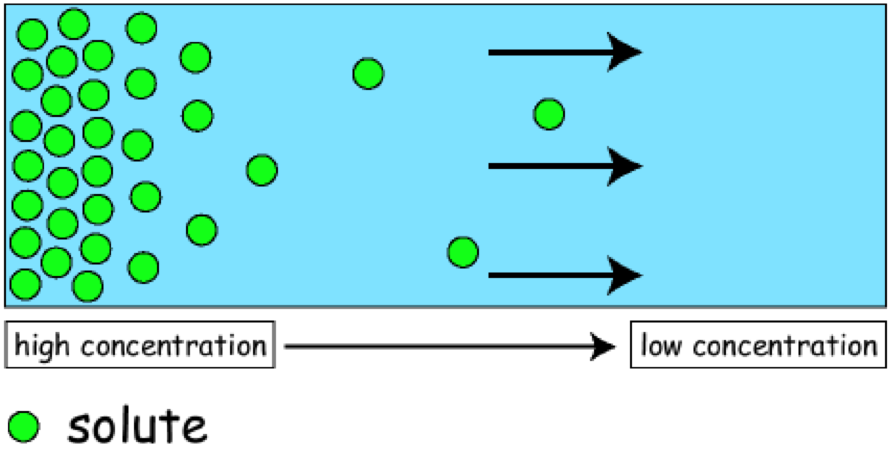
Lecture 25, Fluxes and the Conservation Budget

- Fick’s First Law
- Resistors and Conductors
- Continuity Equation
  - Concept
  - Derivation
  - local and total derivatives
  - constant density, incompressible flow
- Conservation of mass for multicomponent system
  - diffusive flux densities on molar and mass bases
  - Fick's Second Law
- Conservation of Mass, turbulent flow
  - bulk flux density on molar and mass bases
  - Reynolds decomposition
  - derivation

Diffusion is defined as:

process resulting from random motion of molecules by which there is a net flow of matter from a region of high concentration to a region of low concentration.

Diffusion

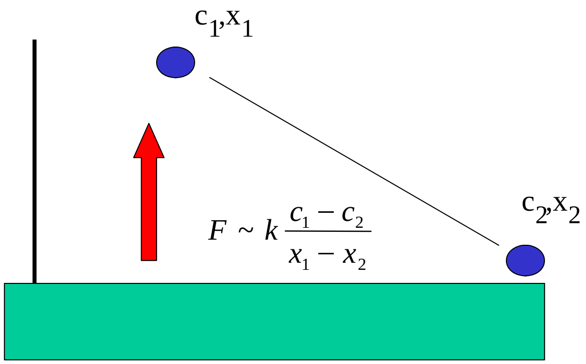


Solute transport is from the left to the right; movement of the solutes is due to the concentration gradient (dC/dx).

Fick’s Law of Diffusion

- *a chemical species diffuses in the direction of decreasing mole fraction. the flux density is proportional to a diffusion coefficient and a gradient*

$$F \sim k\frac{c_1 - c_2}{x_1 - x_2}$$



Computing Flux Density, F

$$F = -D_c \frac{\partial \rho_c}{\partial x}$$

(g m^{-2} s^{-1}): mass density, ρ_c

$$F = -D_c \frac{\partial c}{\partial x}$$

(mol m^{-2} s^{-1}): mole density, c

$$F = -\rho D_c \frac{\partial s}{\partial x}$$

(g m^{-2} s^{-1}): mass fraction, s

$$\mathrm{F} = -\frac{\rho_a}{\mathrm{M_a}} \mathrm{D_c} \frac{\partial C_c}{\partial x}$$

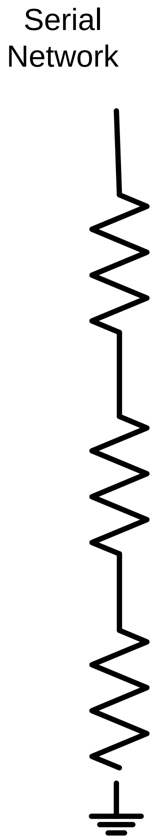
(mol m^{-2} s^{-1}): mole fraction, C_c

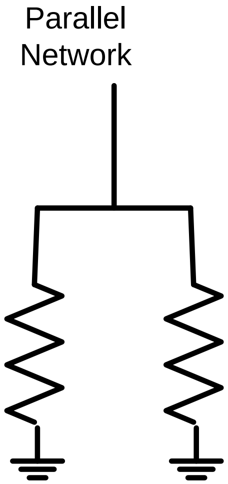
Molecular Diffusivity, D

$$D = D^0 (T / T^0)^n (P^0 / P)$$

T	**D_{h2o}**	**D_{co2}**	**D_{o2}**
^oC	$mm^2\ s^{-1}$	$mm^2\ s^{-1}$	$mm^2\ s^{-1}$
0	21.2	13.9	17.7
10	22.6	14.8	18.8
20	24.0	15.7	20.0
30	25.4	16.7	21.2
40	26.9	17.7	22.5

Resistors, r, and Conductors, g





Ohm's Law

$$I = \frac{V}{R}$$

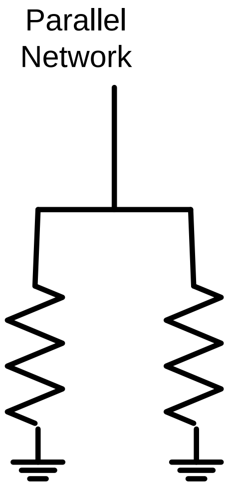
Current = Voltage/Resistance

Parallel Resistance/ Serial Conductances

$$\frac{1}{R} = \frac{1}{r_a} + \frac{1}{r_b}$$

$$R = \frac{r_a r_b}{r_a + r_b}$$

$$G = g_1 + g_2$$



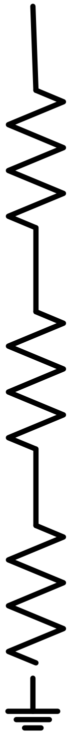
Serial Resistance/ Parallel Conductance Networks

$$R = r_a + r_b$$

$$\frac{1}{G} = \frac{1}{g_a} + \frac{1}{g_b}$$

$$G = \frac{g_a g_b}{g_a + g_b}$$

Serial
Network



Flux-Resistance

$$F = \rho_a \frac{C_a - C_0}{\Sigma r_i}$$

Meteorologists:
R (s/m)

$$F = g(ms^{-1})(\Delta\rho_c(mol \cdot m^{-3}))$$

$$F = \frac{C_a - C_0}{\Sigma r_i}$$

Ecophysiologists:
R (mole^{-1} m^{2} s^{1})

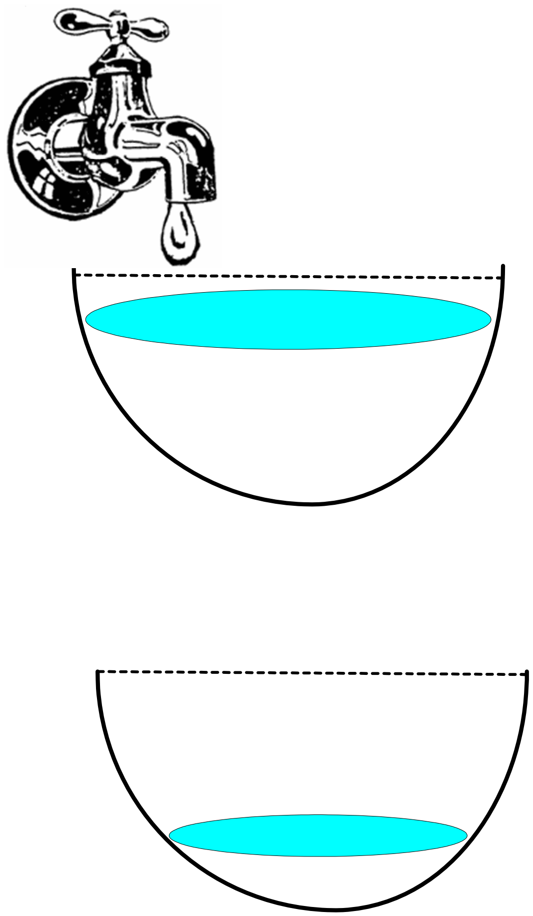
Ecophysiological, Alternative, View of Resistance

$$r(mol^{-1} \cdot m^{2} \cdot s^{1}) = r(m^{-1} \cdot s)\frac{V_o P_o T}{P T_o}$$

$$g(m \cdot s^{-1}) = g(mol \cdot m^{-2} \cdot s^{-1})\frac{V_o P_o T}{P T_o}$$

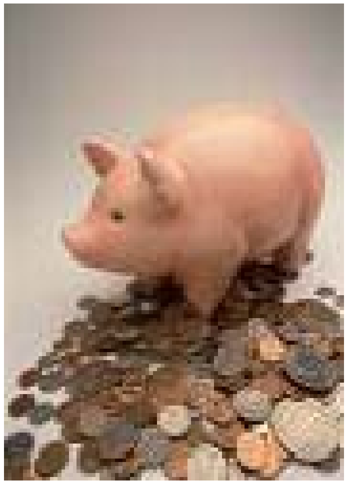
Vo= 0.0224 m^{3} mol^{-1} at STP

Bath tub analogy, change of height of water in a volume



Same Principle with Economy

$$$$ in



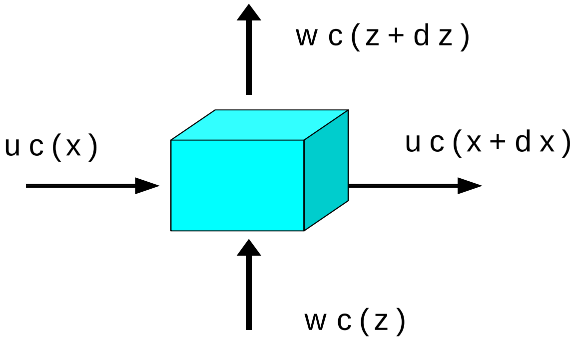
Money in Bank

$$ out

$$\Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t}$$

How air density, ρ, of a volume changes with time

Balance of mass fluxes in and out of horizontal and vertical walls



$$\Delta y \Delta x [\, \rho w|_{z} - \rho w|_{z+\Delta z} \,]$$

$$\Delta y \Delta z [\, \rho u|_{x} - \rho u|_{x+\Delta x} \,]$$

Continuity Equation, how air density, ρ, changes with time

$$\frac{\partial \rho}{\partial t} = -(\frac{\partial u\rho}{\partial x} + \frac{\partial v\rho}{\partial y} + \frac{\partial w\rho}{\partial z})$$

u, longitudinal velocity
v, lateral velocity
w, vertical velocity

Expansion of terms

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} + w\frac{\partial \rho}{\partial z} = -\rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)$$

u, longitudinal velocity
v, lateral velocity
w, vertical velocity

How advection terms arise, relation between total and partial derivatives

$$\frac{dc(t,x,y,z)}{dt} =$$

$$\frac{\partial c}{\partial t} + \frac{dx}{dt}\frac{\partial c}{\partial x} + \frac{dy}{dt}\frac{\partial c}{\partial y} + \frac{dz}{dt}\frac{\partial c}{\partial z} =$$

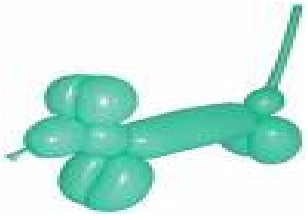
$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z}$$

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z}$$

Incompressible Flow

$$\frac{d\rho}{dt} = 0 = -\rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)$$

$$-\rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = \frac{\partial w}{\partial z}$$



Fick’s Second Law

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2}$$

Time rate of change in C is related to the second derivative with respect to space

Fick’s Second Law

Conservation Equation, Laminar Flow

$$FA - (F + \frac{\partial F}{\partial x} dx)A = \frac{\partial c}{\partial t} A dx$$

$$\frac{\partial c}{\partial t} = -\frac{\partial F}{\partial x}$$

$$F = -D_c \frac{\partial c}{\partial x}$$

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2}$$

Conservation Budget, Turbulent Flow

$$c = \bar{c} + c'$$

$$\frac{\partial \overline{(\bar{c} + c')}}{\partial t} + \frac{\partial \overline{(\overline{u_j} + u_j{}')(\overline{\bar{c} + c'})}}{\partial x_j} = \frac{\partial}{\partial x_j}[D_c \frac{\partial \overline{(\bar{c} + c')}}{\partial x_j}]$$

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}_j \frac{\partial \bar{c}}{\partial x_j} + \frac{\partial \overline{u_j{}' c'}}{\partial x_j} = \frac{\partial}{\partial x_j}[D_c \frac{\partial \bar{c}}{\partial x_j}]$$

2D Simplification

$$\frac{\partial \overline{c}}{\partial t} + \overline{u}\frac{\partial \overline{c}}{\partial x} + \frac{\partial \overline{w'c'}}{\partial z} = \frac{\partial}{\partial z}[D_c \frac{\partial \overline{c}}{\partial z}]$$

Constant Flux Layer, Internal Boundary Layer

$$\frac{\partial \overline{c}}{\partial t} = 0$$

Ideal, steady-state, infinite fetch, no advection

$$\overline{u}_j \frac{\partial \overline{c}}{\partial x_j} = 0$$

$$0 = -\overline{\rho_a}\frac{\partial \overline{w'c'}}{\partial z} = \frac{\partial F}{\partial z}$$

Integral of dF/dZ equals a CONSTANT

Constant Flux Layer, Internal Boundary Layer

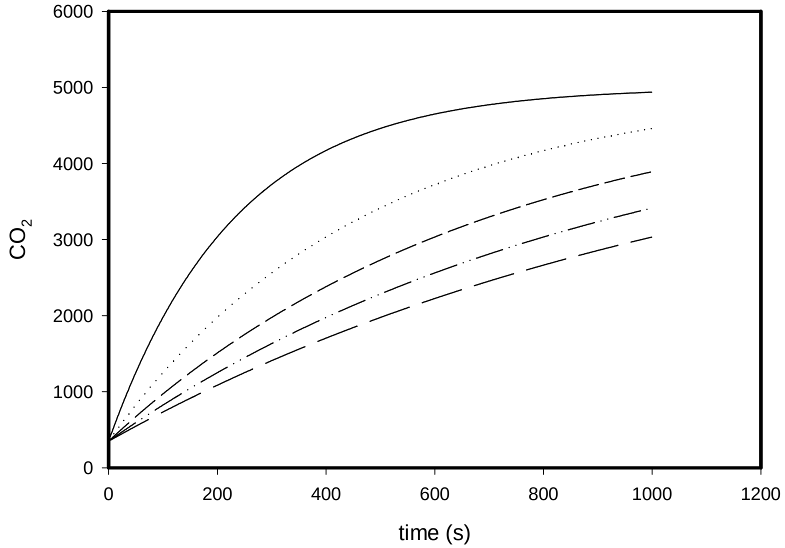
Integrate from Ground up and Define Flux as Sum of flux at the ground and the sum of the Diffusive source-sink from the vegeation

$$\overline{\rho_a}\,\overline{w'c'(h)} = \overline{\rho_a}\,\overline{w'c'(0)} + \int_0^h S(z)dz$$

Case 1, No Advection, Dynamic Response

$$u\frac{\partial c}{\partial x}=0$$

$$\frac{\partial c}{\partial t}=-\frac{\partial F}{\partial x}$$

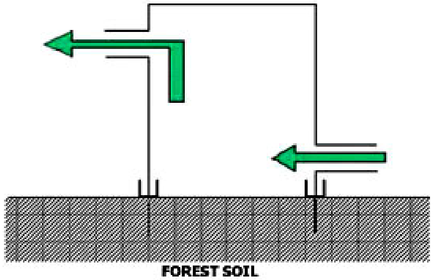


$$\frac{\Delta c}{\Delta t}=-\frac{F(t)}{h}$$

$$F(t)=-h\frac{\Delta c}{\Delta t}$$

Case 2, Steady-State, Advection

$$\frac{\partial c}{\partial t} = 0$$



$$u\frac{\partial c}{\partial x} = -\frac{\partial F}{\partial z}$$

$$u\frac{\Delta c}{\Delta x} = -\frac{F}{h}$$

$$F = -u \cdot h\frac{\Delta c}{\Delta x}$$

Homework

- Use a unit-correct form of the conservation equation to evaluate the change of CO_2 concentration with time (up to 1000 s) in a closed chamber that has horizontal cross section of 0.1 (x) and 0.1 m (y).
  - Perform the calculations for cases where the chamber is 0.1, 0.3, and 0.5 m tall.
  - Start with a CO2 concentration of 350 μmol mol^{-1}.
  - The initial flux density is 2 μmol m^{-2} s^{-1}, the exchange conductance, g, is 4.30 10^{-4} mol m^{-2} s^{-1} and the reference deep soil CO_2 concentration is 5000 μmol mol^{-1}.
  - In performing these calculations consider feedback between the flux density () and build up of CO_2 in the head space. Assume the concentration in the chamber is well mixed.

$$F = g(c(t) - c_{ref})$$

$$u\frac{\Delta c}{\Delta x} = -\frac{\Delta F}{\Delta z}$$

- Use the advection form of the conservation equation to evaluate the flux density of CO2 into an open chamber.

- The chamber is 0.5 (x) by 0.5 (y) by 0.1 (z). The incoming and outgoing CO2 concentrations are 350 and 355 μmol mol^{-1}, respectively. Perform calculations for cases where the flow velocity is 1, 3 and 6 m s^{-1} (the units of flux density should be μmol m^{-2} s^{-1}

- What is the flux of CO_2 into an open chamber, where the volumetric flow rate is 1, 3 and 6 liters per minute? Use the same chamber.