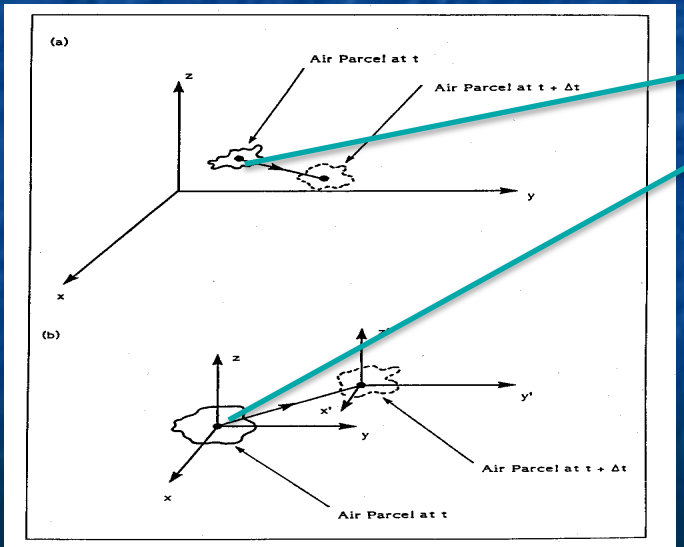
CLIM-319/GGS 319 Air Pollution
Review Guide for Second Exam

Concentration Calculation

- Dispersion Models
  - What is Lagrangian and Eulerian framework?
  - Advantages vs. disadvantages of the frameworks
  - Eulerian Framework
    - In general, used in atmospheric chemistry modeling
  - Lagrangian Framework
    - In general, used in tracer transport and diffusion modeling
      - Gaussian Puff
      - Lagrangian Particle (Monte Carlo)



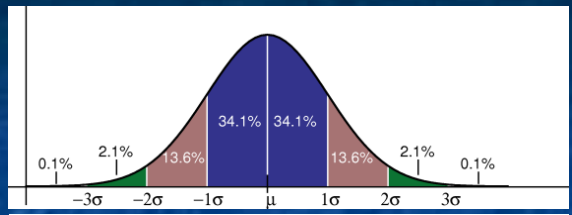
Eulerian (a) and Lagrangian (b) reference systems for the atmospheric motion.

Puff

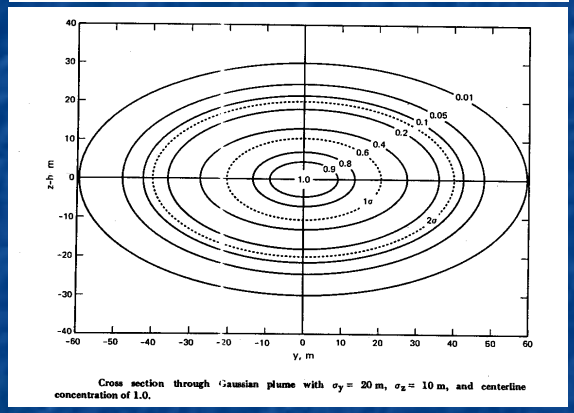
Lecture 7: Concentration Calculation in Lagrangian Framework

Mechanics of concentration calculation

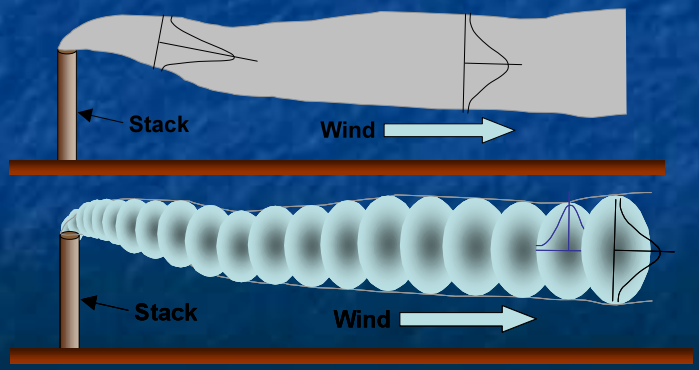
- Gaussian (Normal) distribution
- Gaussian puff identified by
  - Its mass, Q
  - its position, x, y,, z
- Identify source locations
- Source(s) characterization
  - Emission rate
  - Emission duration
- Sequential puff releases



$$\Phi(x,\mu,\sigma)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



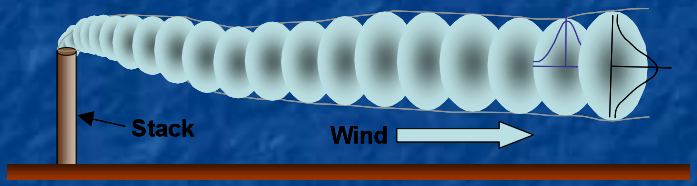
Cross section through Gaussian plume with σ_y = 20 m, σ_z = 10 m, and centerline concentration of 1.0.

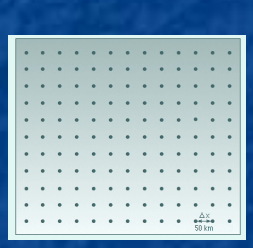


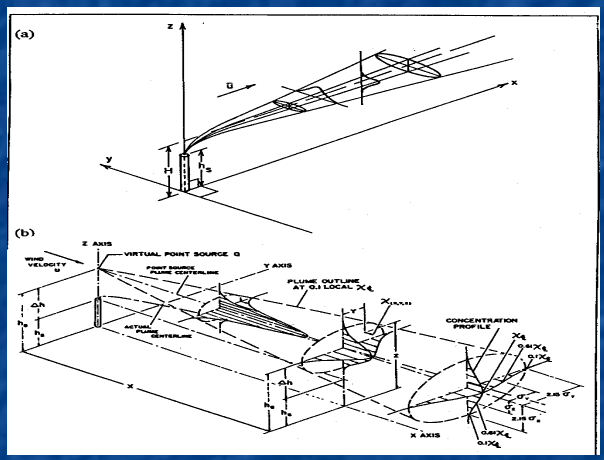
Lecture 7: Concentration Calculation in Lagrangian Framework

- Mechanics of concentration calculation
  - Concentration equation
  - Puff transport + diffusion
    - Puff transport by mean wind
    - Puff diffusion (growth) by turbulence
    - Diffusion (P-G curves)
  - Puff operations
    - Puff split
    - Puff merge
  - Concentration calculation domain
  - Concentration calculation grid
  - Calculation
  - Post-processing
- Uncertainty of the concentration calculation
- Basis and justification for Gaussian models

$$\bar{c}(x,y,z,t) = \frac{Q_{ip}}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right]$$







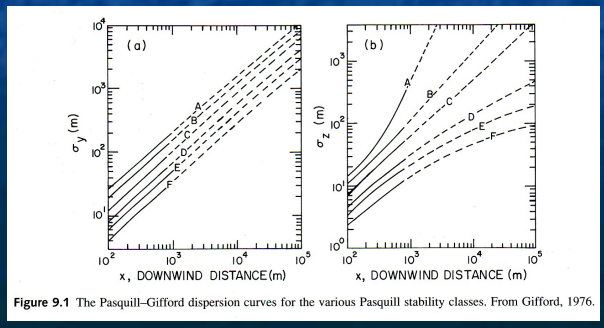


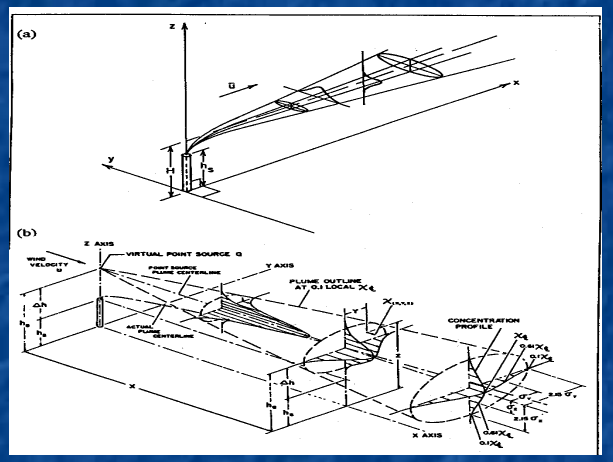
Figure 9.1 The Pasquill–Gifford dispersion curves for the various Pasquill stability classes. From Gifford, 1976.

Lecture 7: Concentration Calculation in Lagrangian Framework

Mechanics of concentration calculation

- Reflecting surface
- Plume rise
- Deposition
- Removal
- Lagrangian particle models
  - Concentration calculation
- Difference between puff & particle models

$$\bar{c}(x,y,z,t;H) = \frac{Q_{ip}}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right]\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right]\right\} \quad (9.12)$$



$$x(t+\Delta t) = x(t) + [u(t) + u_r(t)]\Delta t$$
$$y(t+\Delta t) = y(t) + [v(t) + v_r(t)]\Delta t$$
$$z(t+\Delta t) = z(t) + [w(t) + w_r(t)]\Delta t$$

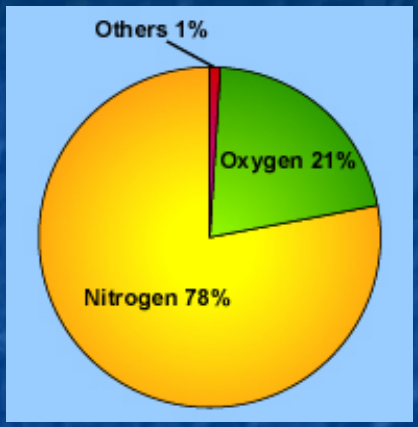
Lecture 8: Concentration Calculation in Eulerian Framework

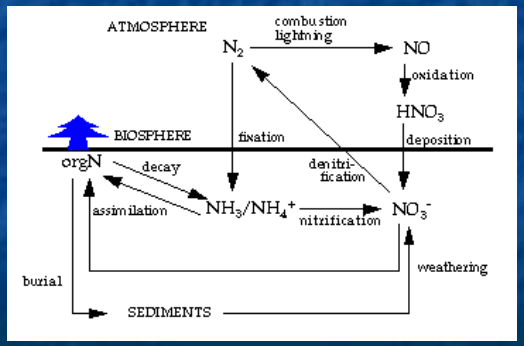
What is Eulerian framework
Advantages vs. disadvantages of the framework
Mechanics of concentration calculation
- Governing equation
- Simulation domain setup
- Grid points
- Initialization
- Numerical method
- Eddy diffusivity coefficient
- Calculation
- Post-processing

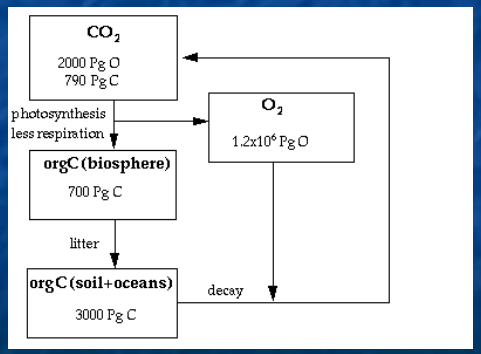
Uncertainty of the concentration calculation
Application of the Eulerian framework

Lecture 9: Geochemical Cycles

What is Earth system?
Early evolution of the atmosphere
The nitrogen geochemical cycle
    No human effect on nitrogen
The oxygen geochemical cycle
    No human effect on O2







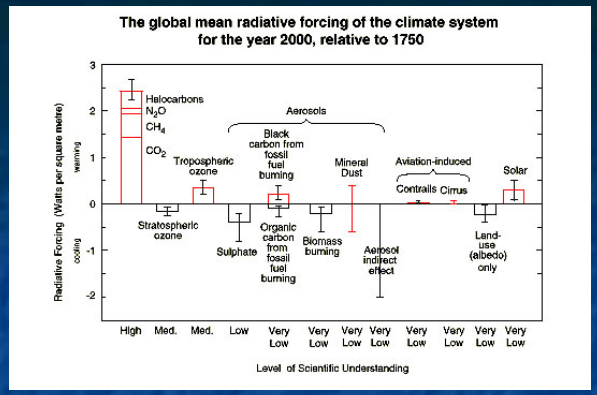
Constituent[a]	Molecular weight	Fractional concentration by volume
Nitrogen (N_2)	28.013	78.08%
Oxygen (O_2)	32.000	20.95%
Argon (Ar)	39.95	0.93%
Water vapor (H_2O)	18.02	0–5%
Carbon dioxide (CO_2)	44.01	380 ppm
Neon (Ne)	20.18	18 ppm
Helium (He)	4.00	5 ppm
Methane (CH_4)	16.04	1.75 ppm
Krypton (Kr)	83.80	1 ppm
Hydrogen (H_2)	2.02	0.5 ppm
Nitrous oxide (N_2O)	56.03	0.3 ppm
Ozone (O_3)	48.00	0–0.1 ppm

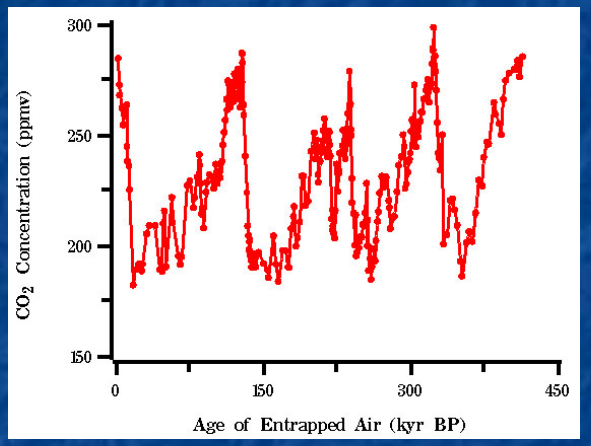
[a] So called *greenhouse gases* are indicated by bold-faced type. For more detailed information on minor constituents, see Table 5.1.

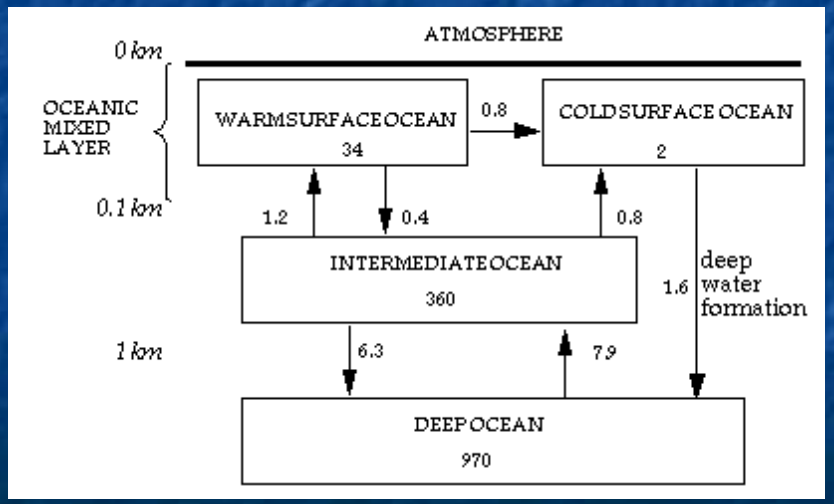
Lecture 9: Geochemical Cycles

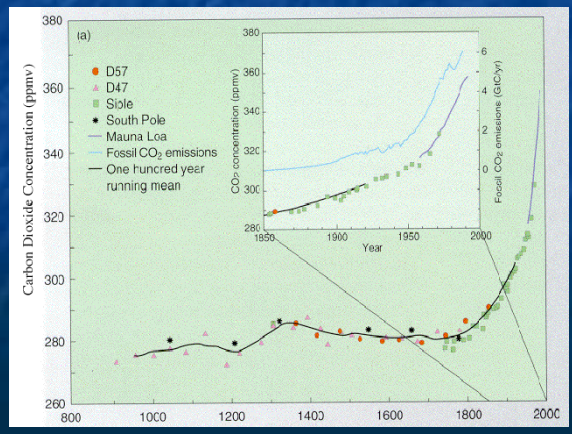
The carbon dioxide geochemical cycle
Background CO2 concentrations

- Increase of ~40 ppm during the last 60 years
- This increase due mostly to fossil fuel combustion
- There is human effect on CO2





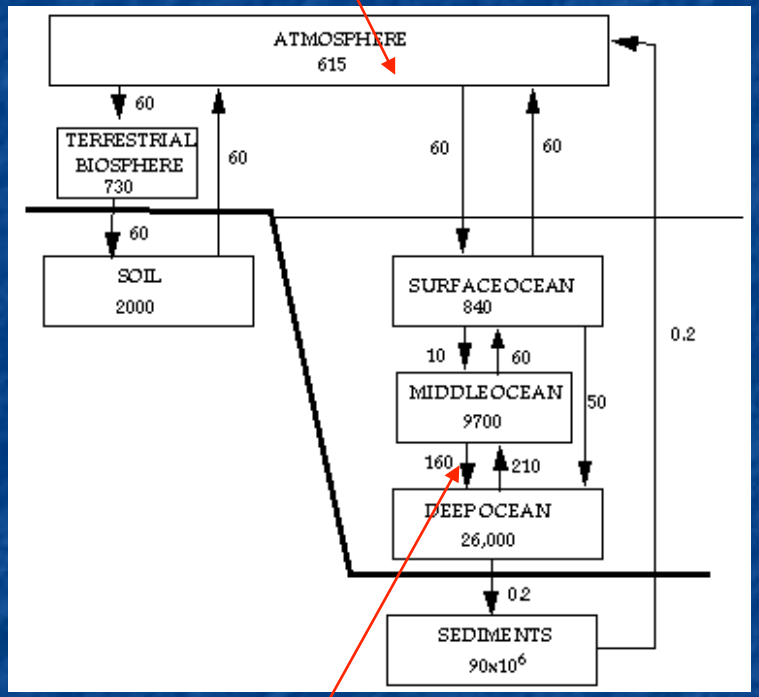




The CO_2 Cycle

- CO_2 partitions between the atmosphere the atmosphere (%50), oceans (%30), and terr. Biosphere (%20)
- CO_2 uptake by the biosphere is subject to limiting plant growth (9 years lifetime)
- CO_2 uptake by the ocean is limited by acidification and slow mixing
- Ultimate removal of the CO_2 added to the atmosphere by fossil fuel combustion requires transfer of oceanic carbon to the lithosphere by formation of sedimentation
- The time scale for this transfer is estimated as 170,000 years
- One can conclude that fossil fuel combustion induces a very long-time perturbation to the global carbon cycle
- Humans effect this perturbation!

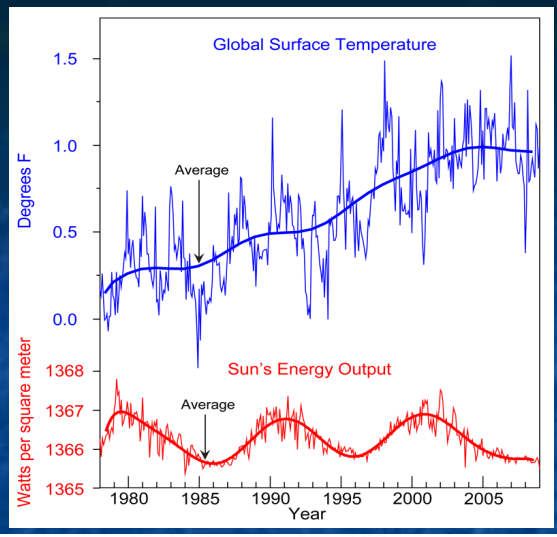
Inventories within the boxes are in Pg

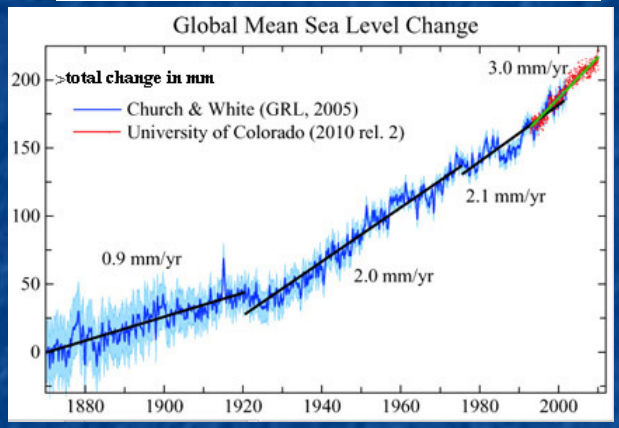


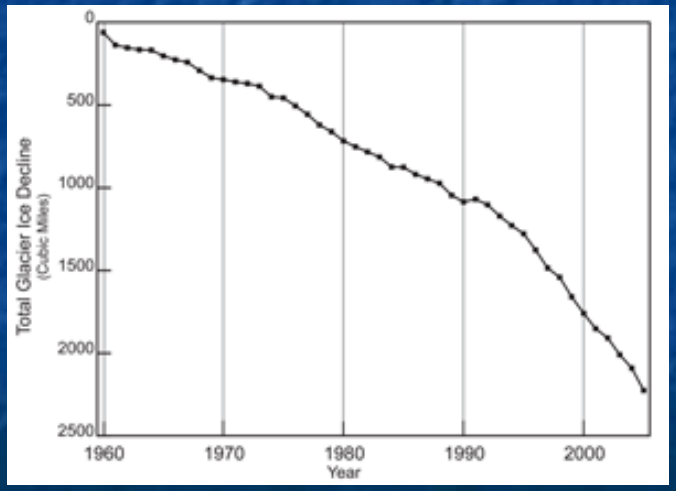
Flows indicated by arrows in Pg/year

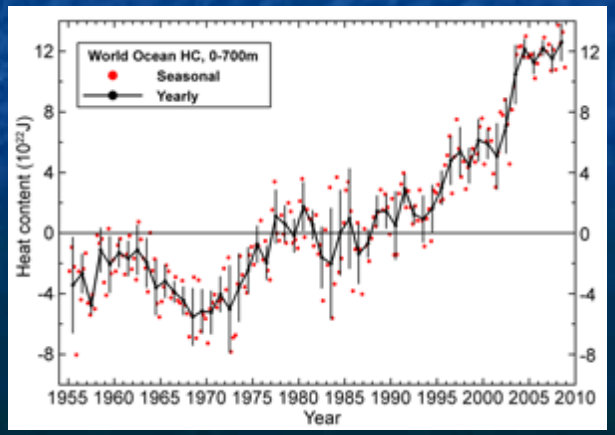
Lecture 10: Greenhouse gases

What are the greenhouse gases?
Natural vs. Anthropogenic greenhouse gases
Relationship between atmospheric temperature and greenhouse gases
Impact on climate & climate change





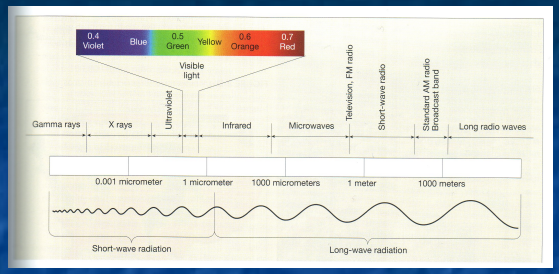


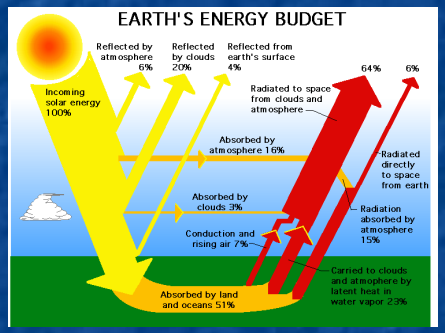


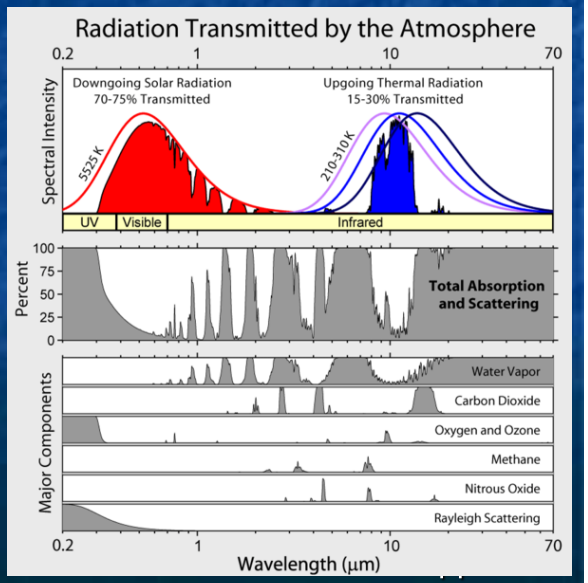
Lecture 10: Greenhouse gases

Relationship between atmospheric temperature and greenhouse gases
Radiation balance
The best estimate of solar energy
Radiation: SW radiation & LW terrestrial radiation
Radiation Laws
- Planck's law
- Wien's displacement law
- Stefan-Boltzman law
- Kirchhoff's law

Scattering
Absorption
What is radiative forcing?



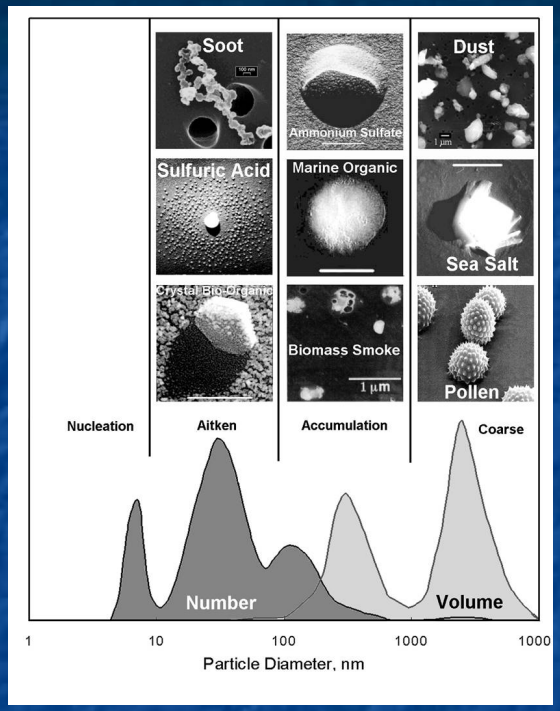


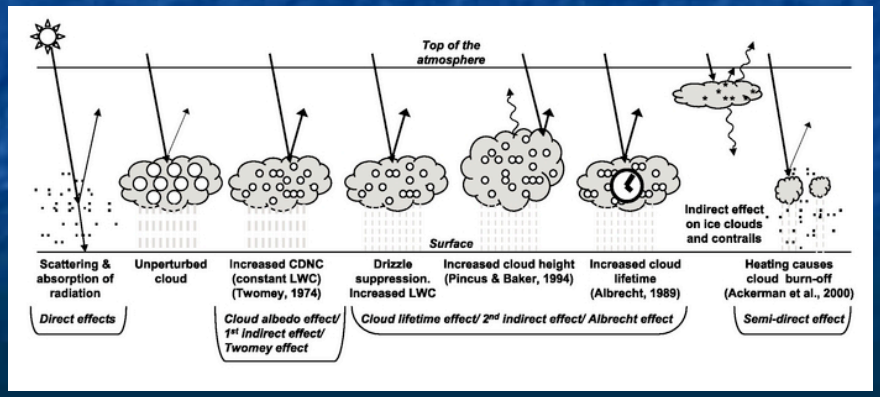


Lecture 11: Aerosols

Definition of aerosol
Natural vs. anthropogenic aerosols
Primary vs. Secondary aerosols
Size distribution (nucleation, Aitken, accumulation, and coarse mode)
Condensation nuclei
Sources and sinks of aerosols
Aerosol effects and their contribution to radiative forcing
- Direct
  - Rayleigh scattering
  - Geometric scattering
  - Mie scattering
- Indirect
- Semi-direct

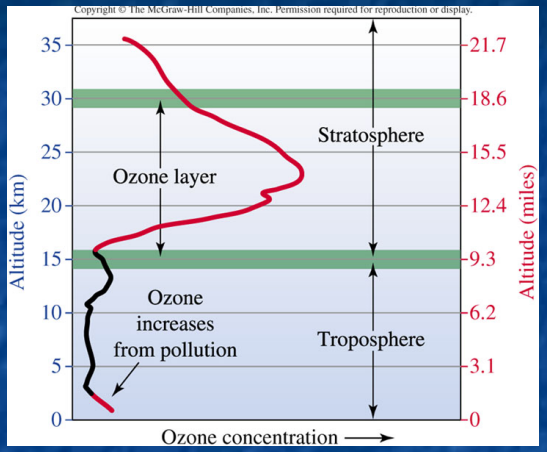
Aerosol properties
- AI, AOD, SSA, AAOD

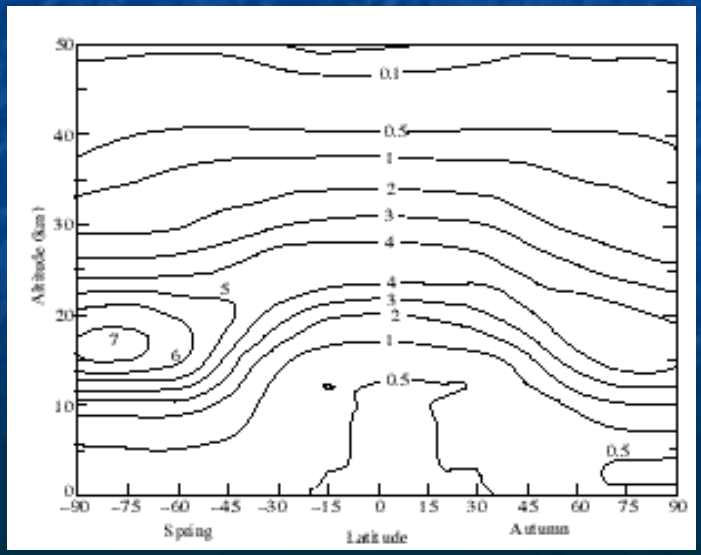


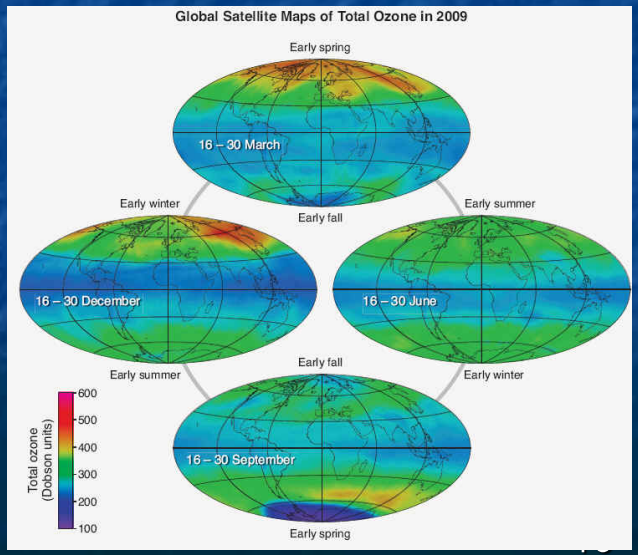


Lecture 12: Stratospheric Ozone

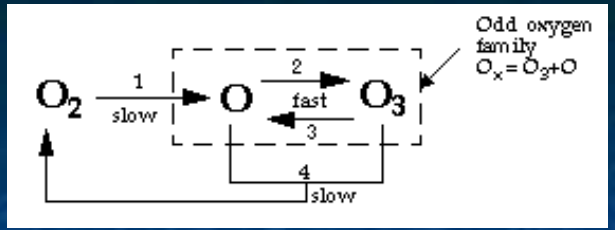
What is ozone?
Importance of stratospheric ozone
Function of ozone layer: UV absorption by ozone
Ozone distribution in the atmosphere
    Vertical distribution
    Horizontal distribution
    Ozone variation with Lat, Lon, and season
    Why seasonal changes more profound in mid and high latitudes?







Lecture 12: Stratospheric Ozone



Ozone formation: The Chapman mechanism

- Initiation step
- Formation
- Deactivation
- Termination

$$O_2 + UV \rightarrow 2O \quad (\lambda < 240\,nm)$$

$$O + O_2 \rightarrow O_3$$

What is wrong with the Chapman mechanism?

- Over estimates values
- Is there another O3 destruction?

$$O_3 + UV \rightarrow O_2 + O \qquad \lambda < 320$$

Catalytic ozone destruction: Missing elements

- Hydrogen oxides
- Nitrogen Oxides
- Chlorine
- Bromine

$$X + O_3 + UV \rightarrow XO + O_2$$
$$XO + O \rightarrow X + O_2$$

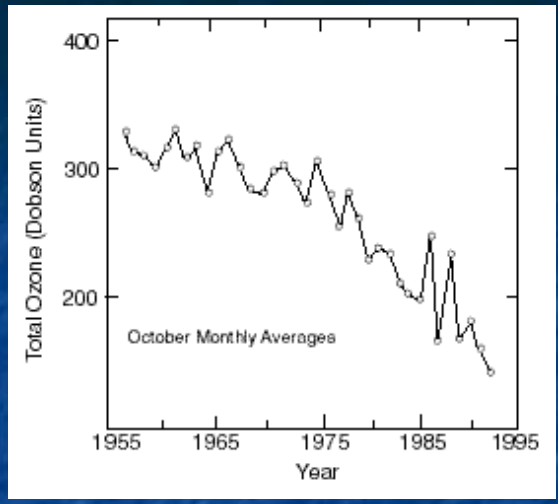
$$Net\ effect \rightarrow O_3 + UV \rightarrow O + O_2$$

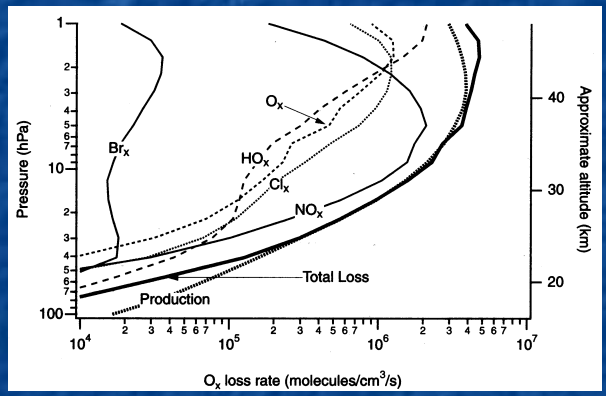
$$O_3 + UV \rightarrow O_2 + O \qquad \lambda < 320\,nm$$
$$O + O_3 \rightarrow 2O_2$$

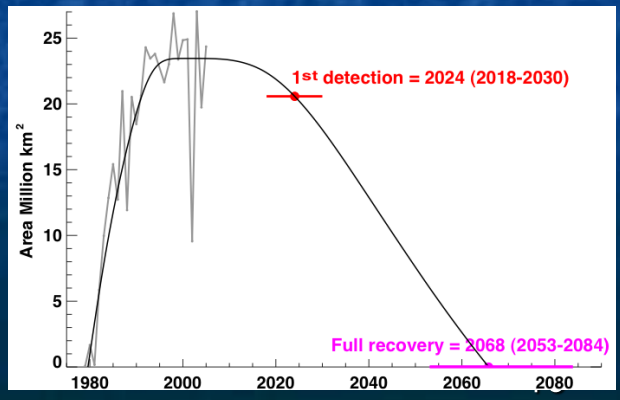
Lecture 12: Stratospheric Ozone

Ozone Hole
What is Dobson unit?
What is responsible of the Antarctic ozone hole?
- Chlorine radicals
- Bromine radicals
- NOx

Antarctic Meteorology
Why is the recovery so slow?
What is the impact of climate change on ozone recovery?







Lecture 13: Tropospheric (Ground Level) Ozone

Good Ozone vs. Bad Ozone
Why are we interested in Tropospheric ozone?

Pollution:
O_3 is an important component of photochemical smog

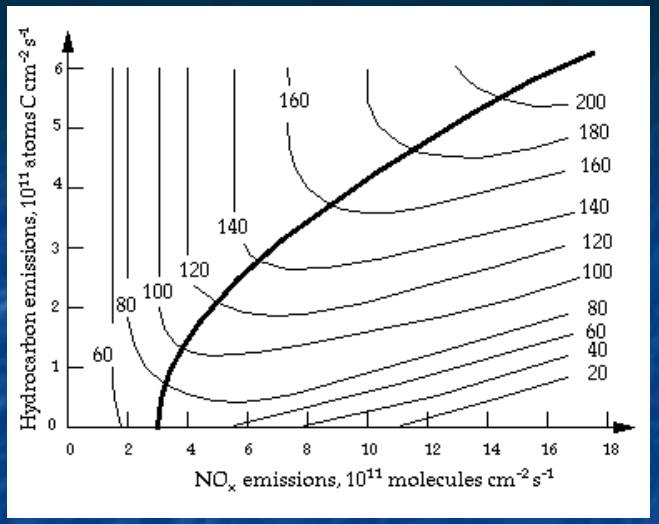
Tropospheric oxidation:
O_3 regulates oxidation through control of OH and controls removal of CH_4, VOCs, etc.

Climate:
Direct: O_3 is a greenhouse gas
Indirect: O_3 governs lifetime of other GHGs via OH

Anthropogenic Influence:
Surface and Tropospheric O_3 is increasing due to human activity

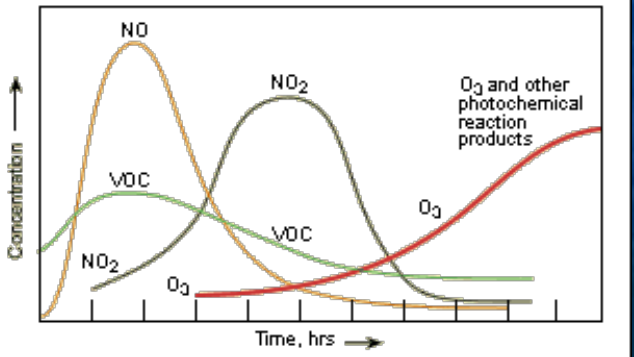
Lecture 13: Tropospheric (Ground Level) Ozone

Chemical formation
Factors controlling the tropospheric ozone budget
Background value
Diurnal cycle of ozone

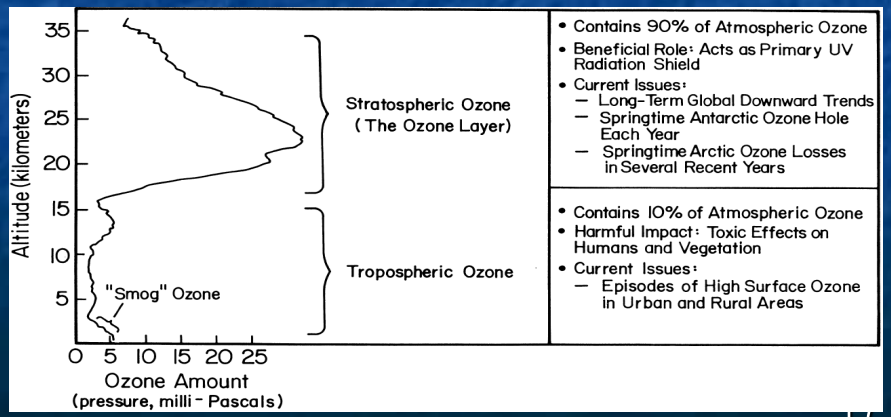


$$NO + VOCs \rightarrow NO_2 + VOC^{*}s$$
$$NO + O_3 \rightarrow NO_2 + O_2$$
$$NO_2 + UV \rightarrow NO + O \qquad (\lambda < 420\,nm)$$
$$O_2 + O \rightarrow O_3$$

Figure 1. Pollutant Concentration Profiles Due to Photochemical Reactions



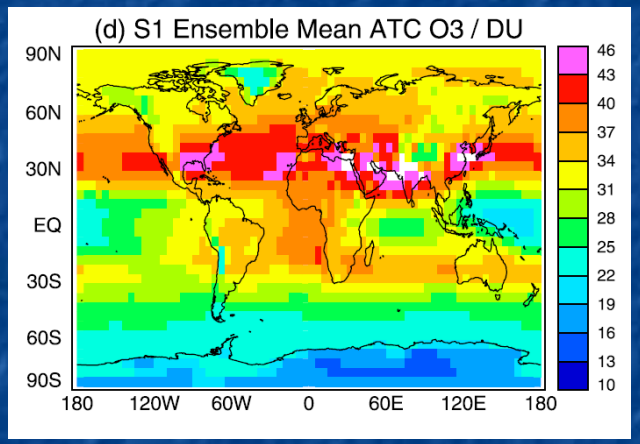
VOC + NOx + Heat + Sunlight = Ozone

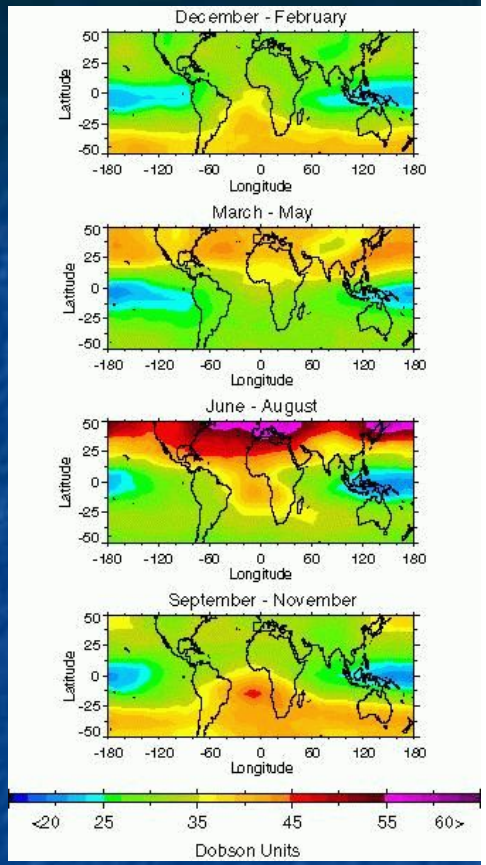


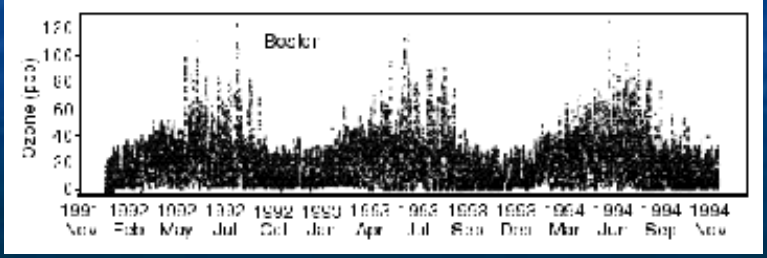
Lecture 13: Tropospheric (Ground Level) Ozone

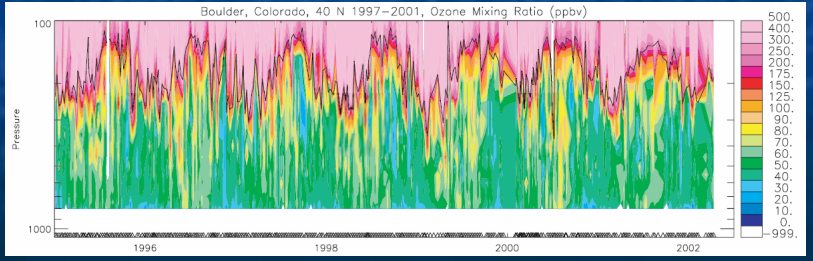
Tropospheric ozone distribution over US region
Chemical lifetime of tropospheric ozone
Transport times of tropospheric ozone
Ozone concentration depends on ….

- Temperature
- Wind
- Time of year
- Topography

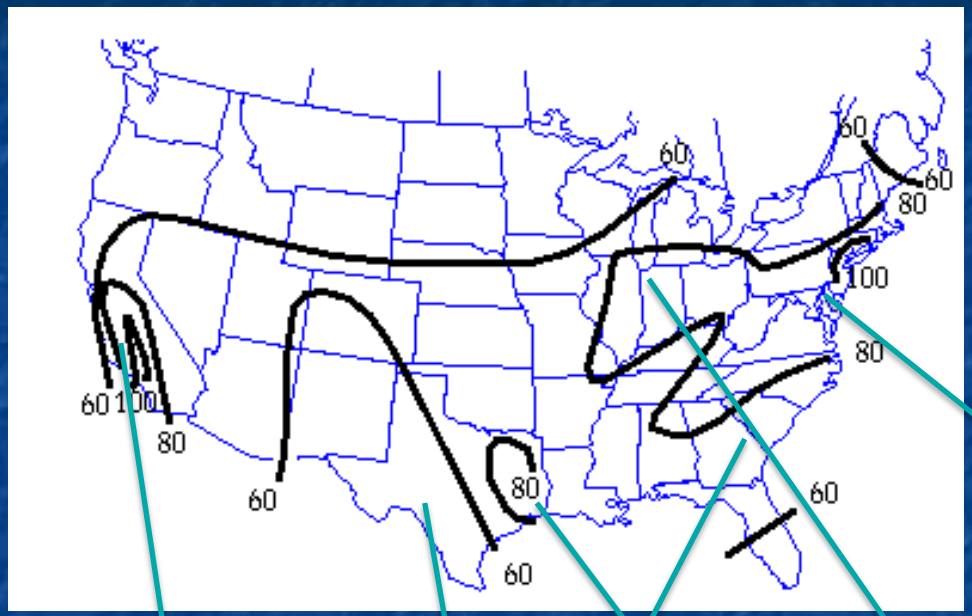


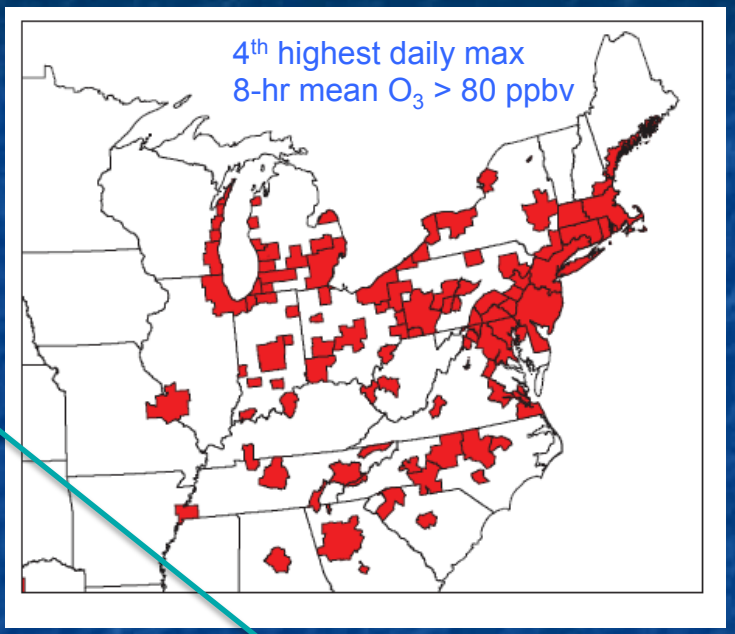






U.S. Ozone Concentration





Mountain barriers limits atmospheric mixing

Local petroleum based industries

In NE, Summer weather and high pressure weather systems

In Southern urban areas, O3 tend to decrease with increasing wind speed

In Northern urban areas, O3 tend to increase with transport of O3 and its precursors

- Higher frequency and duration of days with O3 concentrations shows spatial variability due to various effects

Lecture 13: Tropospheric (Ground Level) Ozone

Ozone Control strategies
Special case: LA ozone problem

