## Solving the Basic Equations for the Atmosphere in 3-D

**Mass Continuity**

$$\frac{\partial \rho}{\partial t} = -\frac{d(u\rho)}{dx} - \frac{d(v\rho)}{dy} - \frac{d(w\rho)}{dz}$$

**Equations of Motion (momentum continuity)**

$$\frac{\partial u}{\partial t} = -\frac{d(uu)}{dx} - \frac{d(vu)}{dy} - \frac{d(wu)}{dz} + ...$$

$$\frac{\partial v}{\partial t} = -\frac{d(uv)}{dx} - \frac{d(vv)}{dy} - \frac{d(wv)}{dz} + ...$$

$$\frac{\partial w}{\partial t} = -\frac{d(uw)}{dx} - \frac{d(vw)}{dy} - \frac{d(ww)}{dz} + ...$$

*+ pressure gradient*

*+ Coriolis force*

*+ gravity*

*+ friction*

**Thermodynamic Equation (energy continuity)**

$$\frac{\partial T}{\partial t} = -\frac{d(uT)}{dx} - \frac{d(vT)}{dy} - \frac{d(wT)}{dz} + \frac{1}{c_v}\left( J - p\frac{D(1/\rho)}{Dt} \right)$$

$J$ : radiation, conduction, latent heat release, etc

$D(1/\rho) / Dt$ : conversion between thermal and mechanical energy in fluid system

**Chemical Continuity Equation**

$$\frac{\partial \chi}{\partial t} = -\frac{d(u\chi)}{dx} - \frac{d(v\chi)}{dy} - \frac{d(w\chi)}{dz}$$

*+ Chemical Production*
*− Chemical Loss*

3. Spatial representations
   a. <u>Finite difference</u> schemes (truncated Taylor expansion at J grid-points)
   b. <u>Spectral</u> techniques (express variables using truncated series of N orthogonal harmonic functions and solve for N coefficients of expansion;) see
   c. <u>Interpolation</u> schemes (interpolates between grid points e.g. using a polynomial)
   d. <u>Finite element</u> schemes (minimizes error between actual and approximate solutions using a "basis function", good for irregular geometries, c.f. (b) above which is good for regular geometries)

4. <u>Explicit and Implicit time stepping</u>

<u>Explicit</u>:     $( \ )_x^{t+\Delta t} = f\left[ ....,( \ )_{x*}^{t},... \right]$

<u>Implicit</u>:     $( \ )_x^{t+\Delta t} = f\left[ ...,( \ )_{x*}^{t},( \ )_{x*}^{t+\Delta t},.... \right]$
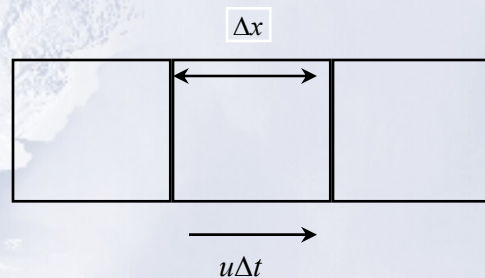
(Implicit methods more stable (but often less accurate) than explicit methods for longer time steps)

# Time stepping and stability

In the numerical model, time is treated in discrete units and the time intervals chosen depend on the size of the model grid boxes. Intuitively, don't want to transport across more than a grid cell over a time step.

## General Rule for stability: the CFL condition

$$\frac{u\Delta t}{\Delta x} \leq 1$$

e.g. Typically in the atmosphere, max u = 100m/s & grid spacing = 200 km, so constraint is $\Delta t < 2000$ seconds (33min)
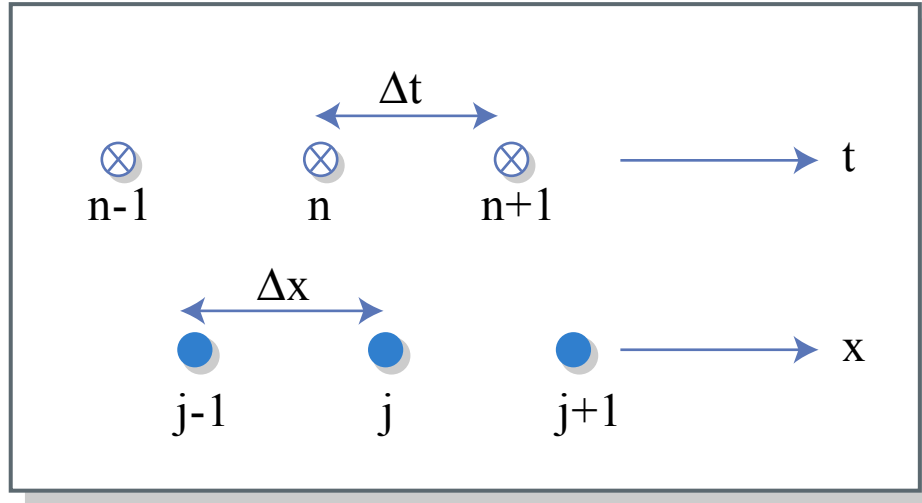
5. Example Finite Difference Schemes



Figure by MIT OCW.

(A) ☐ Advection ☐

    (a) Forward / Upstream (explicit, conditionally* stable)
        (time)    (space)

$$\frac{\partial(\ )}{\partial t} \rightarrow \frac{(\ )_j^{n+1} - (\ )_j^n}{\Delta t} \qquad \text{(first order accurate)}$$

$$u\frac{\partial(\ )}{\partial x} \rightarrow \begin{cases} u_j^n \left\{ \dfrac{(\ )_j^n - (\ )_{j-1}^n}{\Delta x} \right\} & (u_j > 0) \\[2em] u_j^n \left\{ \dfrac{(\ )_{j+1}^n - (\ )_j^n}{\Delta x} \right\} & (u_j \leq 0) \end{cases} \qquad \text{(first order)}$$

*For stability need <u>Courant No.</u> $\dfrac{u\Delta t}{\Delta x} \leq 1$

(b) <u>Centered</u> / <u>Centered</u> or <u>Leap-frog</u> (explicit, neutrally** stable)

$$\frac{\partial(\ )}{\partial t} \rightarrow \frac{(\ )_j^{n+1} - (\ )_j^{n-1}}{2\Delta t} \qquad \text{(second order)}$$

$$u\frac{\partial(\ )}{\partial x} \rightarrow u_j^n \left\{ \frac{(\ )_{j+1}^n - (\ )_{j-1}^n}{2\Delta x} \right\} \qquad \text{(second order)}$$

**No amplitude dissipation but still need Courant No. ≤1 (Note that forward/centered is linearly unstable to small perturbations)

(B) ☐ Diffusion ☐

(i) <u>Forward</u> / <u>Centered</u> (explicit, conditionally*** stable)

$$\frac{\partial(\ )}{\partial t} \quad \text{as in (a) above}$$

$$\frac{\partial}{\partial x}\left(K\frac{\partial(\ )}{\partial x}\right) \rightarrow K_{j+\frac{1}{2}}\left\{\frac{(\ )_{j+1}^n-(\ )_j^n}{(\Delta x)^2}\right\} - K_{j-\frac{1}{2}}\left\{\frac{(\ )_j^n-(\ )_{j-1}^n}{(\Delta x)^2}\right\}$$

***For stability need <u>Fourier No.</u> $\dfrac{K\Delta t}{(\Delta x)^2} \leq \dfrac{1}{4}$

(ii) <u>Backward</u> / <u>Centered</u> (implicit, unconditionally stable)

$\dfrac{\partial(\ )}{\partial t}$ as in (a) above and $\dfrac{\partial}{\partial x}\left(K\dfrac{\partial(\ )}{\partial x}\right)$ as in (i) above but <u>replace n</u> by $\underline{n+1}$

(iii) <u>Backward-forward</u> / <u>Centered</u> (semi-implicit, stable for all $\Delta t$, Crank-Nicholson Scheme)

$\dfrac{\partial(\ )}{\partial t}$ as in (a) above

$\dfrac{\partial}{\partial x}\left(K\dfrac{\partial(\ )}{\partial x}\right)$ is <u>AVERAGE of (i) and (ii) above</u>

(Note that this method second-order accurate in space and time since both centered at time $n+\dfrac{1}{2}$)

(C) $\boxed{\text{Chemistry}}$ (involves a non-linear vectorial equation)

(a) <u>Explicit forward</u>

$$\frac{\vec{X}_j^{n+1}-\vec{X}_j^n}{\Delta t} = \vec{R}\left(\vec{X}_j^n, t_n\right)$$

requires $\Delta t \leq \dfrac{2}{\lambda_{max}}$ where $\lambda_{max}$ is the largest eigenvalue of $\dfrac{\partial \vec{R}}{\partial \vec{X}}$ (often impractical)

(b) <u>Implicit backward</u> (replace n in $\vec{R}$ above by $n+1$) and semi-implicit (average of explicit forward / implicit backward) allow larger $\Delta t$ and are preferred.

(c) For higher order accuracy than above schemes (which are first order accurate) use <u>predictor-corrector</u> methods (e.g. Gear) or <u>generalized Runga-Kutta</u> (e.g. Kaps-Rentrop). These methods are however generally too computationally demanding for 3D chemical transport models.

(d) <u>Hybrid schemes</u>. For 3D models can use: diagnostic equations (steady-state) for species i with $\tau_i = \dfrac{[i]}{L_i} < \dfrac{\Delta t}{10}$; (a) or (b) above for $\tau_i > 100\Delta t$ and the analytical solution assuming constant $P_i$ and $\tau_i$:

$$X_{ij}^{n+1} = \left(P_{ij}\tau_{ij}\right)^n + \left[X_{ij}^n - \left(P_{ij}\tau_{ij}\right)^n\right]\exp\left[-\frac{\Delta t}{\tau_{ij}^n}\right] \quad \text{for } \frac{\Delta t}{10} < \tau_i < 100\Delta t.$$

Note that the hybrid method is inherently non-conservative so corrections required.

(e) Negative mixing ratios/concentrations. Whenever $X_i < 0$ (nonphysical!) then need to replace by $X_i = 0$ and lower either adjacent (grid-point) or global (spectral) $X_i$ to compensate (sometimes called "borrow and fill")

6. <u>Surface fluxes</u> ($\phi_{ij}$)

Consider chemical species i and surface grid points j

   (a) specified <u>natural or anthropogenic emissions</u>

$$\left(\frac{[i]_j^{n+1} - [i]_j^n}{\Delta t}\right)_{\text{emissions}} = \frac{\phi_{ij}^{n+\frac{1}{2}}\Delta x \Delta y}{\Delta x \Delta y \Delta z} = \frac{\phi_{ij}^{n+\frac{1}{2}}}{\Delta z}$$

   (b) <u>interactive fluxes</u> (ocean)
      (two-way)

$$\phi_{ij} = \frac{w_p}{H_L}\left([i]_{eq,j} - [i]_j\right)$$

        ($[i]_{eq,j}$ is the concentration in surface air if gas is in <u>equilibrium</u> with surface ocean)

     where $w_p$ = "piston velocity" (monotonically increases with surface wind speed, determined empirically)

        $H_L$ = dimensionless Henry's Law coefficient (measured in laboratory)

   (c) <u>deposition fluxes</u> (one way)

$$\phi_{ij} = -w_s [i]_j \qquad (w_s = \text{dry deposition velocity; empirical, depends on gas}$$
and surface type)

Wet deposition important for soluble species:

$$\phi_{ij} = -P\left[i_{(aq)}\right]_j \qquad (P = \text{precipitation rate; cm/sec})$$

$$\simeq -\frac{P[i]_j}{H_L} \qquad \text{(equilibrium \underline{assumed} between gas and raindrop)}$$

7. <u>Upper boundary conditions</u>

   • Specified $[i]_j$ (including $[i] = 0$). Specification can be direct or specify $\tau_i \simeq 0$ in uppermost layer.

   • Specified $\phi_{ij}$ (including $\phi_{ij} = 0$). Can usually obtain $\phi_{ij} = 0$ by equating $X_{ij}$ values in top 2-3 layers (depending on finite difference scheme in vertical), or assuming $K_j$ or $w_j = 0$. Recall:

$$\phi_{ij} \simeq -K_j [M]_j \frac{\partial X_{ij}}{\partial z} \qquad \text{(diffusion), or}$$

$$\phi_{ij} = w_j [i]_j \qquad \text{(advection)}$$

8. Subgridscale parameterizations
   a. Eddy diffusion coefficients

- $K_{zz}(R_i)$;  $R_i = g \dfrac{\dfrac{\partial \ln \theta}{\partial z}}{\left(\left(\dfrac{\partial u}{\partial z}\right)^2 + \left(\dfrac{\partial v}{\partial z}\right)^2\right)}$

  (gradient Richardson no.)

  $R_i > 0 \rightarrow$ stable (if $R_i > \dfrac{1}{4}$ get laminar flow)

  $R_i < 0 \rightarrow$ unstable (if $|R_i| \le 1$ then forced convection and if $|R_i| > 1$ then free convection)

  $R_i \simeq 0 \rightarrow$ neutral ($K_{zz} \simeq kzu_*$, $u_* =$ friction velocity)

- $K_{xx}, K_{yy}\left(\dfrac{\partial T}{\partial x}, \dfrac{\partial T}{\partial y}, \dfrac{\partial u}{\partial x}, \dfrac{\partial u}{\partial y}, \text{etc.}\right)$ (e.g. due to baroclinic eddies)
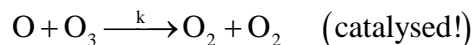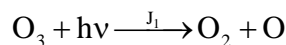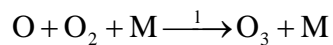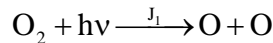
   b. moist convection

- $\dfrac{\partial \theta_E}{\partial z} \le 0$ where $\theta_E =$ equivalent potential temperature implies convective instability

- treatments range from simple "convective adjustment" (transport heat/mass necessary to restore $\dfrac{\partial \theta_E}{\partial z} = 0$), to more complex "process-resolving" models (Kuo, Arakawa-Schubert, Hack (NCAR,CCM2), Tiedtke (ECMWF and ECHAM3), and Emanuel). For chemical models we want the mass fluxes not to the energy fluxes from these various treatments.

9. Chemical rate constants

Consider the simplified ozone layer chemical reactions:

$$O_2 + h\nu \xrightarrow{\ J_1\ } O + O$$

$$O + O_2 + M \xrightarrow{\ 1\ } O_3 + M$$

$$O_3 + h\nu \xrightarrow{\ J_1\ } O_2 + O$$

$$O + O_3 \xrightarrow{\ k\ } O_2 + O_2 \quad (\text{catalysed!})$$

The relevant chemical reaction rates are expressed using first ($J_i$), second (k) and third (l) order rate constants:

$$\frac{d[i]}{dt}\left(\frac{\text{molecule}}{\text{cm}^3\,\text{sec}}\right) = \begin{cases} -J_i[i] & \left(\text{sec}^{-1} \cdot \text{molecule} \cdot \text{cm}^{-3}\right) \\[2mm] -k_{ij}[i][j] & \left(\text{sec}^{-1} \cdot \text{cm}^3 \cdot \text{molecule}^{-1} \cdot \left(\text{molecule} \cdot \text{cm}^{-3}\right)^2\right) \\[2mm] -l_{ijM}[i][j][M] & \left(\text{sec}^{-1} \cdot \text{cm}^6 \cdot \text{molecule}^{-2} \cdot \left(\text{molecule} \cdot \text{cm}^{-3}\right)^3\right) \end{cases}$$

The chemical rate constants (k,l) are measured in the laboratory.

Some typical expressions for their dependence on temperature (T) and density $\left(\left[M\right]\right)$ are:

$$k = A\exp\left(-\frac{B}{T}\right) \qquad \left(\text{measure A and B}\right)$$

$$l = l\left(T_{ref}, \left[M\right]\right)\left(\frac{T}{T_{ref}}\right)^{-\alpha} \qquad \left(\text{measure } l\left(T_{ref,}\left[M\right]\right) \text{ and } \alpha\right)$$

The <u>rate constant for photodissociation</u> is calculated in a non-scattering atmosphere using:

$$J_i = \int_{\lambda_1}^{\lambda_2} \sigma_i\left(\lambda\right)\phi_i\left(\lambda\right)I\left(\infty\right)\exp\left[-\sum_{j=1}^{N}\sigma_j\left(\lambda\right)\frac{M_j\left(z\right)}{\cos\theta}\right]d\lambda$$

where

$\sigma_i\left(\lambda\right) = $ absorption cross-section at wavelength $\lambda$ $\left(cm^2\cdot molecule^{-1}\right)$

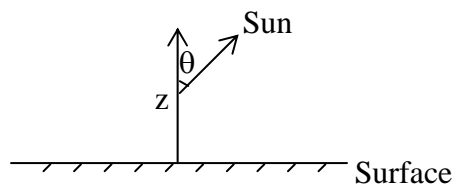$\phi_i\left(\lambda\right) = $ photodissociation yeild $\left(dimensionless\right)$

$\lambda_2 - \lambda_1 = $ width of electronic absorption band

$I\left(\infty\right) = $ solar photon flux at altitude $z = \infty$ $\left(photon\cdot cm^{-2}\cdot sec^{-1}\right)$

$N = $ number of gases $\left(j\right)$ absorbing at wavelength $\lambda$

$M_j\left(z\right) = $ molecules of j per unit area above z $\left(molecule\cdot cm^{-2}\right)$

$\theta = $ solar zenith angle



10. <u>Some essential chemistry and radiation components</u>
    a. <u>UV fluxes</u> for photodissociation rates
    b. For all species <u>involving OH</u> in their chemistry need to include:
        1. $O_3, O_2, O\left(^1D\right)$
        2. $H, OH, HO_2, H_2O_2,$ with latter 3 in gas and aqueous phase
        3. $NO, NO_2, NO_3, N_2O_5, HNO_3$ with latter 2 in gas and aqueous phase
        4. $CH_4, CH_3, CH_3O_2, CH_3O, CH_3O_2H, CH_2O, CHO, CO$ (also <u>selected heavier hydrocarbons</u> such as <u>isoprene and terpenes in forested areas</u> and <u>anthropogenic hydrocarbons in urban areas</u>)
11. Spectral (spherical harmonic) models

$$Y_n^m(\lambda, \mu) \equiv P_n^m(\mu)e^{im\lambda} \qquad \text{natural since eigensolutions of barotropic wave equation}$$

grid value: $\xi(\lambda_i, \mu_j) = \sum\limits_{m=-M}^{M} \sum\limits_{n=|m|}^{N(m)} \xi_n^m P_n^m(\mu_j) e^{im\lambda_i}$

spectral coefficient: $\xi_n^m = \sum\limits_{j=1}^{J} \left\{ \dfrac{1}{2M} \sum\limits_{l=1}^{2M} \xi(\lambda_l, \mu_j) e^{im\lambda_l} \right\} P_n^m(\mu_j) w_j$

($w_j$ - Gaussian weights)

where $\lambda$ and $\mu$ respectively denote the zonal and meridional independent variables, $P_n^m$ are the associated Legendre functions for which m denotes zonal wavenumber, n-m denotes a form of meridional wavenumber, M and N are the spectral truncation limits, and J is the order of the north-south transform grid, a function of the truncation parameters.
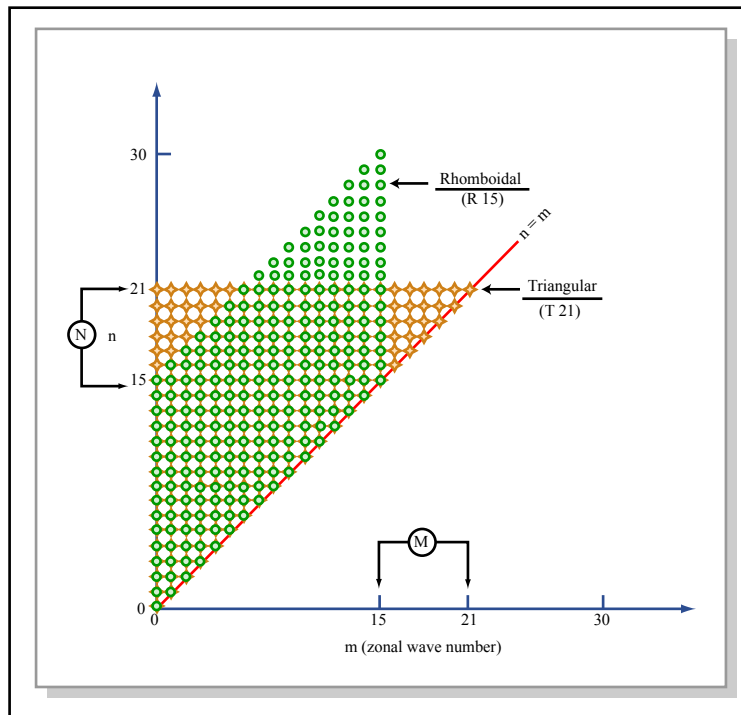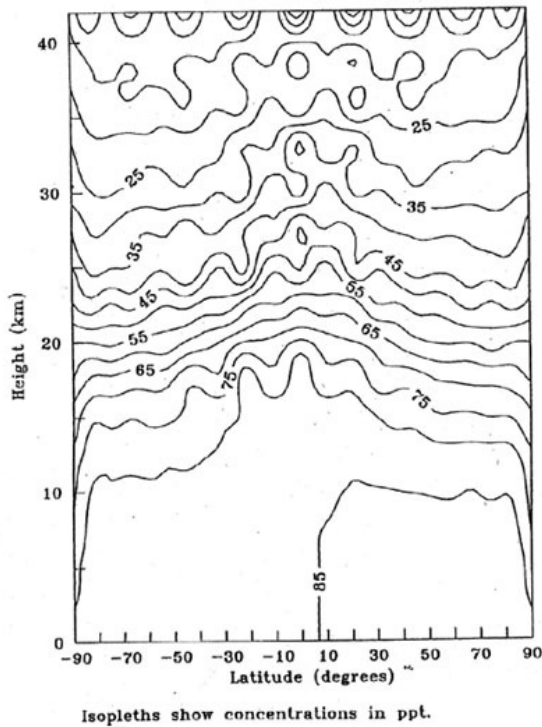


Figure by MIT OCW.

Note: Physics and chemistry are computed on the equivalent grid points and then transformed to spherical harmonic representation.
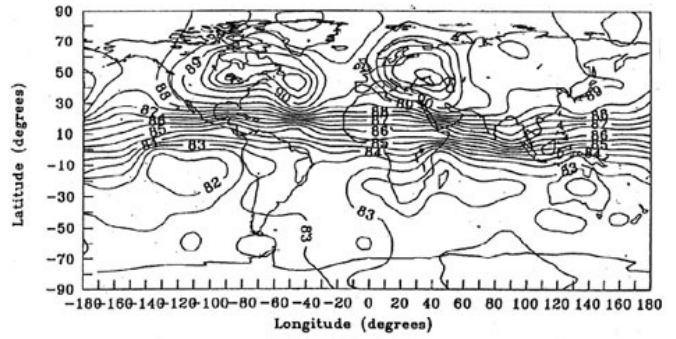
12. Examples

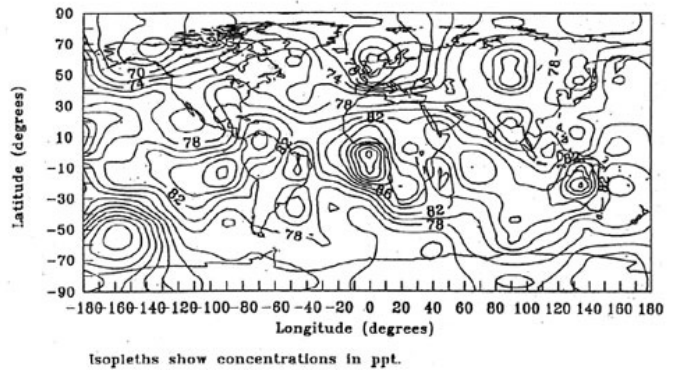(a) MIT (1989) Chemistry-Dynamics Model

CHClF$_2$ simulations

F22--Zonal Average--October

Isopleths show concentrations in ppt.

F22--surface--October

Isopleths show concentrations in ppt.

F22--100 mb level--October

Isopleths show concentrations in ppt.

MIT 3D
Model details:
Horizontal – R6 (spectral), 15 lat x 16 long (grid)
Vertical – ln P (surface to $\approx$ 72 km), 26 levels
Explicit chemistry and radiation
"balance-type" dynamics, parameterized trop. hating time – 4 x 1 hour, Lorenz n-cycle.