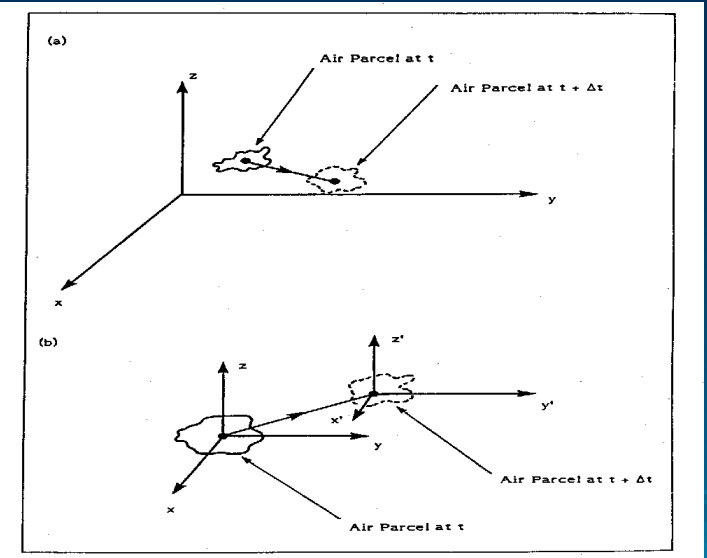
GGS 319
Air Pollution Fundamentals

- ✓ **Concentration Calculation in Eulerian Framework**



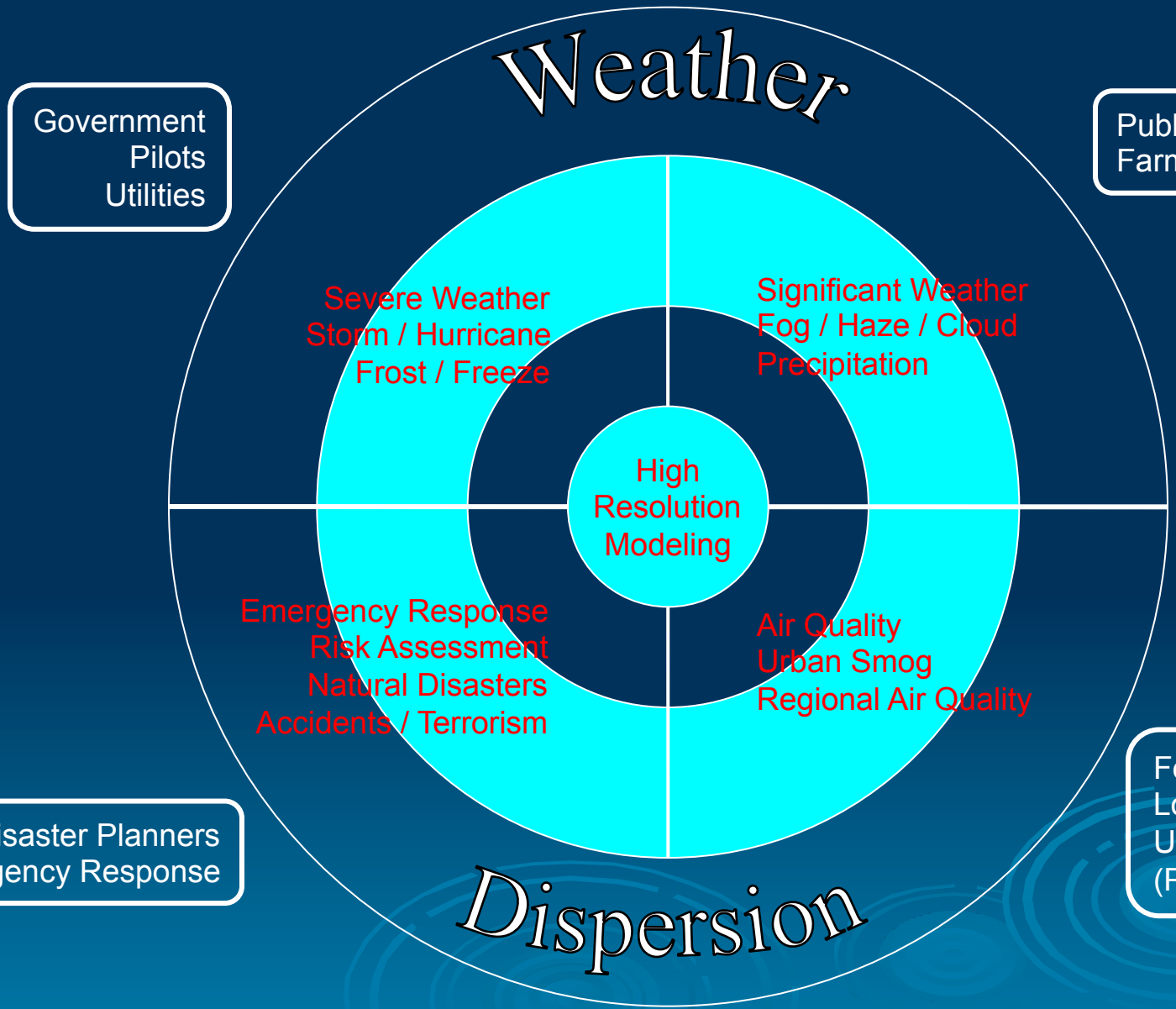
Concentration Calculation

- Eulerian Framework
  - In general, used in atmospheric chemistry modeling
- Lagrangian Framework
  - Gaussian Puff
  - Particle (Monte Carlo)
- Coupled Meteorology - Dispersion Models



Eulerian (a) and Lagrangian (b) reference systems for the atmospheric motion.

High Resolution Modeling

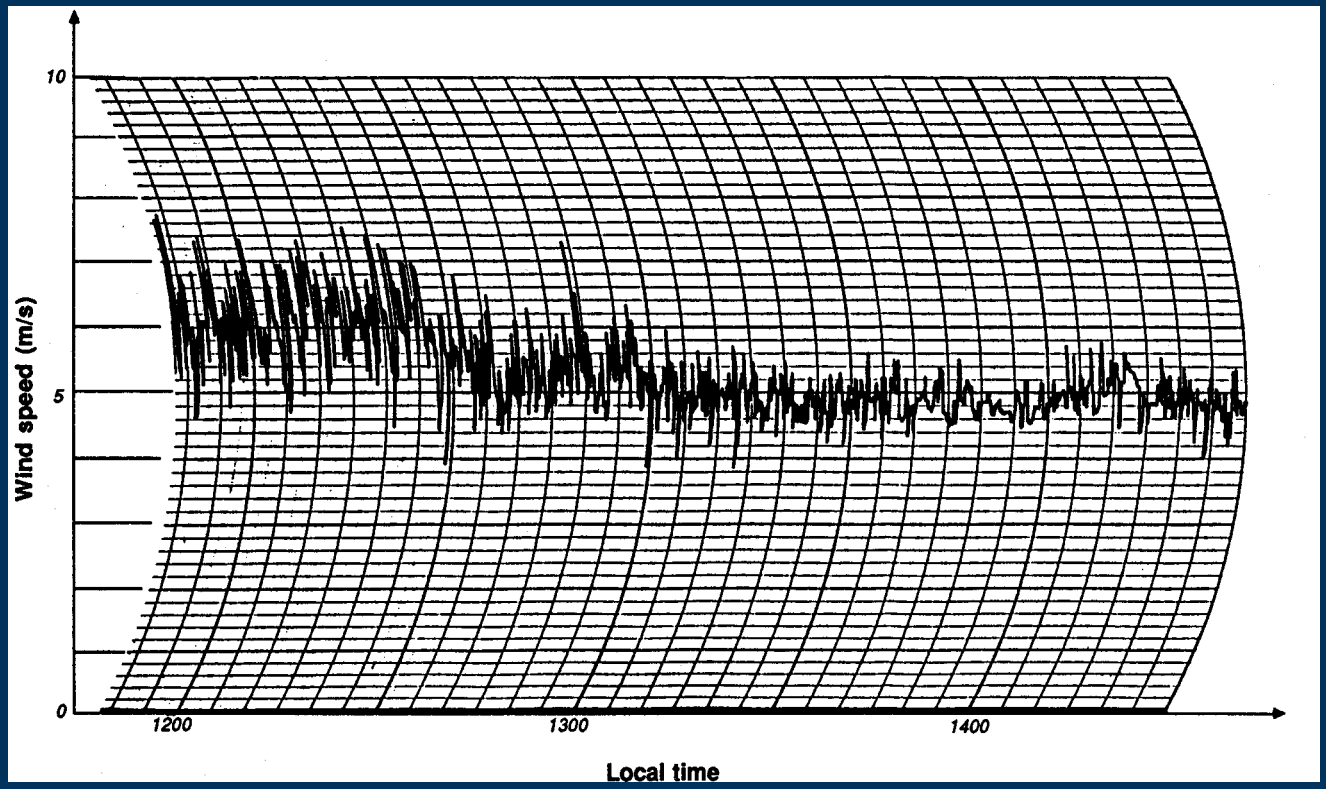


Government
Pilots
Utilities

Public
Farmers

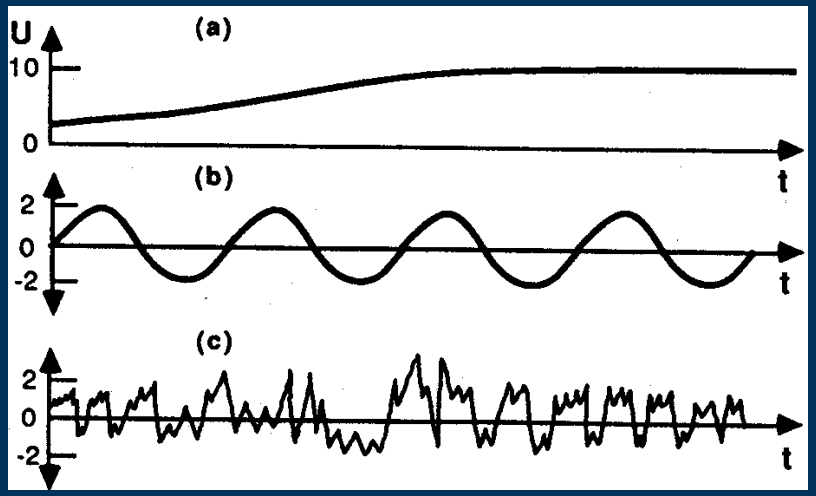
Disaster Planners
Emergency Response

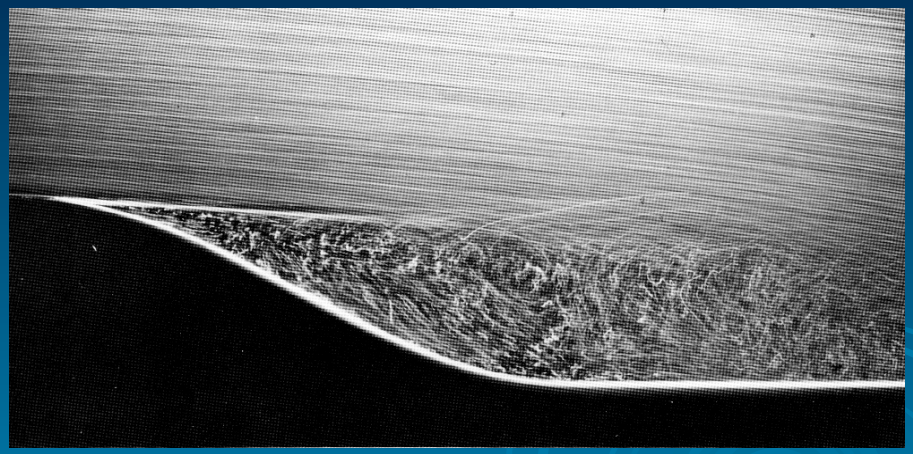
Federal / State /
Local Gov't
Utilities
(Pollution Credit)



- TA common approach is to split variables such as temperature and wind into a mean part and a perturbation part.
- Mean part represents the effects of the mean temperature and mean wind .
- The perturbation part can represent either wave effect or the turbulence effect that is super imposed on the mean wind.

Transport by mean wind, waves and turbulence





- Air flow = mean wind + waves + turbulence
- Each can exist separately, or in the presence of any of the others
- Transport quantities such as moisture, heat, momentum, and pollutants are transported by
  - Mean wind
  - Waves
  - Turbulence

Transport by mean wind, waves and turbulence

- Mean wind
  - Responsible for horizontal transport, or **advection**.
  - **2** to **10 m/s** are common.
  - Friction causes the mean speed to be slowest near the ground.
  - Vertical mean winds are much smaller (on the order of **mm**)
- Waves
  - Frequently occur in the nighttime PBL
  - Generated locally by wind shear and obstacles
  - Effective at transporting momentum and energy
- Turbulence
  - Almost always exist in the PBL
  - This makes PBL different than the rest of the atmosphere
  - Outside of the PBL, CAT exist in convective clouds and jet stream

Mean and Turbulent Parts

$$U = \bar{U} + u'$$

$$V = \bar{V} + v'$$

$$W = \bar{W} + w'$$

$$\theta_v = \overline{\theta_v} + \theta_v'$$

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

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

- Prime quantities represent the part of the flow that varies with periods shorter than about one hour and responsible for diffusion
- The mean (or average) represents the part that varies with a period longer than about one hour and responsible for transport

Eulerian Framework

- Solves a conservation equation for a tracer field
- The Eulerian system is fixed with respect to the earth
- The conservation of mass of a single pollutant species of concentration c(x, y, z, t)

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-V \cdot \nabla c}_{transport} + \underbrace{\nabla^2 Kc}_{diffusion} + \underbrace{S}_{source/sink}$$

Conservation equation

$$\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \rightarrow operator$$

$$K \rightarrow eddy\ diffusivity$$

$$u, v, w \rightarrow wind\ components$$

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/sink}$$

Eulerian Framework

- Wind components (u,v,w) are known
- Source (S) characteristics are known
  - Geographical location
  - Release rate & duration
- Eddy diffusivity coefficient (K) is specified from PBL turbulence field
- So the only unknown is pollutant field (c)

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/\sin k}$$

The rate of change of pollutant wrt time

The rate of change of pollutant wrt space

Eulerian Framework

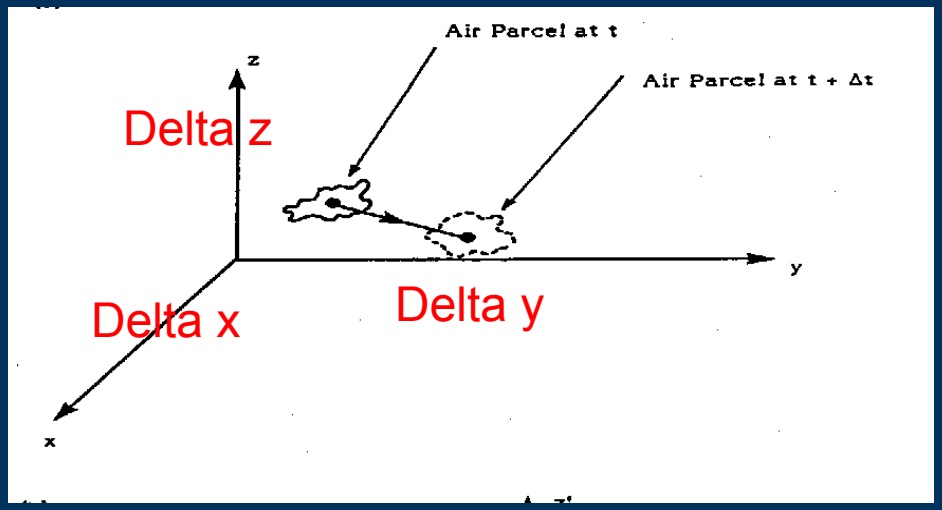
$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/\sin k}$$

How do we solve the transport equation?

- Assign a coordinate system
- Choose a concentration calculation domain
- Set grid calculation points
- Set surface characteristics values (such as terrain height, vegetation cover, etc.)
- Initialize pollutant field
- Set boundary conditions
- Use a numerical method to solve the transport equation
- Ensure the conservation of mass
- The results will give temporal and spatial variations of the pollutant fields

Eulerian Framework (Coordinate System)

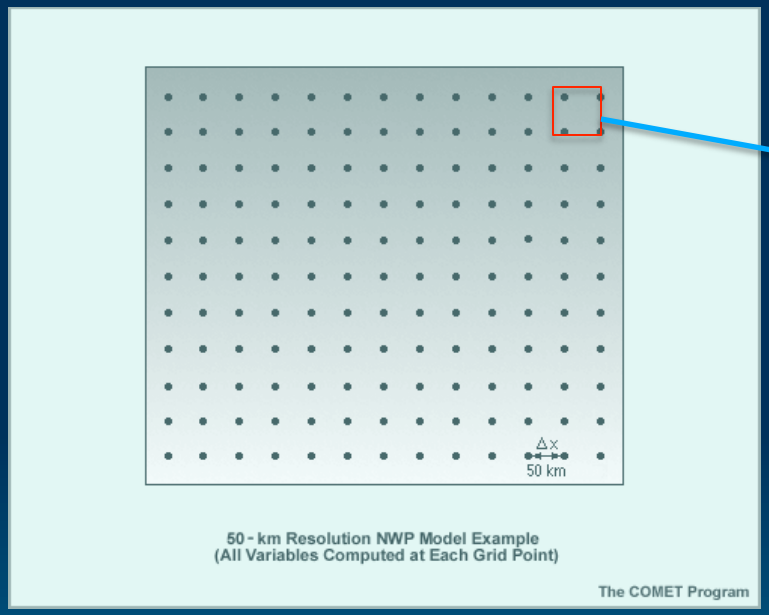
- Assign a coordinate system

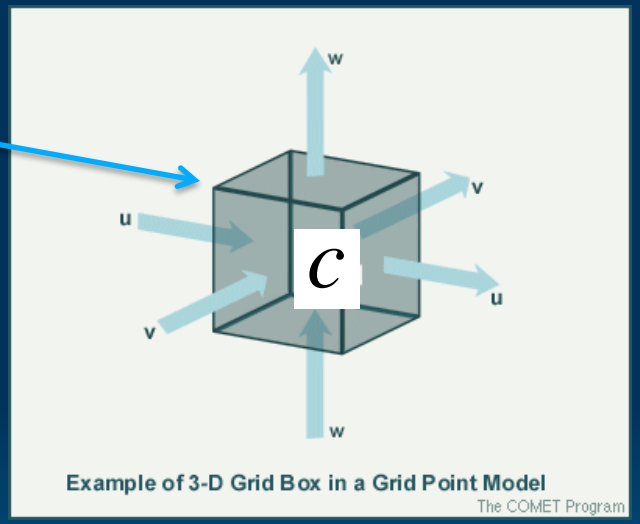


$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/\sin k}$$

Eulerian Framework

- Choose a concentration calculation domain
- Set grid calculation points

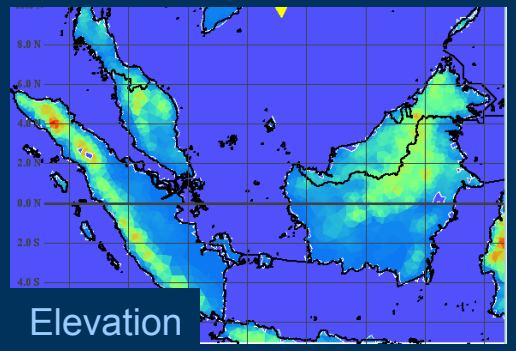


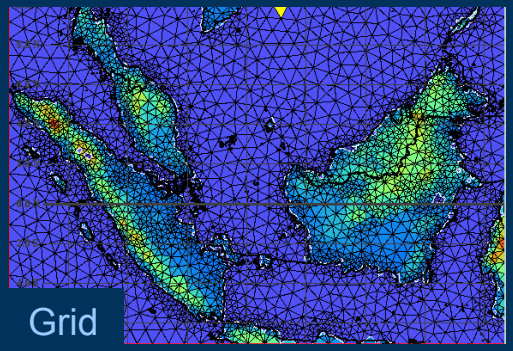


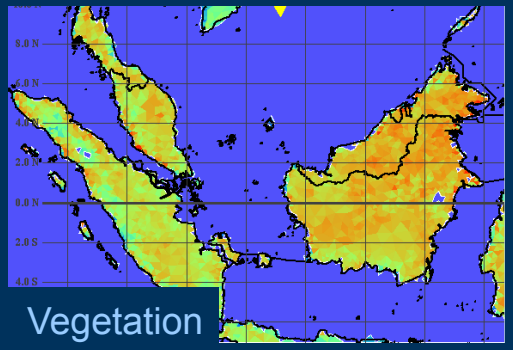
$$\underbrace{\frac{\partial c}{\partial t}}_{\text{time variation}} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{\text{transport term}} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{\text{diffusion term}} + \underbrace{S}_{\text{source/sink}}$$

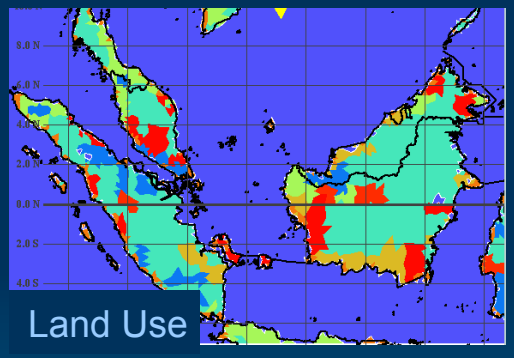
Eulerian Framework

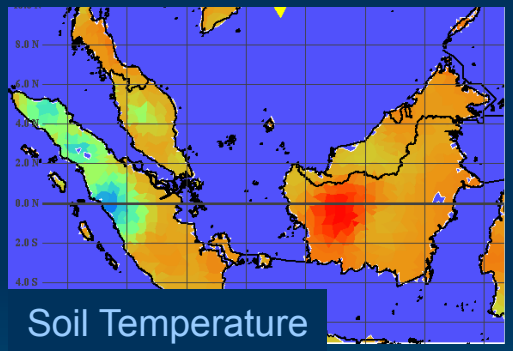
- Set surface characteristics values (such as terrain height, vegetation cover, etc.)

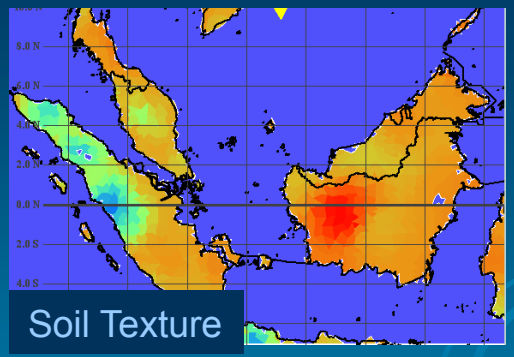


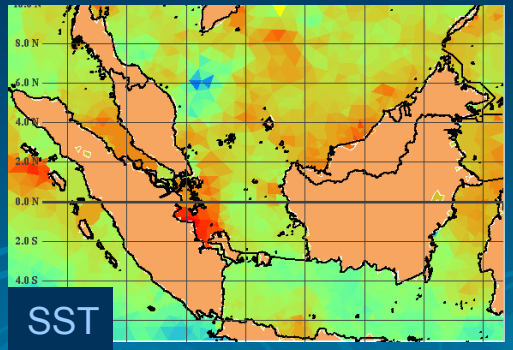


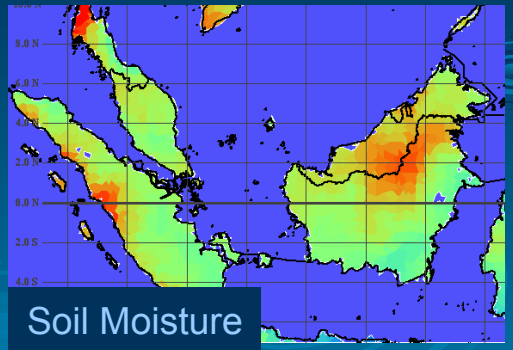






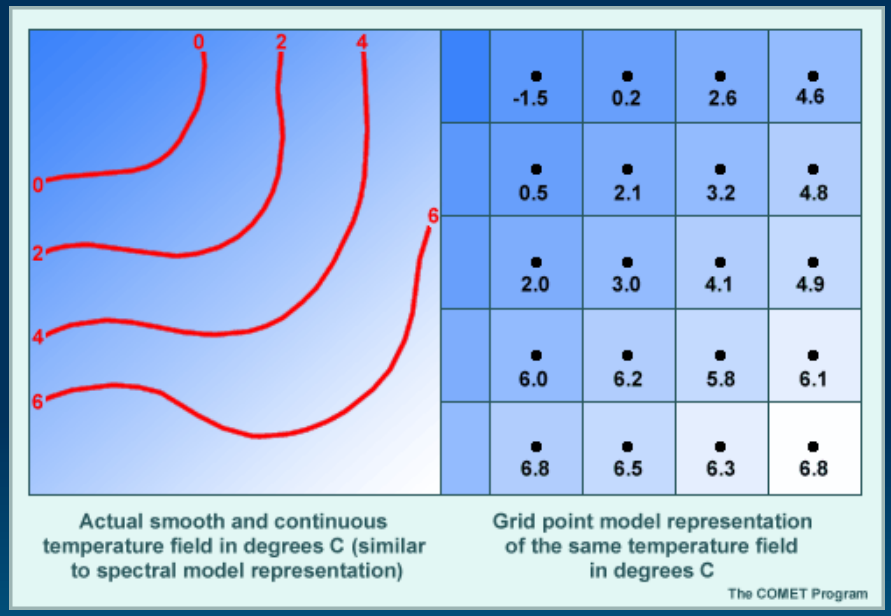






Eulerian Framework

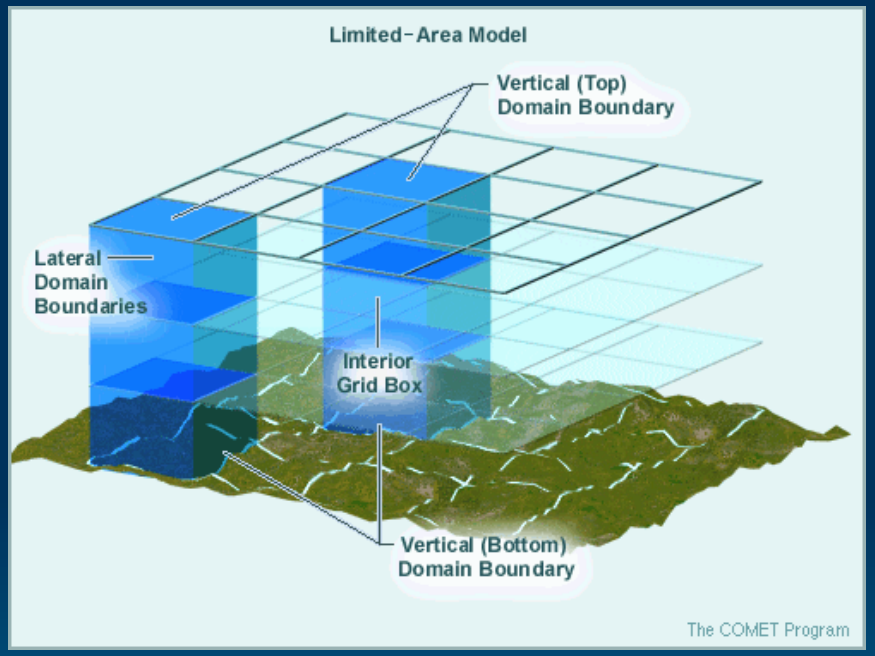
- Initialize pollutant fieldas terrain height, vegetation cover, etc.)

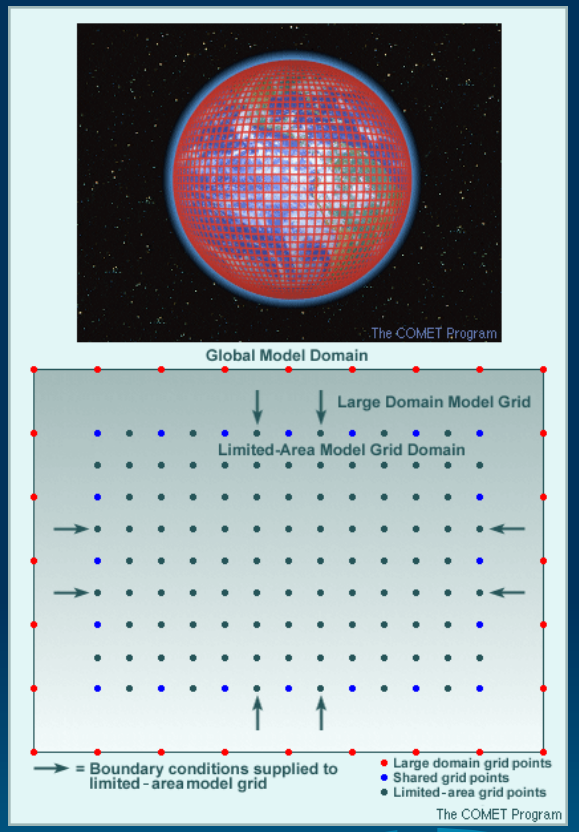


$$\underbrace{\frac{\partial c}{\partial t}}_{\text{time variation}} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{\text{transport term}} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{\text{diffusion term}} + \underbrace{S}_{\text{source/sink}}$$

Eulerian Framework

- Set boundary conditions

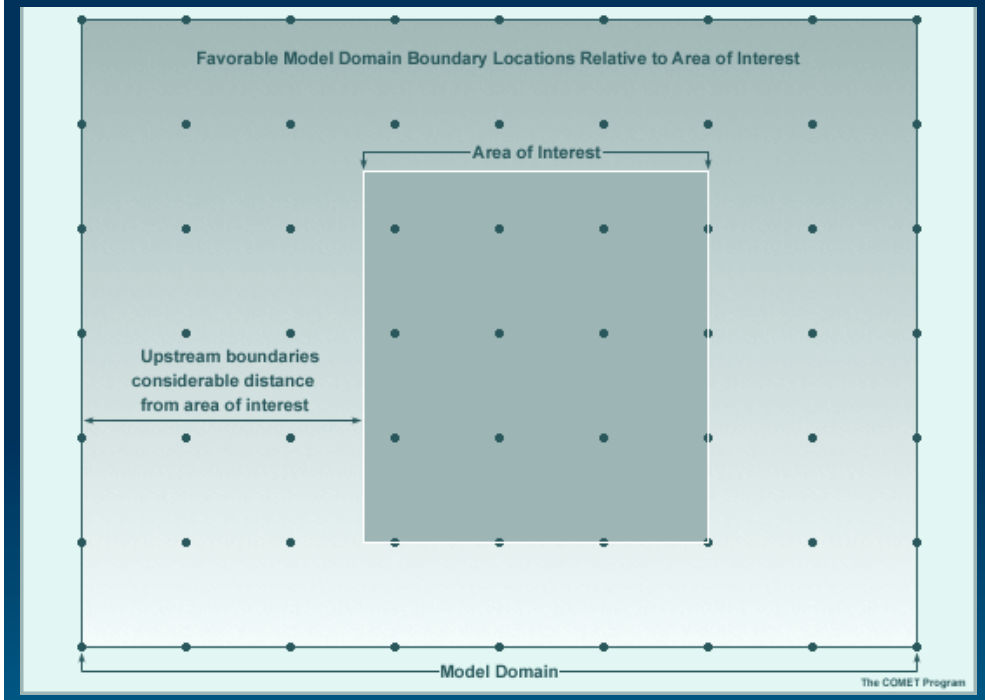


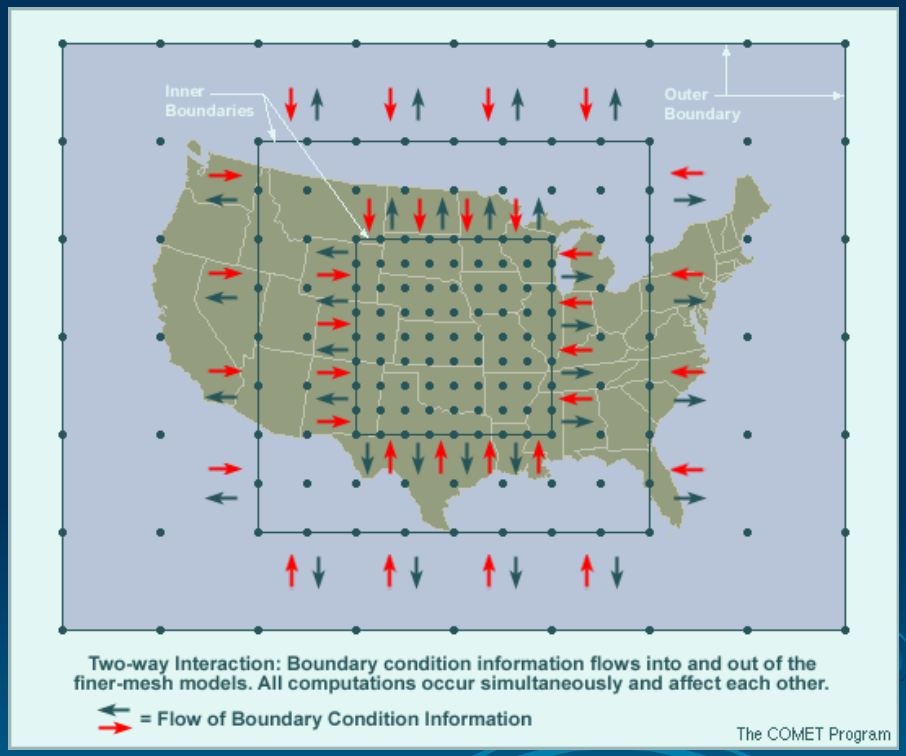


$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/sink}$$

Eulerian Framework

- Set boundary conditions





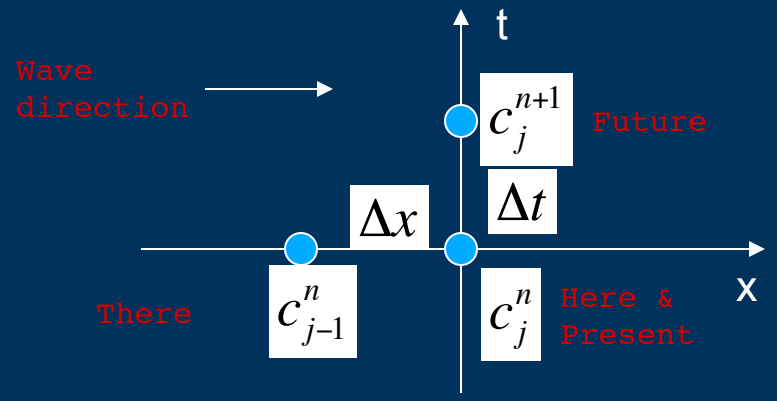
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Eulerian Framework

- Use a numerical method to solve the transport equation
- Finite difference method

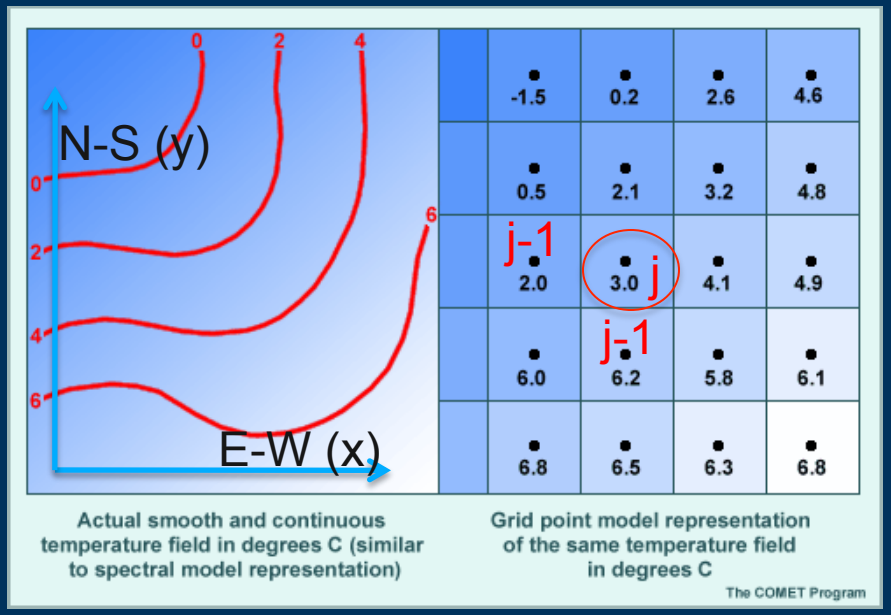
$$\underbrace{\frac{\partial c}{\partial t}}_{\text{time variation}} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{\text{transport term}}$$

$$\frac{c_j^{n+1} - c_j^n}{\Delta t} = -u\left[\frac{c_j^n - c_{j-1}^n}{\Delta x}\right] - v\left[\frac{c_j^n - c_{j-1}^n}{\Delta y}\right] - w\left[\frac{c_j^n - c_{j-1}^n}{\Delta z}\right]$$



$$\underbrace{\frac{\partial c}{\partial t}}_{\text{time variation}} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{\text{transport term}} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{\text{diffusion term}} + \underbrace{S}_{\text{source/sink}}$$

Eulerian Framework



- Assume u=1 m/s & v=1m/s
- Δx = 10km
- Δt = 60 s

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y}}_{transport\ term}$$

$$\frac{c_j^{n+1} - c_j^n}{\Delta t} = -u\left[\frac{c_j^n - c_{j-1}^n}{\Delta x}\right] - v\left[\frac{c_j^n - c_{j-1}^n}{\Delta y}\right]$$

$$c_j^{n+1} = c_j^n - \left[u\left(\frac{c_j^n - c_{j-1}^n}{\Delta x}\right) + v\left(\frac{c_j^n - c_{j-1}^n}{\Delta y}\right)\right]\Delta t$$

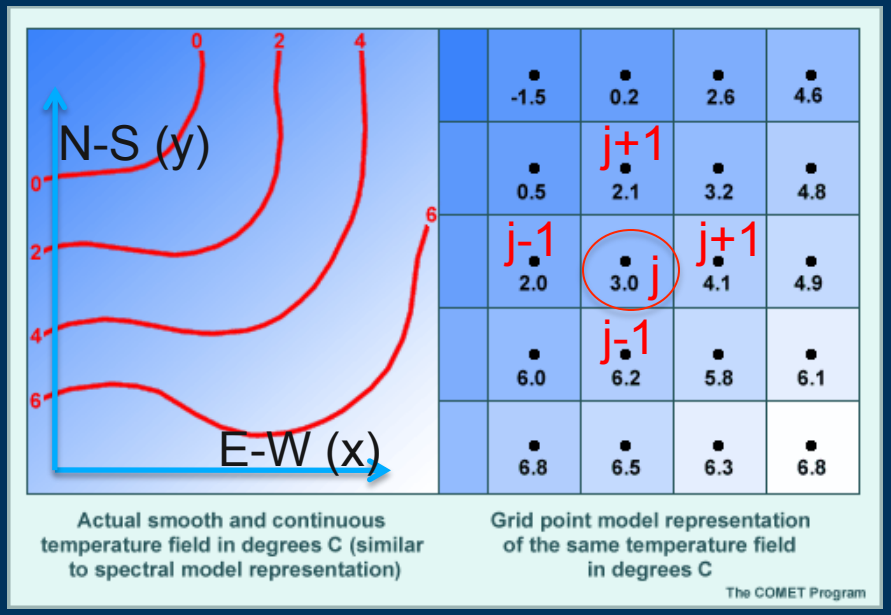
$$c_j^{n+1} = 3.0gm/kg - \left[1m/s\left(\frac{3.0gm/kg - 2.0gm/kg}{10000m}\right) + 1m/s\left(\frac{3.0gm/kg - 6.2gm/kg}{10000m}\right)\right]60s$$

$$c_j^{n+1} = 3.0gm/kg - \left[1m/s \times \frac{1.0gm/kg - 3.2gm/kg}{10000m}\right]60s$$

$$c_j^{n+1} = 3.0gm/kg - 0.0132gm/kg$$

$$c_j^{n+1} = 2.9868gm/kg$$

Eulerian Framework



- Assume u=1 m/s & v=1m/s
- Δx = 10km
- Δt = 60 s

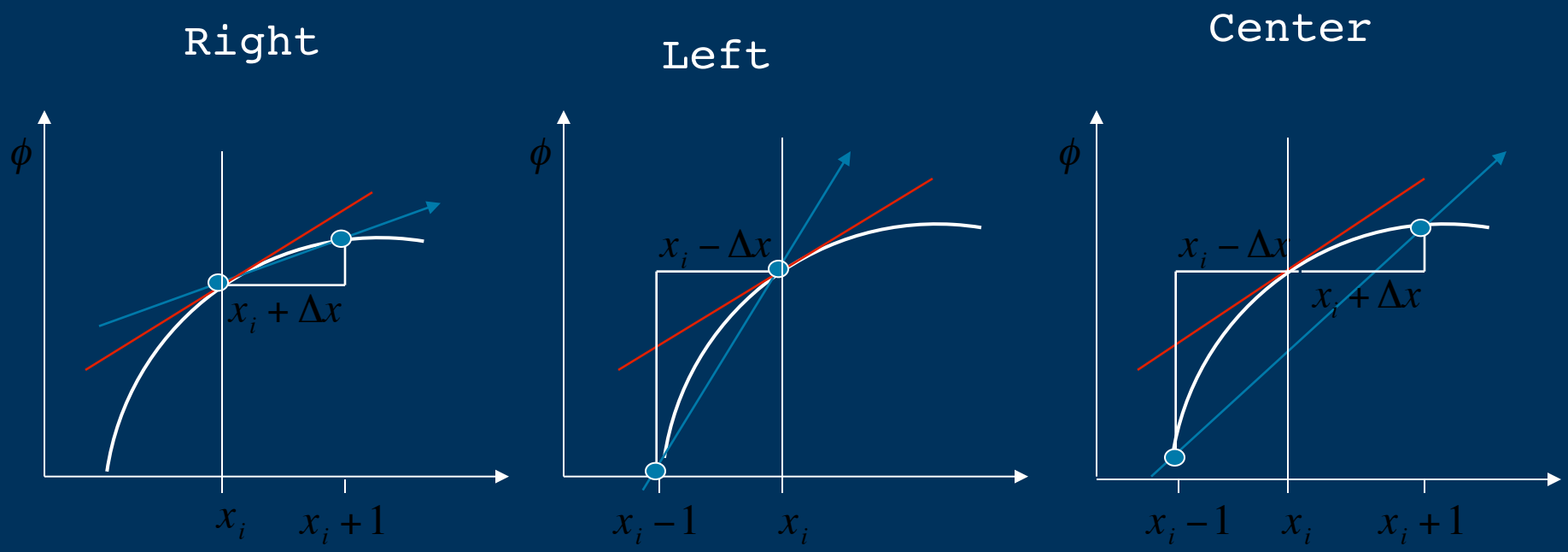
$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y}}_{transport\ term}$$

$$\frac{c_j^{n+1} - c_j^n}{\Delta t} = -u\left[\frac{c_{j+1}^n - c_{j-1}^n}{2\Delta x}\right] - v\left[\frac{c_{j+1}^n - c_{j-1}^n}{2\Delta y}\right]$$

$$c_j^{n+1} = c_j^n - \left[u\left(\frac{c_{j+1}^n - c_{j-1}^n}{2\Delta x}\right) + v\left(\frac{c_{j+1}^n - c_{j-1}^n}{2\Delta y}\right)\right]\Delta t$$

HW = Calculate j point future value based on the center difference scheme

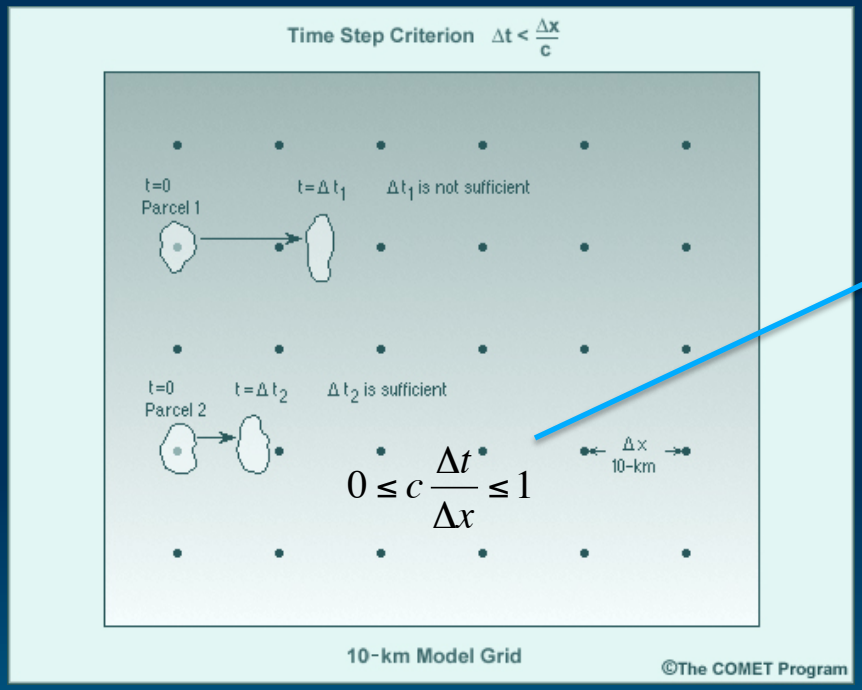
Eulerian Framework



- Blue line – estimate of derivative, red line – true derivative
- Discretizing space creates a grid spacing Δx
- Therefore, we introduce errors that should increase as Δx get larger.

Eulerian Framework

- Use a numerical method to solve the transport equation

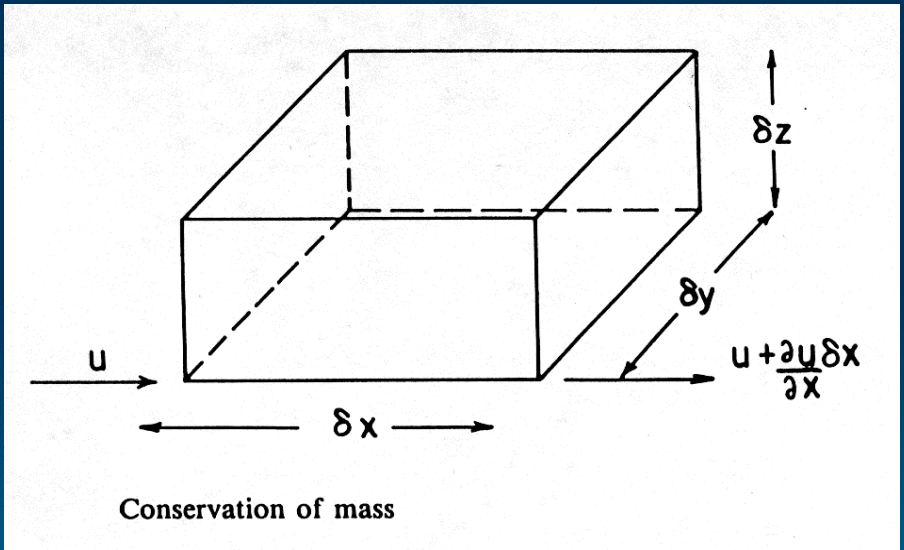


CFL stability condition

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/sink}$$

Eulerian Framework

- Conservation of Mass
- Inflow mass = outflow mass



Conservation of mass

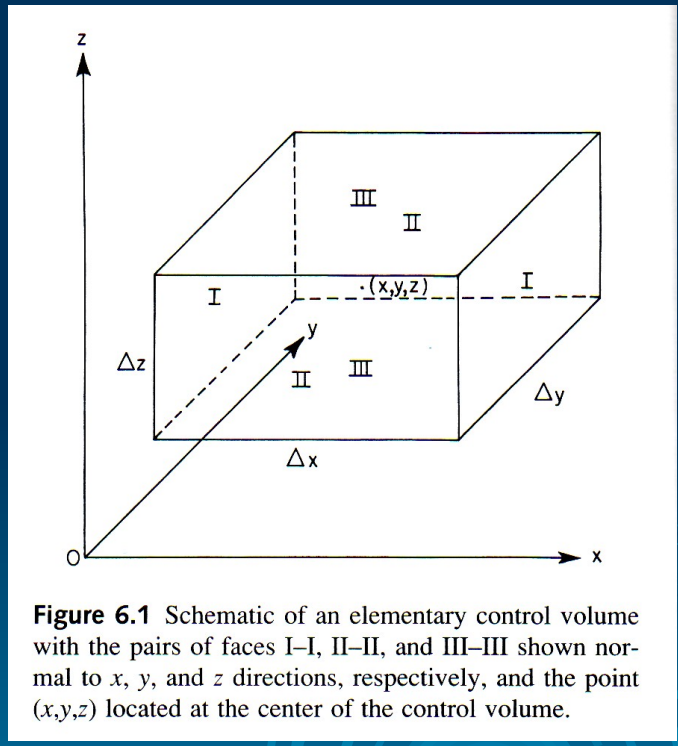


Figure 6.1 Schematic of an elementary control volume with the pairs of faces I–I, II–II, and III–III shown normal to x, y, and z directions, respectively, and the point (x,y,z) located at the center of the control volume.

Eulerian Framework

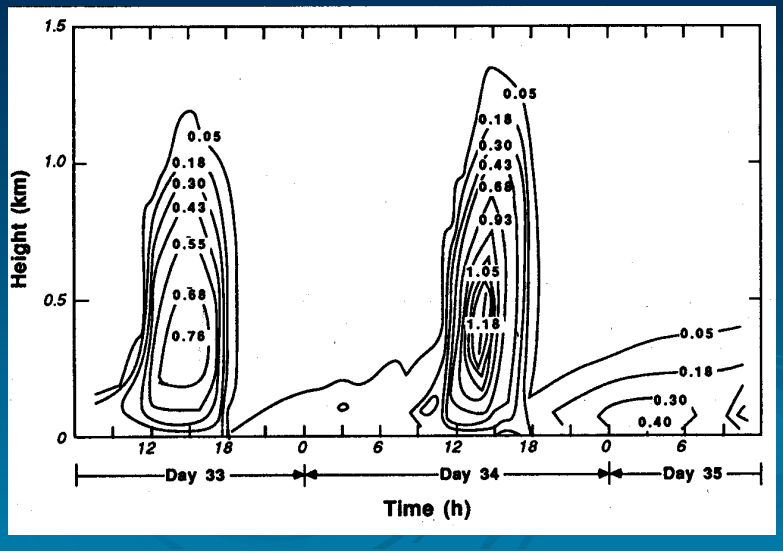
- So far we have solved the transport term
- What about the diffusion term?
- Solving diffusion term is not a trivial task!
- K (eddy diffusivity) needs to be specified (e.g., as a function of turbulent kinetic energy).

  K ~ 1.5 10-5 m^2/s for air
- Therefore, we will examine the solution graphically.

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/sink}$$

Turbulence Kinetic Energy

- **Term: Storage**
  - There is a substantial variation in the magnitude of TKE with time at any one height
  - An increase in TKE from a small early morning value to a larger early afternoon value represents a net storage of TKE in the air
  - During the later afternoon and evening, a corresponding decrease of TKE with time occurs where dissipation and other losses exceed the production of turbulence
  - The storage term is thus negative during this transition phase

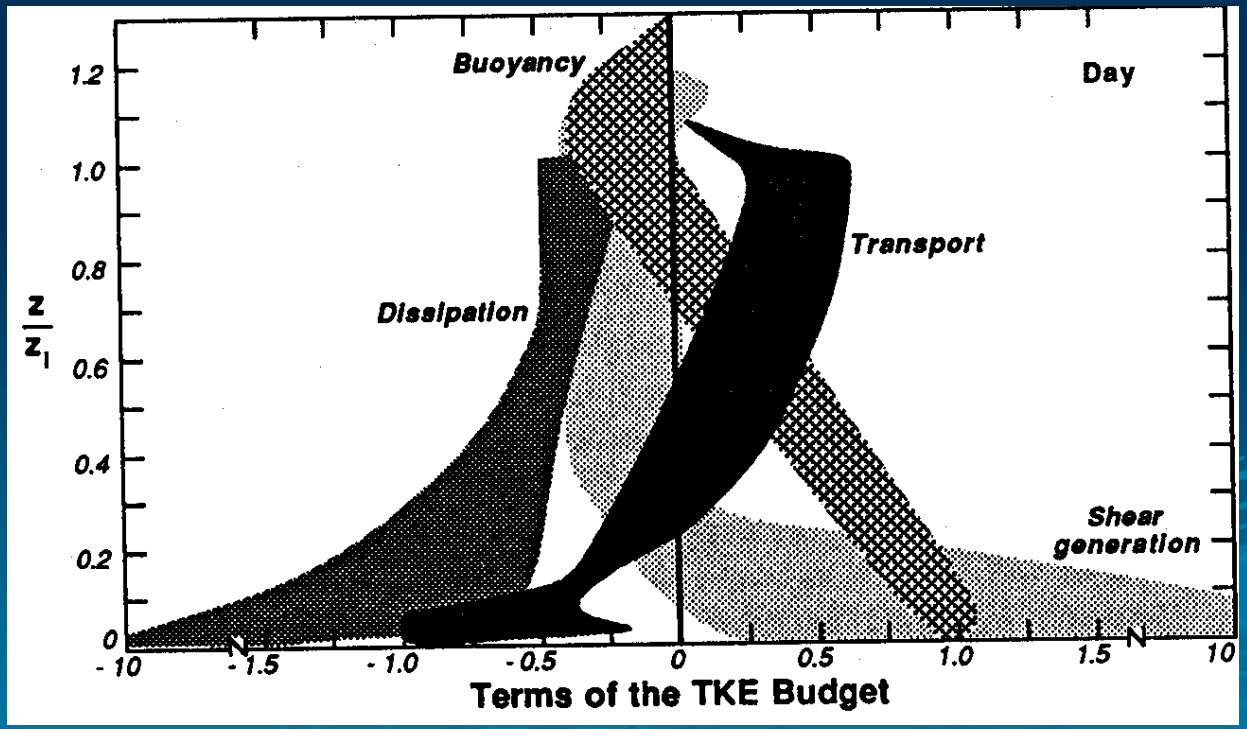


Turbulence Kinetic Energy

- **Term: Transport**
  - Little is known about this term
  - When averaged over a horizontal area larger than about 10 km by 10 km, it is often assumed that there is little horizontal variation in TKE
  - Thereby making the advection term negligible
  - On a smaller scale, however, it is clear that this term must be important (e.g., reservoir of water)
  - Over ocean surfaces, the advection term would probably be negligible even on the small scales

Turbulence Kinetic Energy

- **Term: Buoyant production/consumption**
  - The figure shows the variation of a number of TKE budget terms with height within a fair-weather convective boundary layer



Turbulence Kinetic Energy

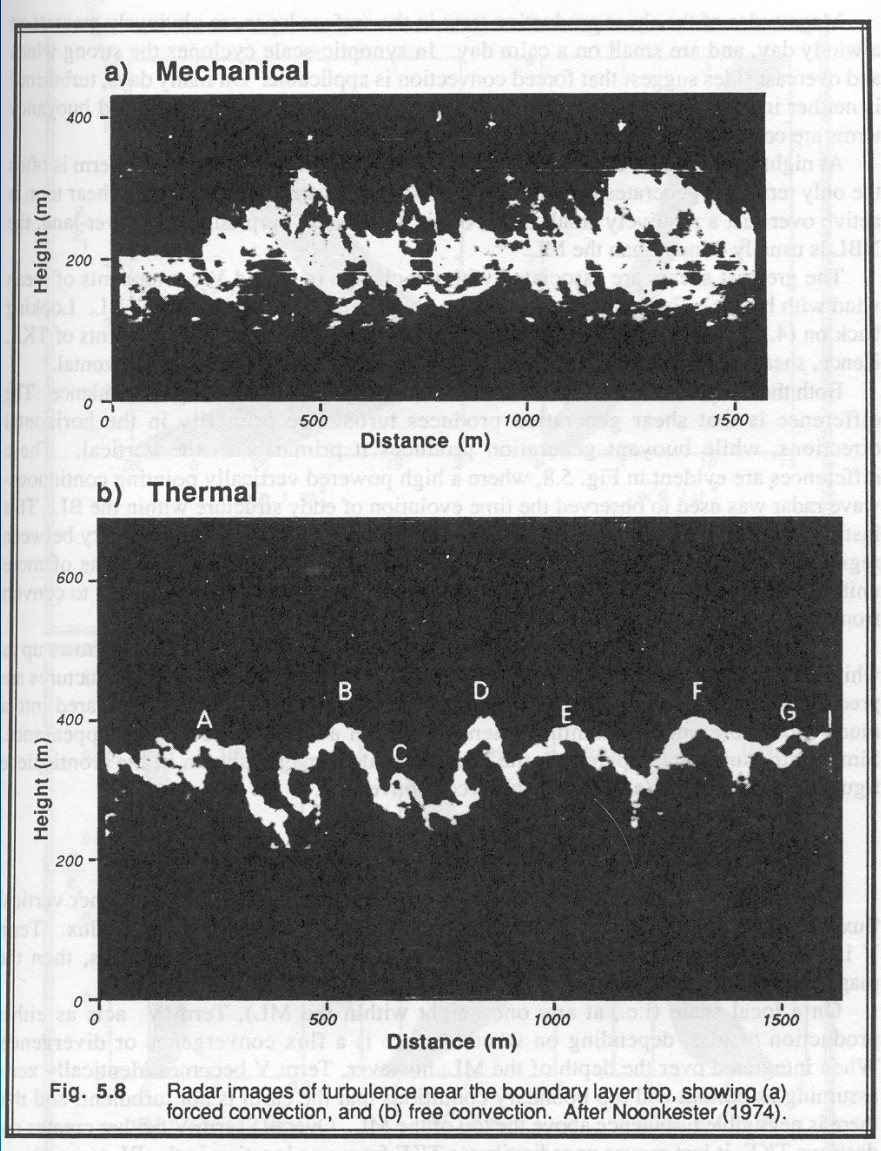


Fig. 5.8 Radar images of turbulence near the boundary layer top, showing (a) forced convection, and (b) free convection. After Noonkester (1974).

- ✓ Both the buoyant and shear production terms can generate anisotropic turbulence
- ✓ The difference is that shear generation produces turbulence primarily in the horizontal directions, while buoyant generation produces it primarily in the vertical
- ✓ For forced convection, the eddies are sheared into a much more horizontal orientation, with much more chaotic apprearance

Turbulence Kinetic Energy

- **Term : Dissipation**
  - Molecular destruction of turbulent motions is greatest for the smallest size eddies
  - The more intense this small-scale turbulence. The greater the rate of dissipation
  - Small-scale turbulence is, in turn, driven by the cascade of energy from the larger scales

Turbulence Kinetic Energy

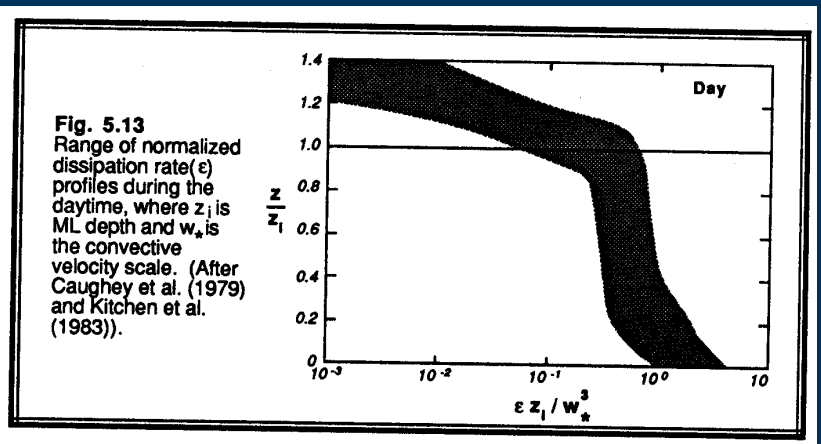


Fig. 5.13
Range of normalized dissipation rate(ε) profiles during the daytime, where z_i is ML depth and w_* is the convective velocity scale. (After Caughey et al. (1979) and Kitchen et al. (1983)).

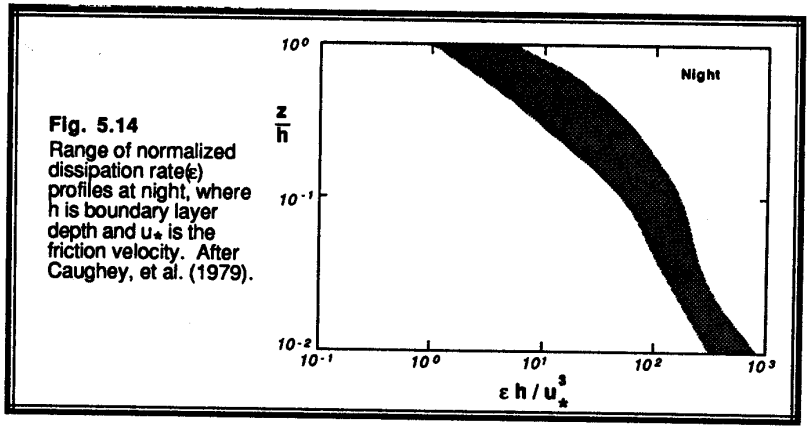


Fig. 5.14
Range of normalized dissipation rate(ε) profiles at night, where h is boundary layer depth and u_* is the friction velocity. After Caughey, et al. (1979).

- **Term: Dissipation**
  - Daytime dissipation rates are often largest near the surface, and then become relatively constant with height in the ML. Above the ML top, the dissipation rate rapidly decreases to near zero
  - At night, both TKE and dissipation rate decrease very rapidly with height
  - Because turbulence is not conserved, the greatest TKEs and hence greatest dissipation rates are frequently found where TKE production is the largest, near the surface

Turbulence Kinetic Energy

Contributions to the TKE Budget

- **Term VII : Dissipation**
  - However, the dissipation rate is not expected to perfectly balance the production rate because of various transport terms in the budget equation
  - The close relationship between TKE production rate, intensity of turbulence, and dissipation rate is shown in the Fig.
  - At night where only shear can produce turbulence, the dissipation rate is small because the associated TKE is small
  - After sunrise buoyant greatly increases the turbulence intensity, resultin

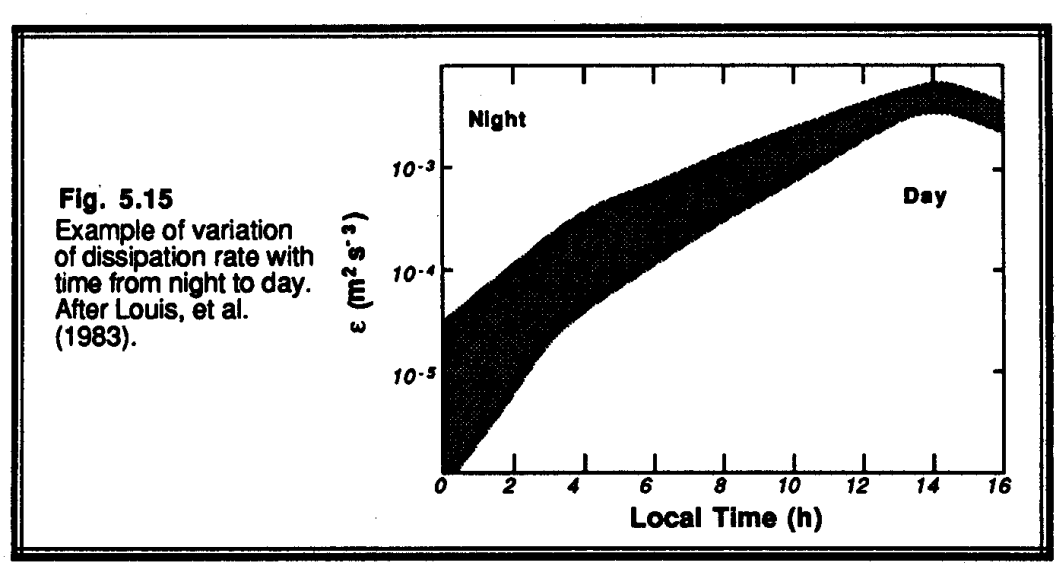
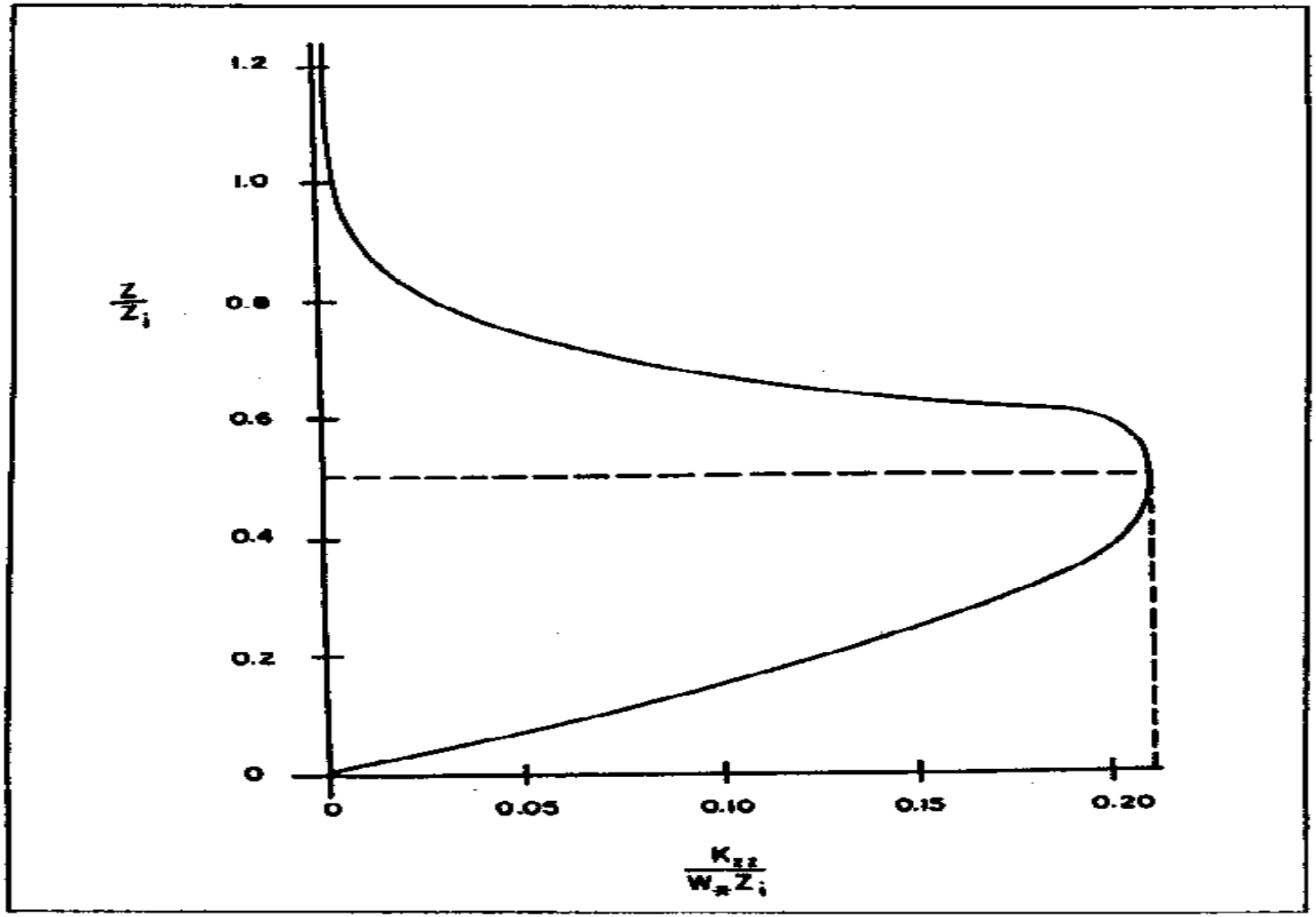


Fig. 5.15
Example of variation of dissipation rate with time from night to day. After Louis, et al. (1983).

K-Theory

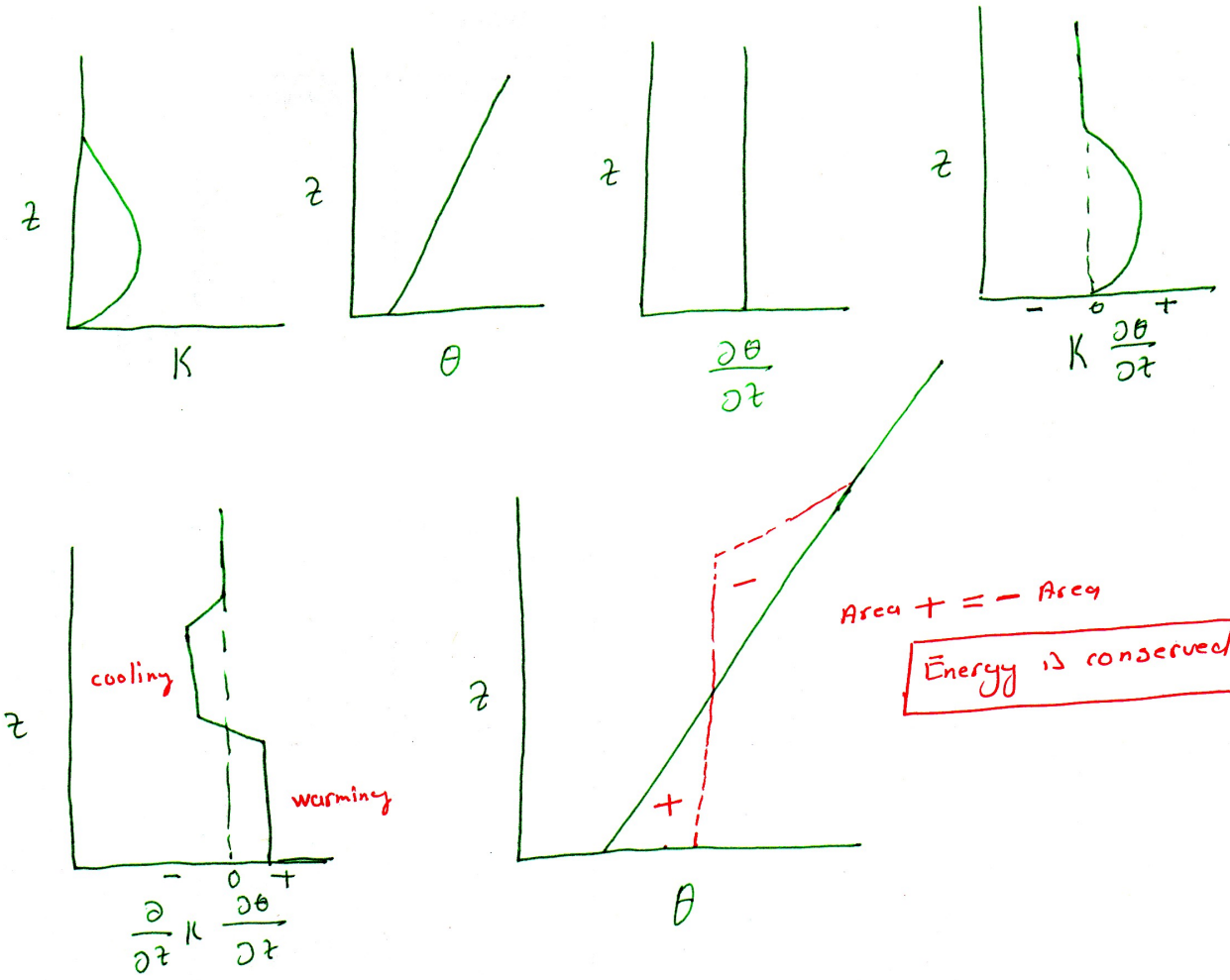
- K is known by a variety of names
  - Eddy viscosity
  - Eddy diffusivity
  - Eddy-transfer coefficient
  - Turbulent transfer coefficient
  - Gradient transfer coefficient
- The eddy diffussivity is best not kept constant, but should be parameterized as a function of the flow
- The parameterizations for K should satisfy the following constraints
  - K=0 where there is no turbulence
  - K = 0 at the ground (z=0)
  - K increases as TKE increases
  - K varies with static stability
  - K is non-negative



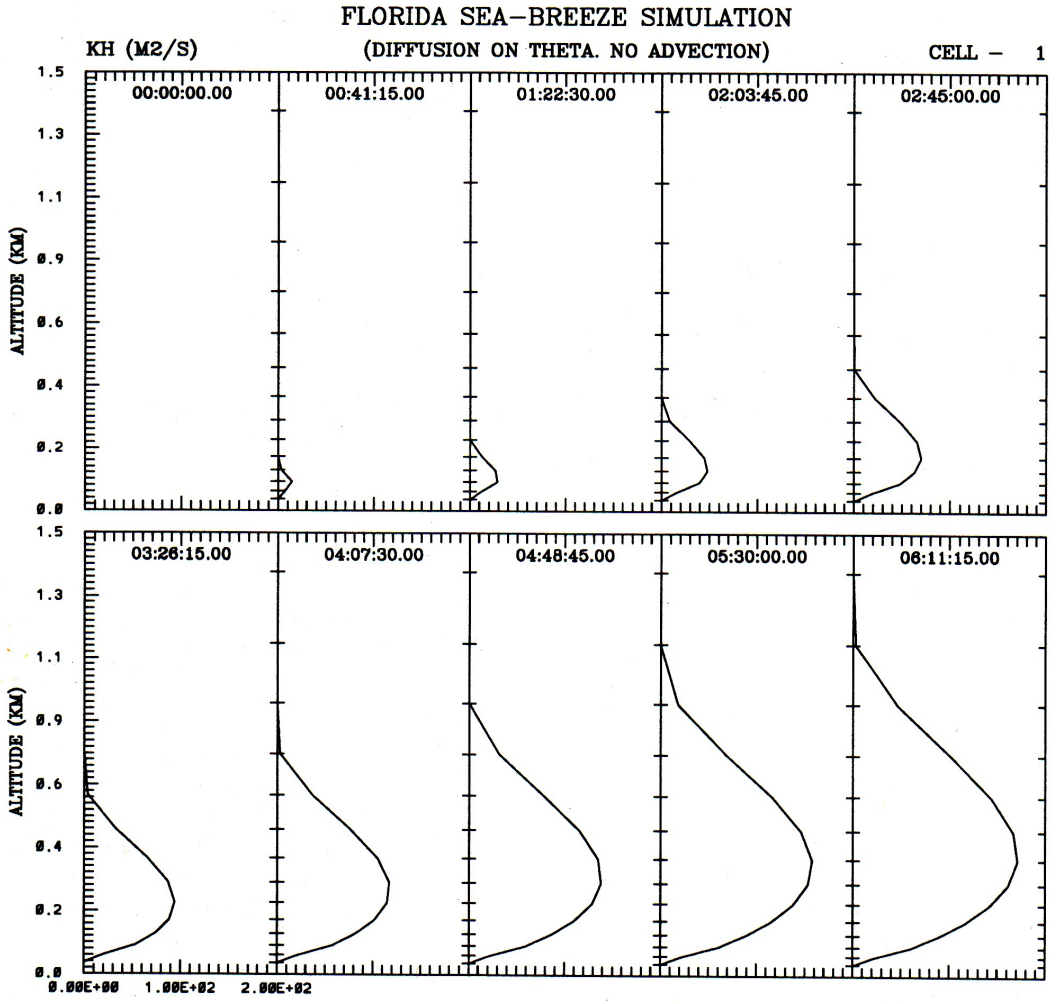
Vertical turbulent diffusivity profile under unstable conditions (from McRae et al., 1982). [Reprinted with permission from Academic Press.]

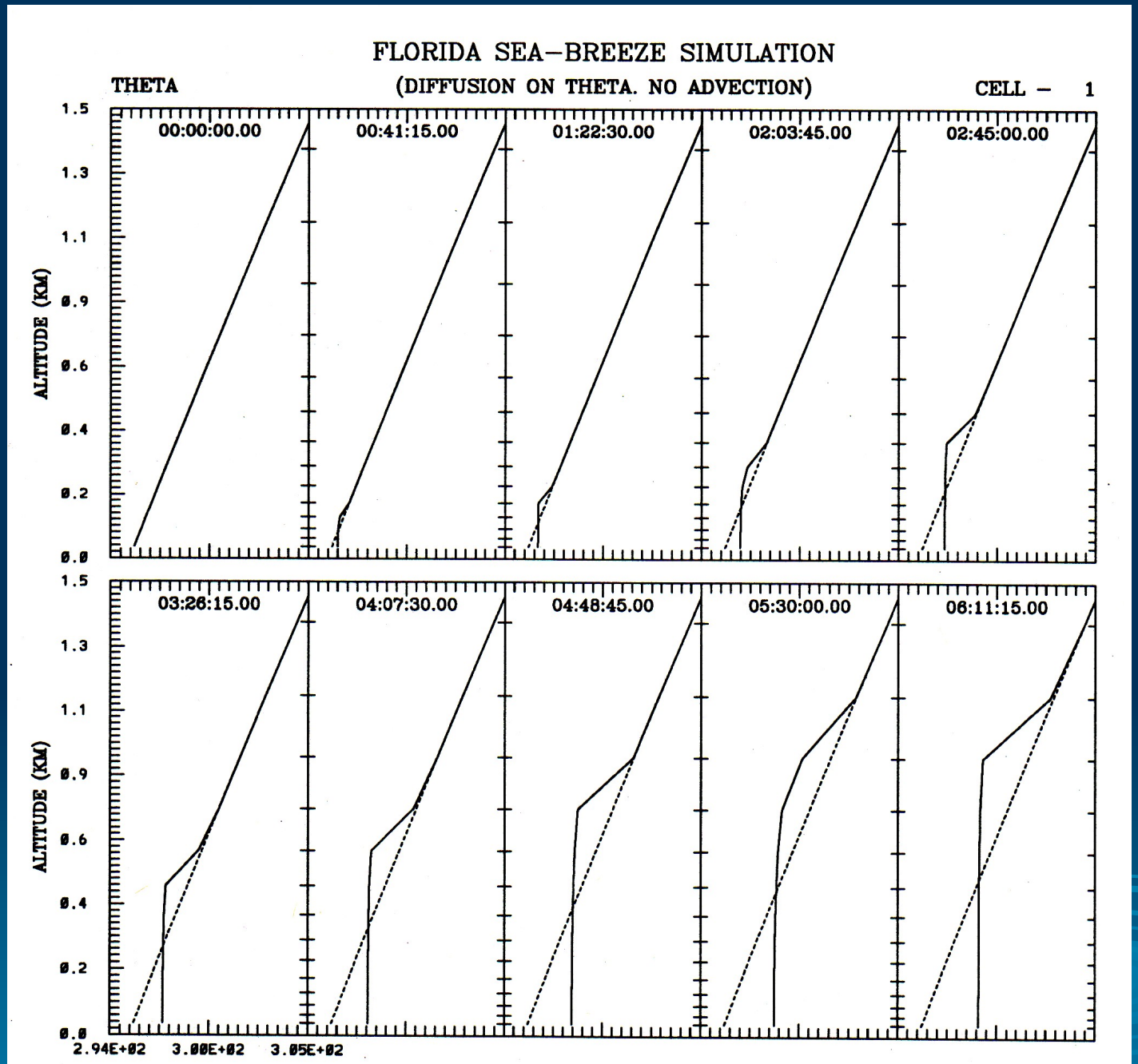
DIFFUSION

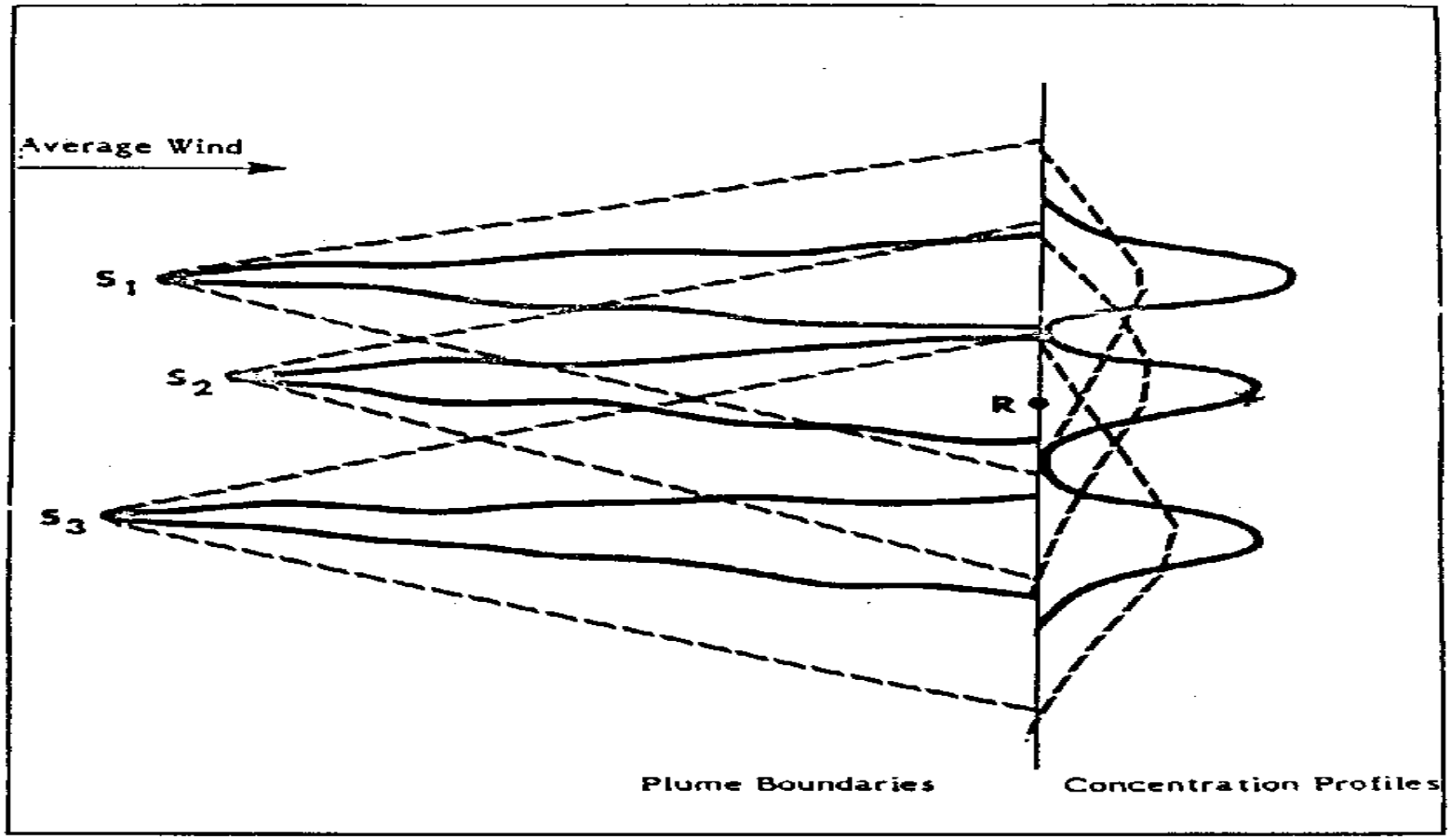
$$\frac{\partial \theta}{\partial t} = - - - \quad \frac{\partial}{\partial z} K \frac{\partial \theta}{\partial z}$$



$$\frac{\partial \theta}{\partial t} = \cdots \frac{\partial}{\partial z} K \frac{\partial \theta}{\partial z}$$




FLORIDA SEA–BREEZE SIMULATION
THETA
(DIFFUSION ON THETA. NO ADVECTION)
CELL – 1
00:00:00.00
00:41:15.00
01:22:30.00
02:03:45.00
02:45:00.00
03:26:15.00
04:07:30.00
04:48:45.00
05:30:00.00
06:11:15.00
ALTITUDE (KM)
1.5
1.3
1.1
0.9
0.6
0.4
0.2
0.0
2.94E+02
3.00E+02
3.05E+02



An example of the consequence of overestimating horizontal diffusion on the concentration at the receptor R. Solid lines show the actual average plume, while dotted lines show the plume as simulated by the model.

Eulerian Framework

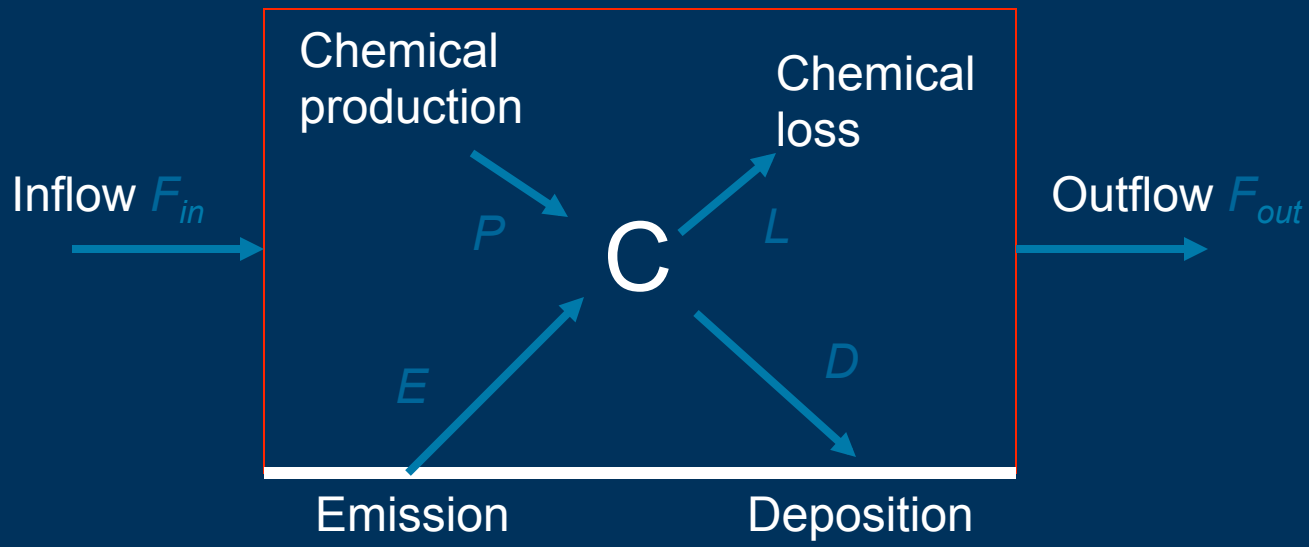
- Mass Conservation
  - Knowledge of source characteristics, such as
    - type of release,
    - source location and geometry, and
    - source strength
  - is a necessary starting point for diffusion estimates

Table 6.2 Idealized Source Characteristics Used for Representing Pollutant Sources in Diffusion Models/Theories

Type of Release	Source Location	Source Geometry
Instantaneous	Ground surface	Point or volume source
Continuous	Elevated in PBL	Line source
Intermittent	Free atmospheric	Area source

  - Note that a source may be characterized by any combination of the type of release, source location and source geometry.

Source & Sink Term



Mass balance equation: $\frac{dm}{dt} = \sum \text{sources} - \sum \text{sinks} = F_{in} + E + P - F_{out} - L - D$

$$\underbrace{\frac{\partial c}{\partial t}}_{time\ variation} = \underbrace{-u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}}_{transport\ term} + \underbrace{\frac{\partial}{\partial x}K\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}K\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}K\frac{\partial c}{\partial z}}_{diffusion\ term} + \underbrace{S}_{source/sink}$$