R. G. Prinn
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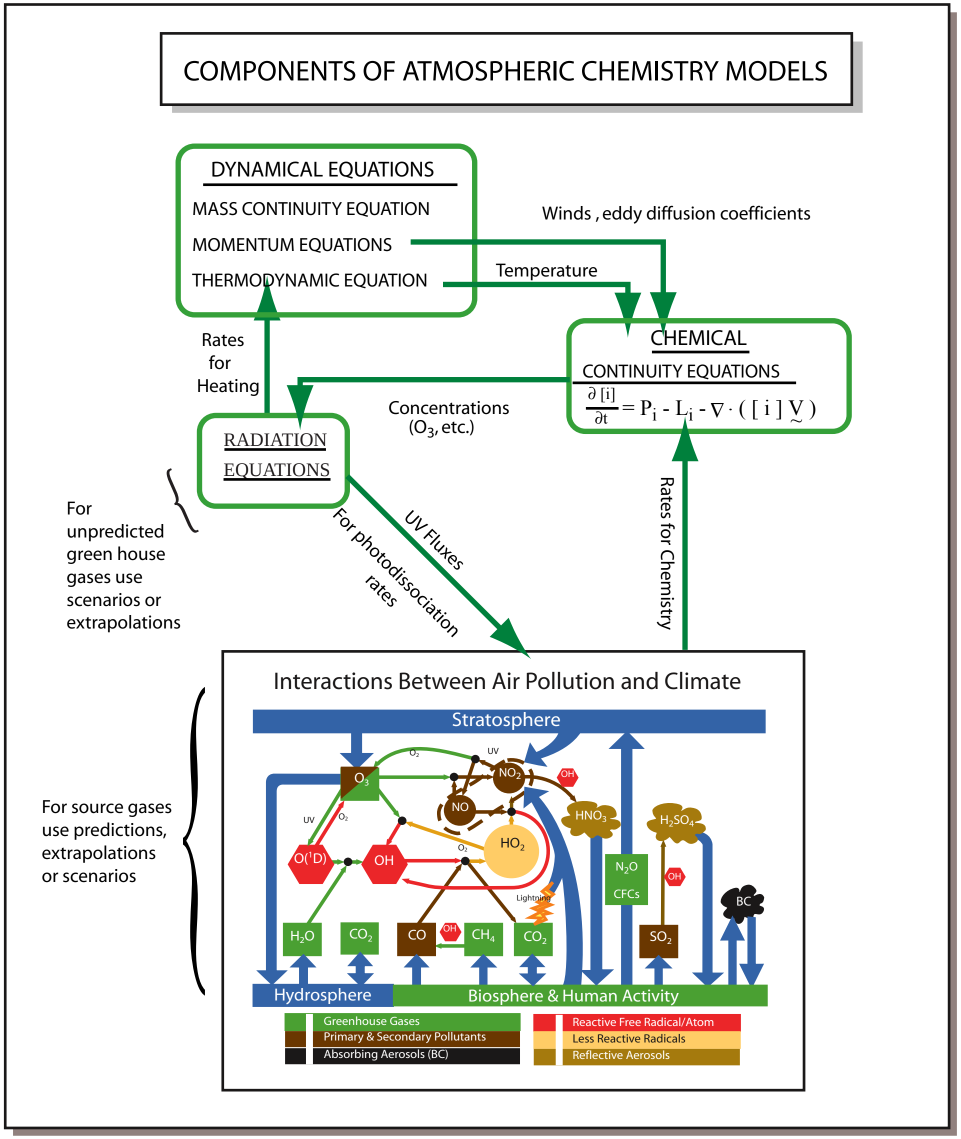


Figure by MIT OCW.

To solve the model equations,we divide the atmosphere into a finite number of boxes (grid cells).

Assume that each variable has the same value throughout the box.

Write a budget for each each box, defining the changes within the box, and the flows between the boxes.

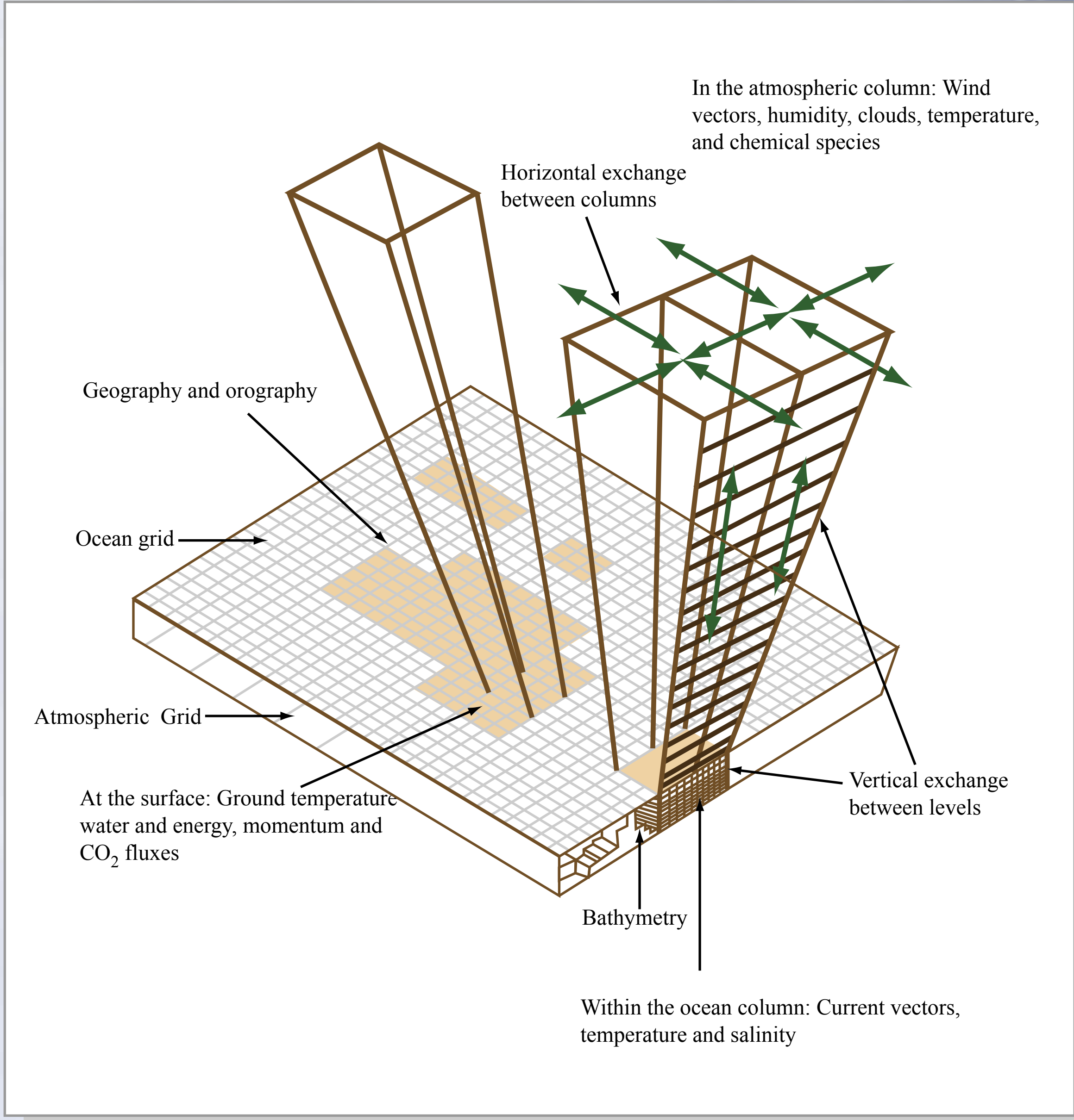


Figure by MIT OCW.

Combining Chemistry and Transport: The Continuity Equation

Physical picture:
(Eulerian)

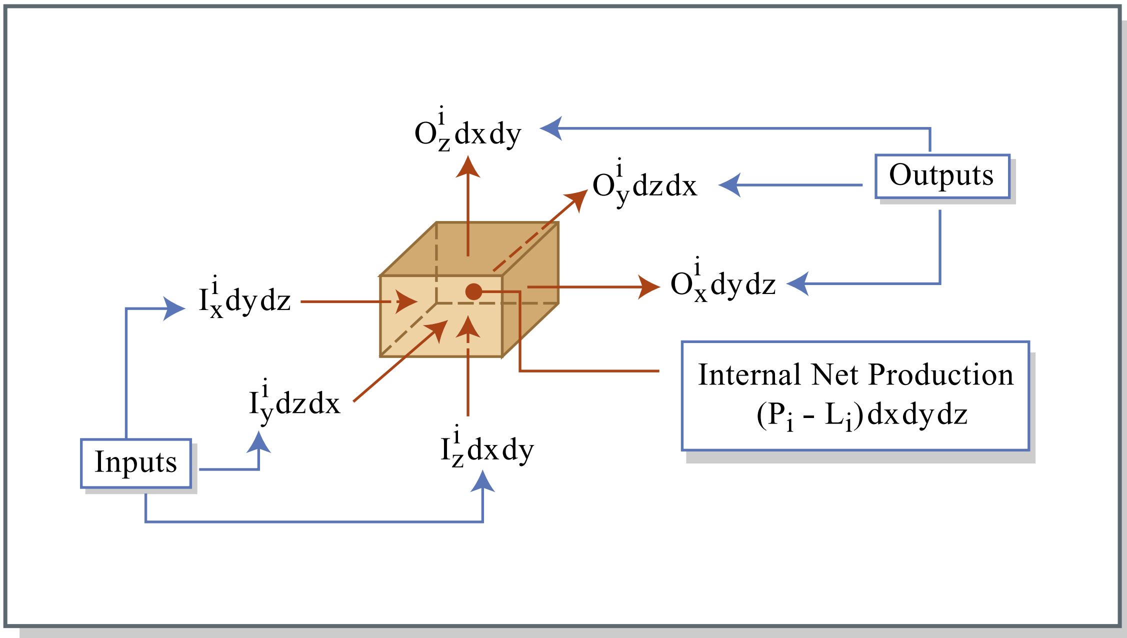


Figure by MIT OCW.

Notation:

Inputs $= I_x^i dydz + I_y^i dzdx + I_z^i dxdy$

Outputs $= O_x^i dydz + O_y^i dzdx + O_z^i dxdy$

$$= \left[I_x^i + \frac{\partial I_x^i}{\partial x} dx \right] dydz + \left[I_y^i + \frac{\partial I_y^i}{\partial y} dy \right] dzdx + \left[I_z^i + \frac{\partial I_z^i}{\partial z} dz \right] dxdy$$

$I_x^i = [i]u,\ I_y^i = [i]v,\ I_z^i = [i]w$ (input fluxes)

$u = \frac{dx}{dt},\quad v = \frac{dy}{dt},\quad w = \frac{dz}{dt}$ (wind velocities)

$P_i,\ L_i$ = rates of chemical production, loss

$[i]$ = concentration of i

Local rate of change of [i] given by:

$$\frac{\partial [i]}{\partial t} = \frac{\text{Inputs - Outputs + Internal net production}}{dxdydz}$$

$$= P_i - L_i - \frac{\partial}{\partial x}([i]u) - \frac{\partial}{\partial y}([i]v) - \frac{\partial}{\partial z}([i]w)$$

$$= P_i - L_i - \nabla \cdot ([i]\vec{V}) \qquad (1)$$

Continuity equation for i

For total molecular concentration $[M]$, $P_M - L_M \simeq 0$ so:

$$\frac{\partial [M]}{\partial t} = -\nabla \cdot ([M]\vec{V}) \qquad (2)$$

Continuity equation for M

Defining mixing ratio $= [i]/[M] = X_i$:

$$\frac{\partial X_i}{\partial t} = \frac{\partial}{\partial t}\left([i]/[M]\right) = \frac{\frac{\partial [i]}{\partial t}[M] - \frac{\partial [M]}{\partial t}[i]}{[M]^2}$$

$$= \frac{\left(P_i - L_i - \nabla\cdot\left(X_i[M]\vec{V}\right)\right)[M] + \nabla\cdot\left([M]\vec{V}\right)X_i[M]}{[M]^2} \quad \text{(Using equations (1) and (2))}$$

$$== \frac{\left(P_i - L_i - X_i\nabla\cdot\left([M]\vec{V}\right) - [M]\vec{V}\cdot\nabla X_i\right)[M] + \nabla\cdot\left([M]\vec{V}\right)X_i[M]}{[M]^2}$$

$$= \frac{\left(P_i - L_i - [M]\vec{V}\cdot\nabla X_i\right)[M]}{[M]^2}$$

$$= \frac{P_i - L_i}{[M]} - \vec{V}\cdot\nabla X_i \qquad (3)$$

Continuity Equation for i (mixing ratio form)

Theorem: If there is no gradient in the mixing ratio of i $\left(\nabla X_i = 0\right)$ then there can be no local changes in i due to transport.

Rate of change of X_i traveling with the air given by (Lagrangian view):

(a)

$$\frac{dX_i}{dt} = \frac{d}{dt}\left[X_i(x, y, z, t)\right]$$

$$= \frac{\partial X_i}{\partial x}\frac{dx}{dt} + \frac{\partial X_i}{\partial y}\frac{dy}{dt} + \frac{\partial X_i}{\partial z}\frac{dz}{dt} + \frac{\partial X_i}{\partial t} \quad \text{(chain rule)}$$

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

$$= \vec{V}\cdot\nabla X_i + \frac{P_i - L_i}{[M]} - \vec{V}\cdot\nabla X_i \quad \text{(using equation (3))}$$

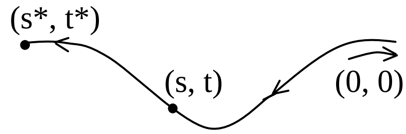
$$= \frac{P_i - L_i}{[M]} \qquad (4)$$

Theorem: If there is no "net chemical production" ($P_i - L_i = 0$), then the mixing ratio of i is conserved moving with the air.

(b)

$$X_{it^*} = X_{i0} + \int_0^{s^*} \frac{dX_i}{dt}\frac{dt}{ds}\,ds$$

$$= X_{i0} + \int_0^{s^*} \frac{P_{is} - L_{is}}{[M]u_s}\,ds \qquad \text{(using equation (4))} \quad (5)$$



<u>Theorem</u>: The change in mixing ratio in an air mass from its initial value is a line integral of the "net chemical production" over the trajectory of the air mass.

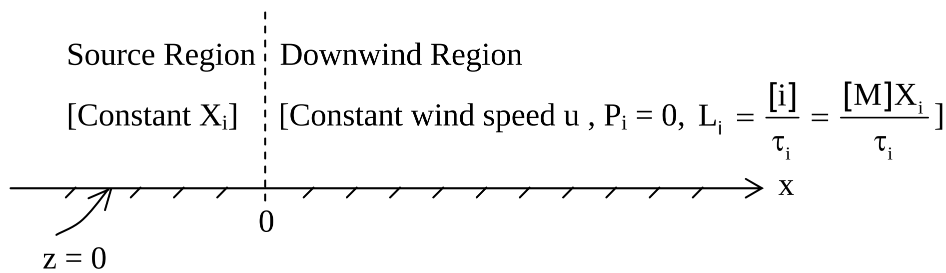
<u>A steady state exists when the local rate of change is zero</u>:

$$\left.\begin{aligned} &\frac{\partial[i]}{\partial t} = 0 \qquad \text{i.e. } P_i - L_i = \nabla\cdot\left([i]\vec{V}\right) \\ &\frac{\partial[M]}{\partial t} = 0 \qquad \text{i.e. } \nabla\cdot\left([M]\vec{V}\right) = 0 \end{aligned}\right\} (6)$$

(6)

$$\frac{\partial X_i}{\partial t} = 0 \qquad \text{i.e. } \frac{P_i - L_i}{[M]} = \vec{V}\cdot\nabla X_i \qquad (7)$$

One-Dimensional (Horizontal) Model



Equation (7) with $v = w = 0$ gives:

$$P_i - L_i = 0 - [M]\frac{X_i}{\tau_i}$$

$$= [M]u\frac{dX_i}{dx}$$

i.e. $$\frac{d\ln X_i}{dx} = -\frac{1}{u\tau_i}$$

i.e. $$X_i(x) = X_i(0)\exp\left(-\frac{x}{u\tau_i}\right) \qquad (8)$$

[chemical (e-folding) distance, $h = u\tau_i$]
[advection time = x/u]

i.e.

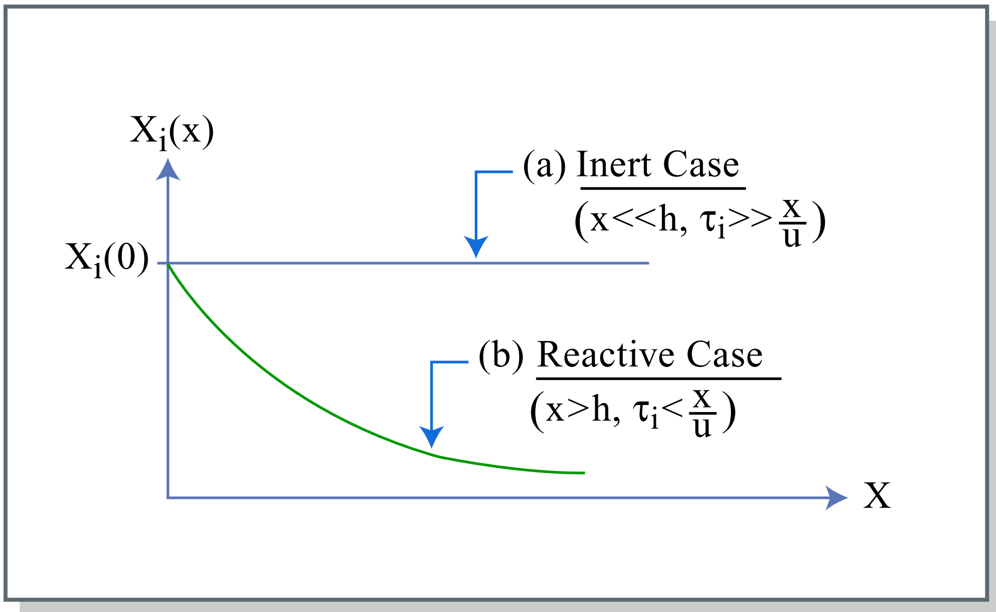


Figure by MIT OCW.