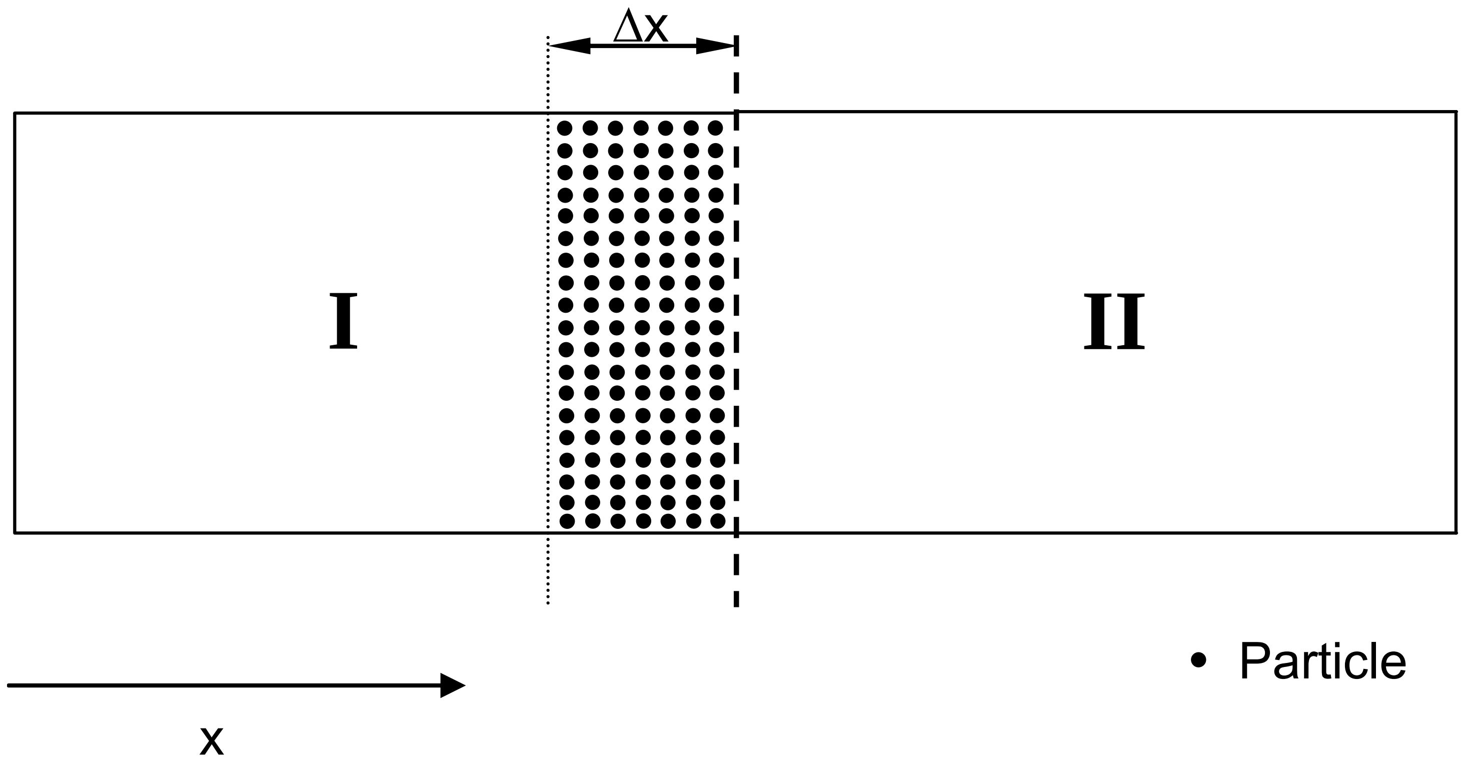
- The transport equation is derived for a conservative tracer (material)
- The control volume is constant as the time progresses
- The flux (J) can be anything (flows, dispersion, etc.)

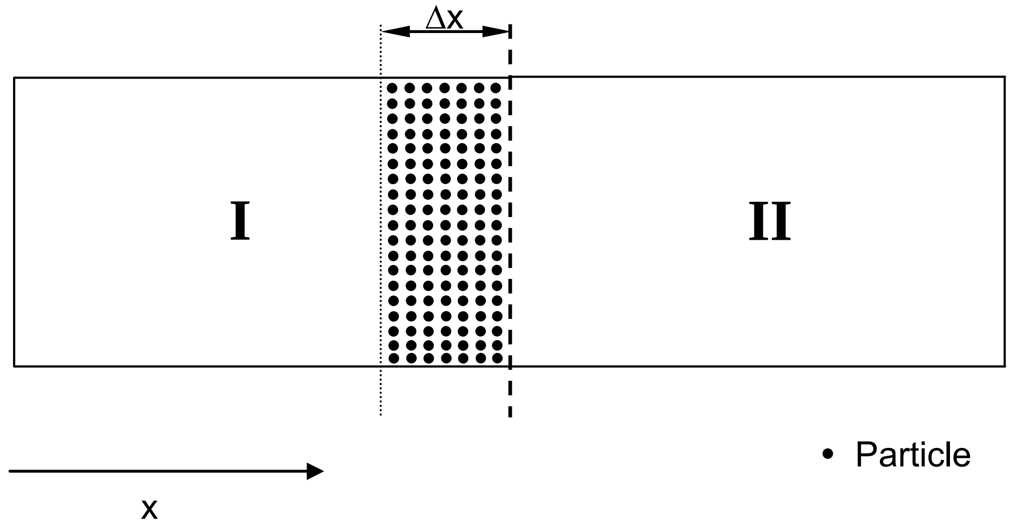
The Advective Flux

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.**



Δx is defined as the distance, which a particle can pass in a time interval of **Δt.** **The assumption is that the particles move on the direction of positive x only.**

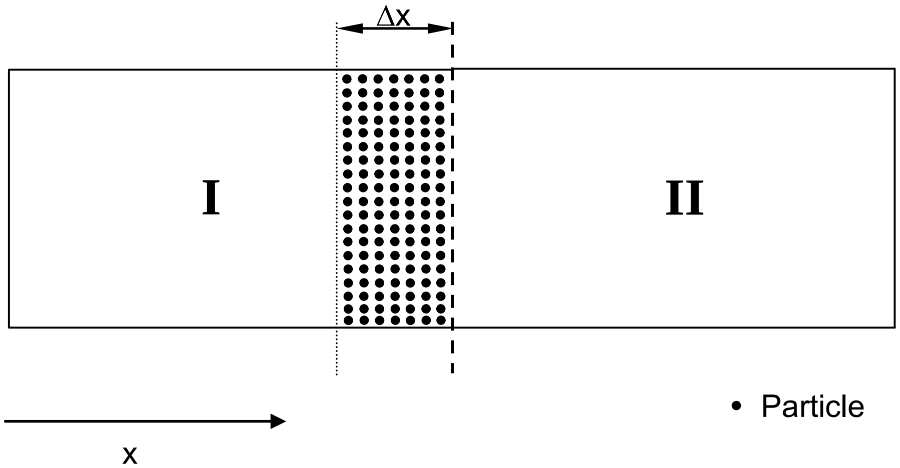




The number of particles (analogous to mass) moving from control volume I to control volume II in the time interval Δt can be calculated using the Equation below, where

$$Q = C \cdot \Delta x \cdot A \qquad \text{Equation 11}$$

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



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

Number of particles passing from I to II in Δt

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

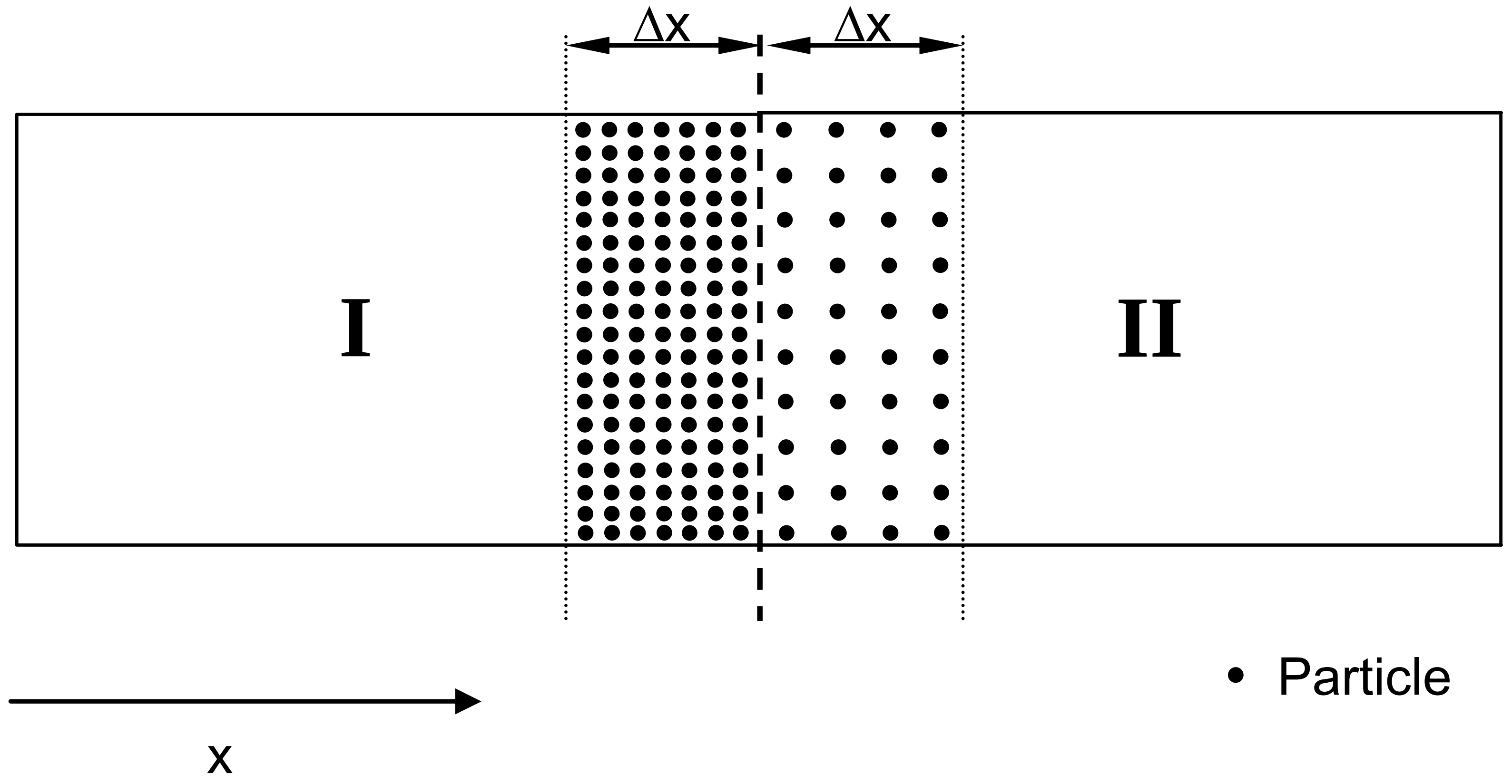
Equation 12

The Advective Flux

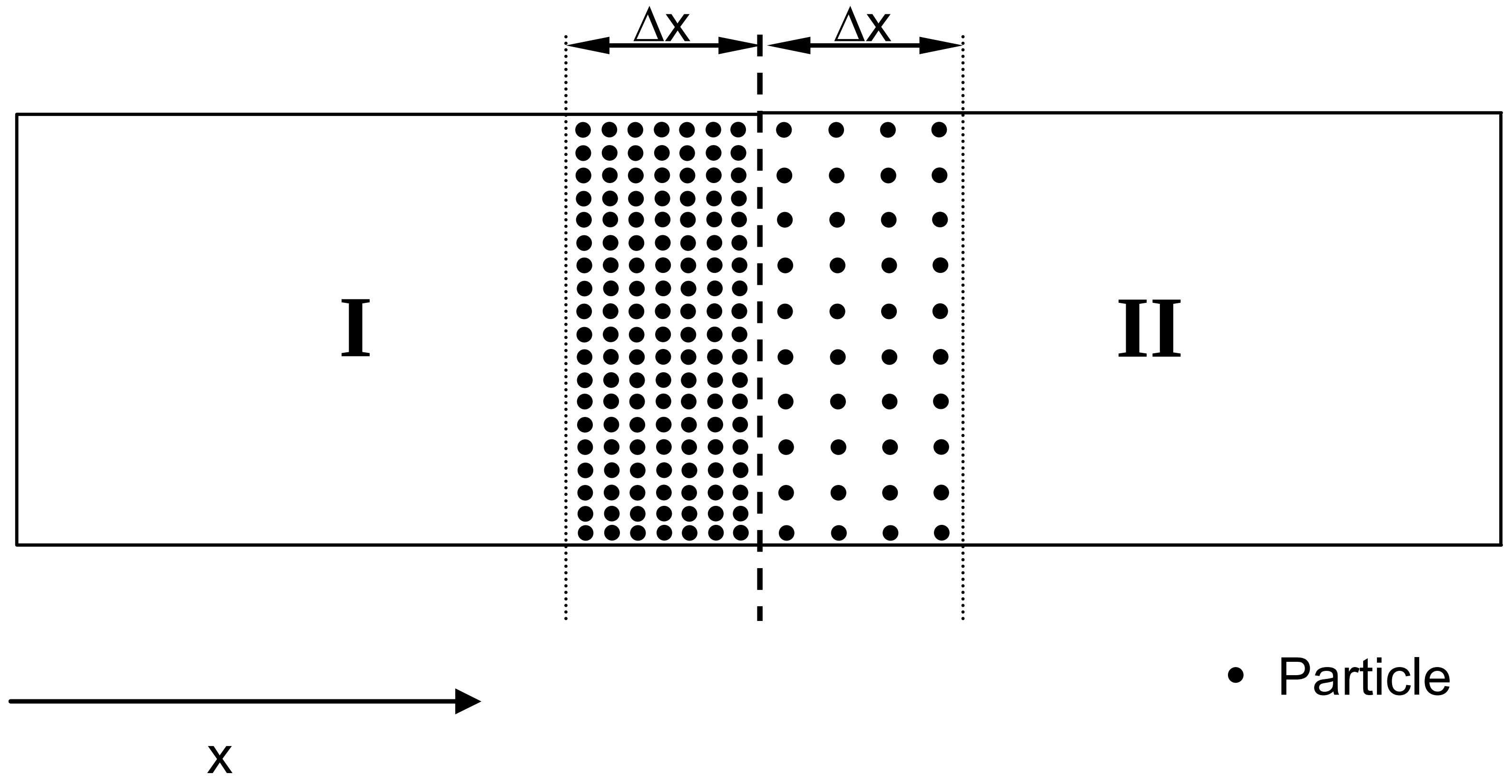
$$J_{ADV} = \frac{\partial x}{\partial t} \cdot C \qquad \text{Equation 12}$$

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.**

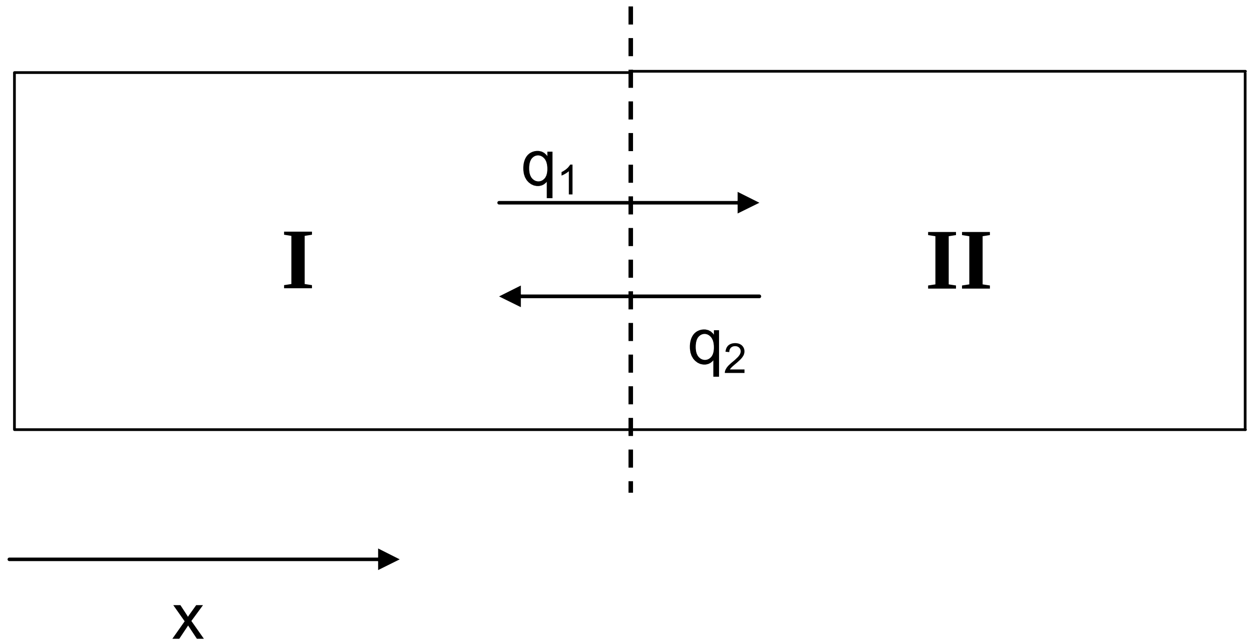


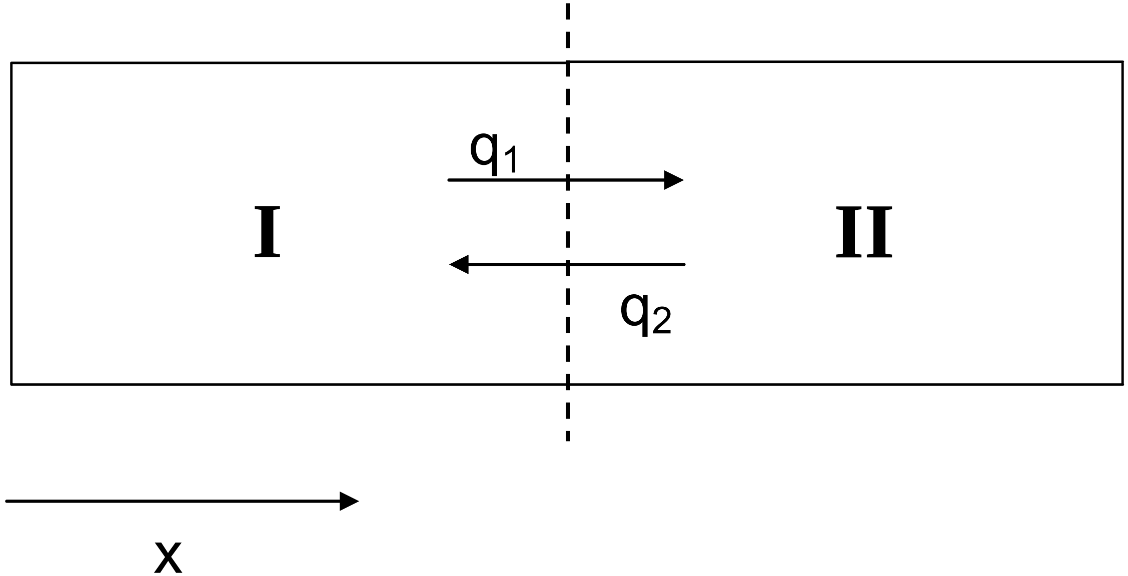
Δx is defined as the distance, which a particle can pass in a time interval of **Δt**. The assumption is that the particles move on positive and negative x directions. **In this case there are two directions, which particles can move in the time interval of Δt**.



Another assumption is that a particle does not change its direction during the time interval of **Δt** 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





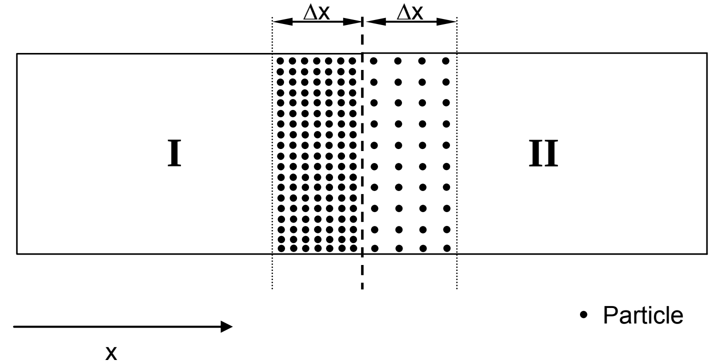
$$q_1 = \overbrace{0.5}^{\text{50 \% probability}} \cdot C_1 \cdot \Delta x \cdot A \qquad \text{Equation 13}$$

$$q_2 = 0.5 \cdot C_2 \cdot \Delta x \cdot A \qquad \text{Equation 14}$$

$$Q = q_1 - q_2 \qquad \text{Equation 15}$$

$$Q = 0.5 \cdot \Delta x \cdot A \left(C_1 - C_2 \right) \qquad \text{Equation 16}$$

Number of particles passing from I to II in Δt



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

Equation 16

Divide by time

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

Equation 17

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

Equation 18

Number of particles passing from I to II in unit time

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

Equation 19

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

Equation 20

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

Equation 21

Divide by Area

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

Equation 22

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

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

Equation 22

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

Equation 23

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

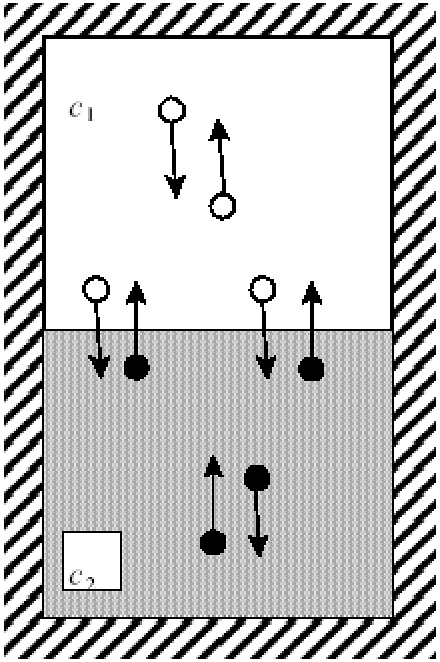
Equation 24

$$\Rightarrow \quad J_{DISP} = -D \cdot \frac{\partial C}{\partial x}$$

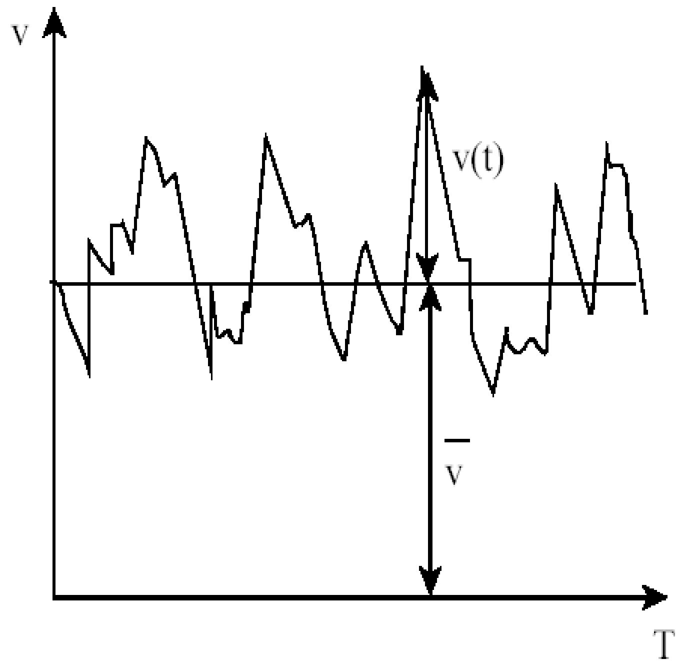
Equation 25

$$\left.\begin{array}{l} 0.5 \rightarrow [\;] \\ \Delta x \rightarrow [L] \Rightarrow (\Delta x)^2 \rightarrow [L^2] \\ \Delta t \rightarrow [T] \end{array}\right\} \Rightarrow D = \frac{0.5 \cdot (\Delta x)^2}{\Delta t} \rightarrow \left[\frac{[\;] \cdot [L^2]}{[T]}\right] = [L^2 \cdot T^{-1}]$$

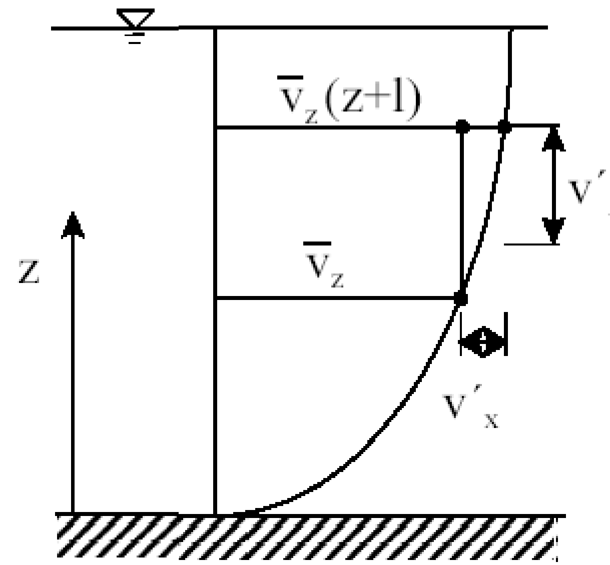
Dispersion



Molecular diffusion



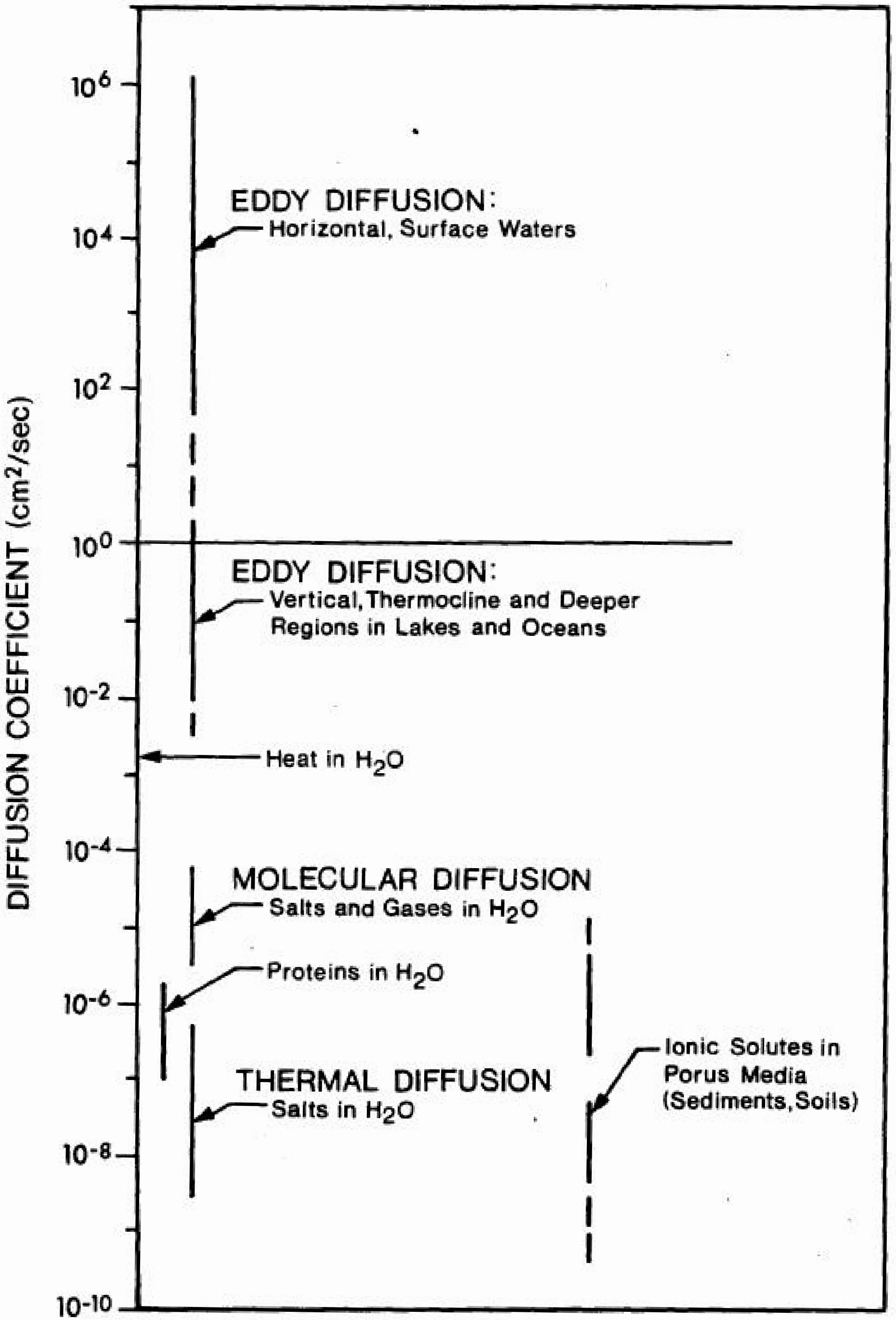
Turbulent diffusion



Longitudinal dispersion

GENERALLY

Molecular diffusion << Turbulent diffusion << Longitudinal dispersion



Ranges of the Dispersion Coefficient (D)

The Dispersive Flux

$$J_{DISP} = -D \cdot \frac{\partial C}{\partial x}$$ 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

General transport equation

$$J_{advection} = \frac{\partial x}{\partial t} \cdot C$$ Equation 12

Advective flux

$$J_{dispersion} = -D \cdot \frac{\partial C}{\partial x}$$ Equation 25

Dispersive flux

$$J = J_{advection} + J_{dispersion}$$ Equation 26

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

The Advection-Dispersion Equation

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

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} J_{advection} - \frac{\partial}{\partial x} J_{dispersion} \quad \text{Equation 28}$$

$$J_{advection} = \frac{\partial x}{\partial t} \cdot C \qquad J_{dispersion} = -D \cdot \frac{\partial C}{\partial x}$$

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{\partial x}{\partial t} \cdot C\right) - \frac{\partial}{\partial x}\left(-D \cdot \frac{\partial C}{\partial x}\right) \quad \text{Equation 29}$$

The Advection-Dispersion Equation

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{\partial x}{\partial t}\cdot C\right) - \frac{\partial}{\partial x}\left(-D\cdot\frac{\partial C}{\partial x}\right) \qquad \text{Equation 29}$$

Velocity u in x direction

$$u\cdot\frac{\partial C}{\partial x} \qquad -D\cdot\frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} = -u\cdot\frac{\partial C}{\partial x} + D\cdot\frac{\partial^2 C}{\partial x^2} \qquad \text{Equation 30}$$

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

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

Velocity times concentration over space

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

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

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

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

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

$$\frac{\partial C}{\partial t} = \sum_{i=1}^{3}\left(-u_i \cdot \frac{\partial C}{\partial x_i} + D_i \cdot \frac{\partial^2 C}{\partial {x_i}^2}\right)$$

Equation 31

$x_1 = x$, $u_1 = u$, $D_1 = D_x$

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

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

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

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

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

Equation 33

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

Equation 34

Transport Equation with all Components

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

Equation 35

$$- w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2} + \sum k \cdot C - \upsilon_{sedimentation} \cdot \frac{\partial C}{\partial z}$$

$$\pm \text{ external sources and sinks}$$

Sedimentation in z direction

- **External loads**
- **Interaction with bottom**
- **Other sources and sinks**

Dimensional Analysis of Components

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

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

$$\left(\frac{\partial C}{\partial t}\right)_{\text{sedimentation}} = -\upsilon_{\text{sedimentation}} \cdot \frac{\partial C}{\partial z}$$

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

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

Must be given in $[M \cdot L^{-3} \cdot T^{-1}]$

Advection-Dispersion Equation with all components

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

$$- w \cdot \frac{\partial C}{\partial z} + D_z \cdot \frac{\partial^2 C}{\partial z^2}$$

$$+ \sum k \cdot C - \upsilon_{\text{sedimentation}} \cdot \frac{\partial C}{\partial z}$$

$$\pm \text{external sources and sinks}$$

Equation 35