Lecture 23, 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

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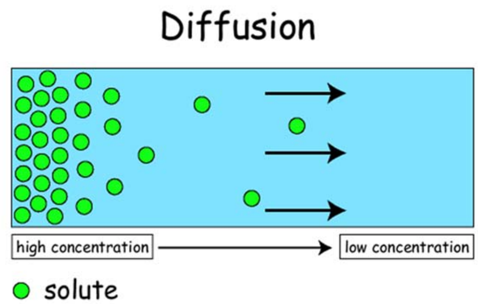
Now we discuss Fluxes. To do so we start with their definitions and description of the conservation budgets

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.



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

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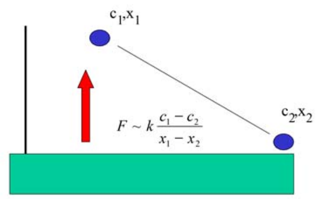
We will discuss diffusive fluxes separately from turbulent fluxes

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*

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



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In turbulence we use an analog to Fick's law, but it principle it is for diffusion

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

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

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

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Get your units straight

Molecular Diffusivity, D

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

T	**D_{h2o}**	**D_{co2}**	**D_{o2}**
°C	$mm^2\ s^{-1}$	$mm^2\ s^{-1}$	$mm^2\ s^{-1}$
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

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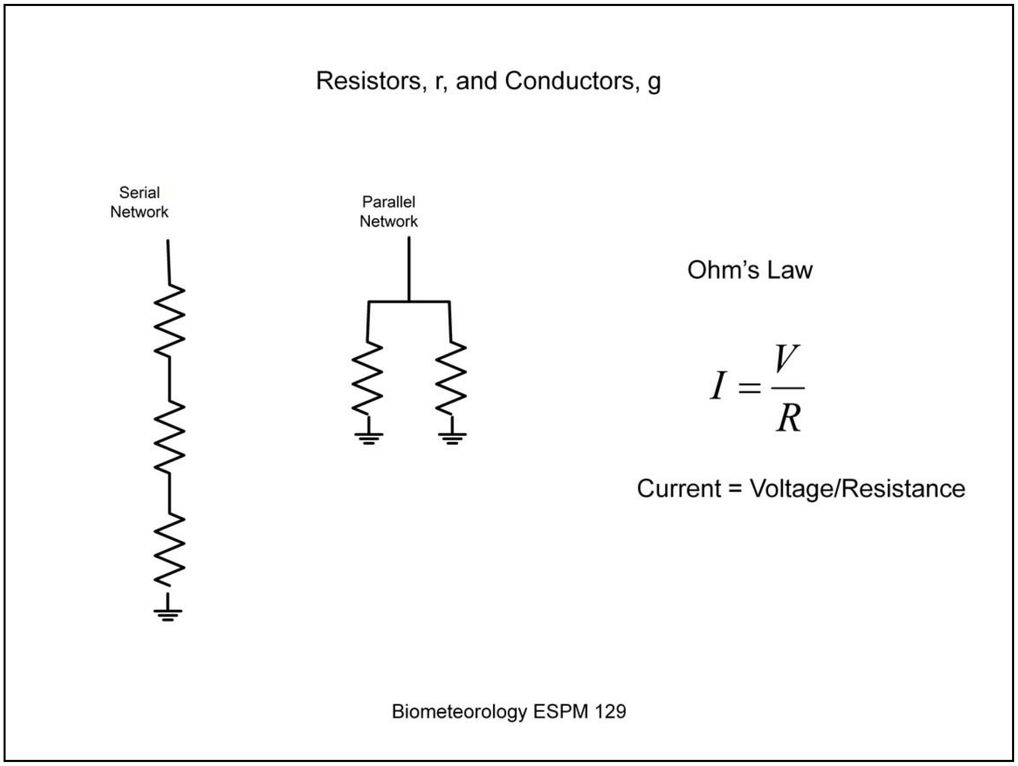
Molecular diffusivity is a function of the molecular mass, pressure and temperature. Differences in diffusion among molecules are a reason why stable isotopes, like 13C are important tracers for ecological studies. There is fractionation by diffusion between 12C and 13C

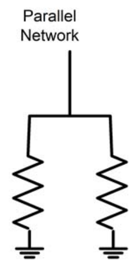


Now we will focus on Ohm's Law as an analog for describing fluxes and defining networks and their rules. First we want to distinguish between parallel and serial networks

Parallel Resistance/ Serial Conductances

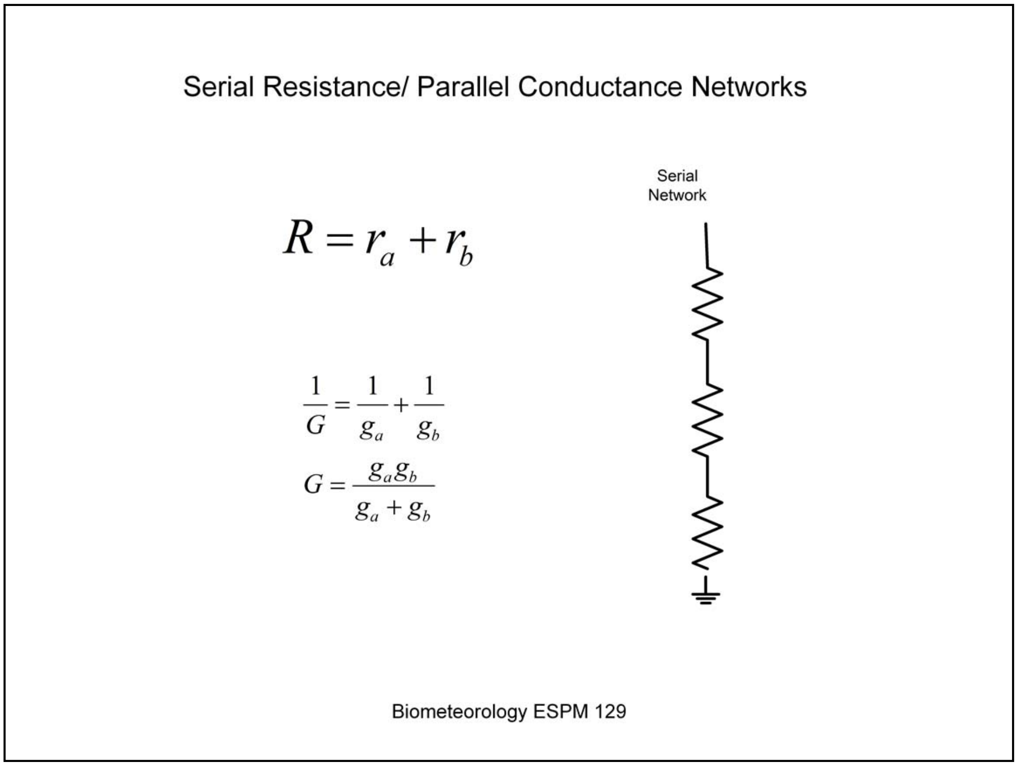
$$\frac{1}{R} = \frac{1}{r_a} + \frac{1}{r_b}$$

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



$$G = g_1 + g_2$$

The resistances of a parallel network are summed in terms of their inverse. But conductances are additive and are in serial



In serial networks, the resistances are additive

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)

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This equation was introduced in lecture 2 and is the basis of biometeorology as the sum of the resistances have biophysical meanings

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

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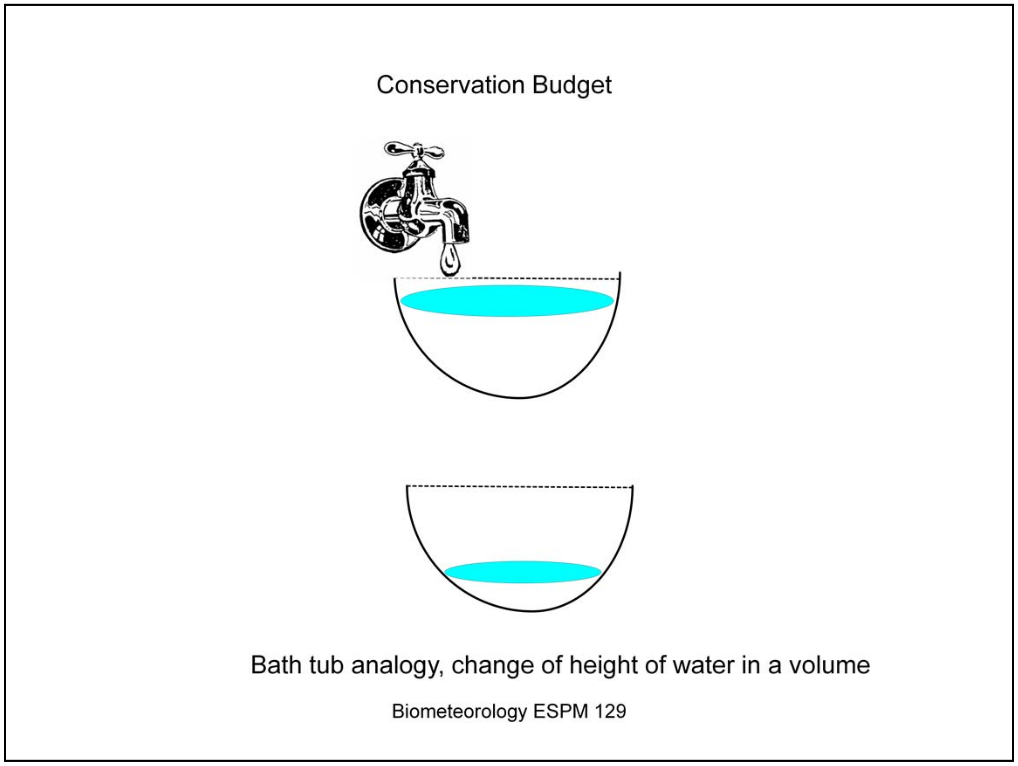
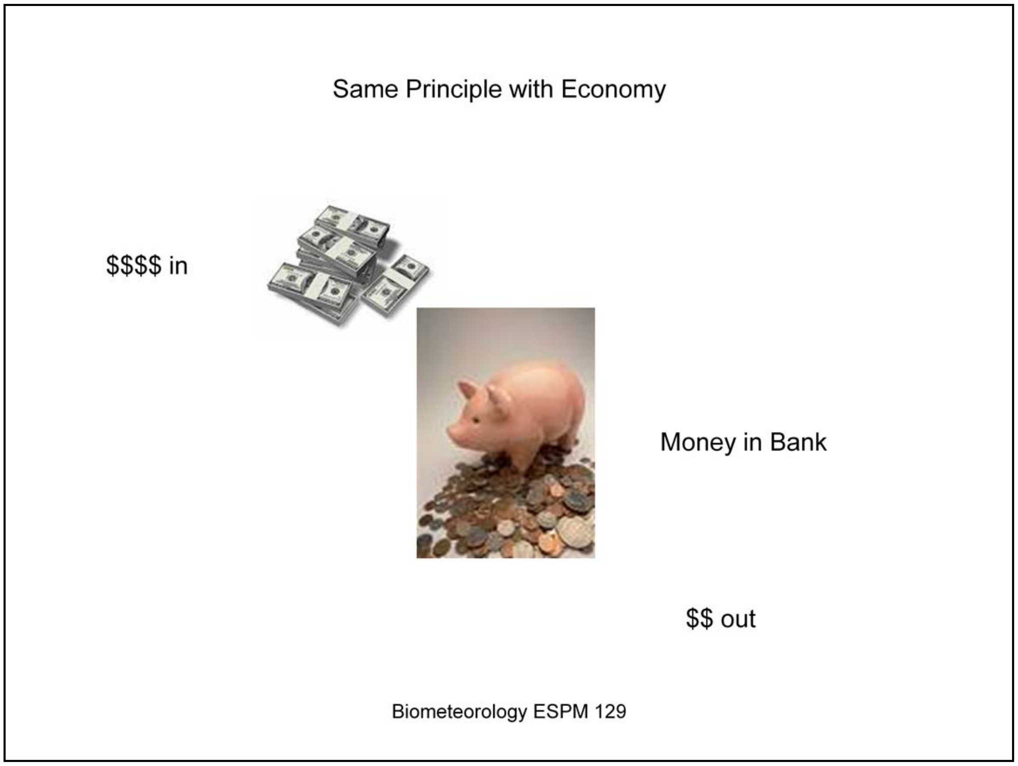
In meteorology and fluid mechanics a resistance is an inverse velocity. Ecologists prefer to adjust it into flux density units as they work across elevational gradients.



The conservation budget is no more complicated that thinking about the flows of water in and out of your bath tub.

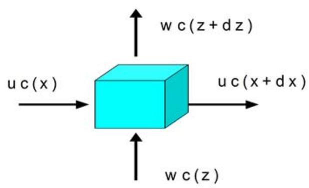


Or bank account. Material in a controlled volume builds up if the flux in is greater than the flux out, and vice versa

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

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

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



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

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

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Lets consider the fluxes in and out of a controlled volume and how that changes the density with time. Density times velocity is a flux density, mole m-2 s-1

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

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Add these up and here is what you get.

Expansion of terms

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

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

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We can expand the terms to find those associated with time rate of change, advection and flux divergence

How advection terms arise, relation between total and partial derivatives

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

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

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

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

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Looking under the hood. Expanding the total derivative gives us another way to discover the advection term

Incompressible Flow

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

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

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For incompressible flows, those we deal with. Think about squeezing a balloon and watch which way the air moves. This happens in the boundary layer as air moves around and over objects

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

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For diffusive flows, we can simply the budget equations into a one dimensional balance between time rate of change and flux divergence, by substituting Fick’s first law. Hence we see a second derivative in c with respect to space.

Fick's Second Law

Conservation Equation, Laminar Flow

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

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

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

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A simple derivation of the previous relation

Conservation Budget, Turbulent Flow

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

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

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

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Next we introduce turbulent flow, substitute c with the sum of the mean and fluctuation components and do the math. A new term arises associated with the flux divergence of the turbulenc flux covariance

2D Simplification

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

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2 d simplification. We assume mean vertical velocity is zero, so the w dc/dz term drops out.

Constant Flux Layer, Internal Boundary Layer

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

Ideal, steady-state, infinite fetch, no advection

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

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

Integral of dF/dZ equals a CONSTANT

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This equation is the basis of use of the eddy covariance method. Under steady state conditions and no advection, large fetch, the flux divergence is zero, so the flux is constant with height!!!

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

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

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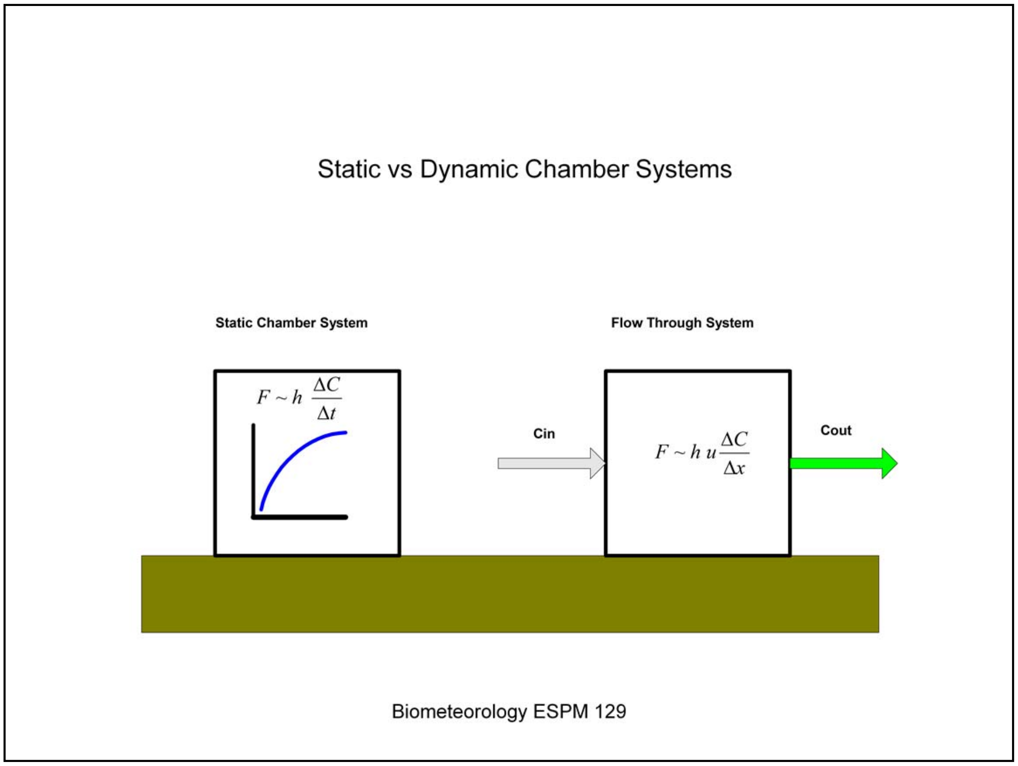
In practice the eddy flux measured above a canopy is the sum of the sources and sinks of the leaves and soil, underneath. This is for passive scalars. If you are looking at reactive chemical species there could be a flux divergence due to chemical reactions.



Now we apply these theories to understand how ecologists and biometeorologists measure soil or leaf gas exchange with chambers. We have two options, a closed static chamber and an open steady-state chamber

Case 1, No Advection, Dynamic Response

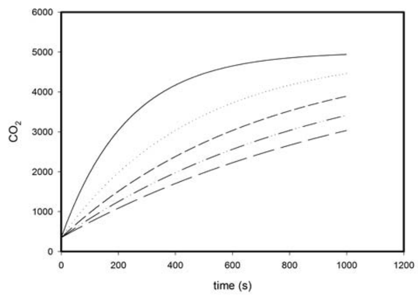
$$u\frac{\partial c}{\partial x}=0$$

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

$$\frac{\Delta c}{\Delta t}=-\frac{F(t)-0}{h-0}$$

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

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



Evaluate Flux at t=0!!

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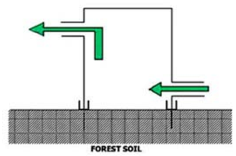
Case 1. Take budget equation, assume advection is zero and there is no flux out of the top of the chamber. All we need to measure is the time rate of change in C and height of the chamber h. Notice that the time rate of change in C is non linear, so there are negative feedbacks on fluxes. If you keep the chamber on the soil too long it will inhibit the flux. So we want to evaluate the flux in terms of dc/dt at time 0. Important points

Case 2, Steady-State, Advection

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



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

$$u\frac{\Delta c}{\Delta x} = -\frac{F-0}{h-0} \qquad u\frac{\Delta c}{\Delta x} = -\frac{F}{h}$$

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

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Case two, steady state, so dc/dt is zero. Air flows in and out of the chamber so there is now a balance between advection and flux divergence. This method is a function of the volume of flow, height of the chamber and cross section x. In practice u must be slow as if too large it will induce pressure differences that can inhibit efflux from the soil. Pressure differences of only a few pascals are large enough to cause biases.

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.