# *Pollution and climate modelling*

## *An Introduction*

**Sources:** *"Fundamentals of Atmospheric Modelling", M. Jacobson (2005); "Chemical Transport Models", online book by D. Jacobson (http://acmg.seas.harvard.edu/education/)*

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**SPAT PG Lectures, 1st of December 2016**

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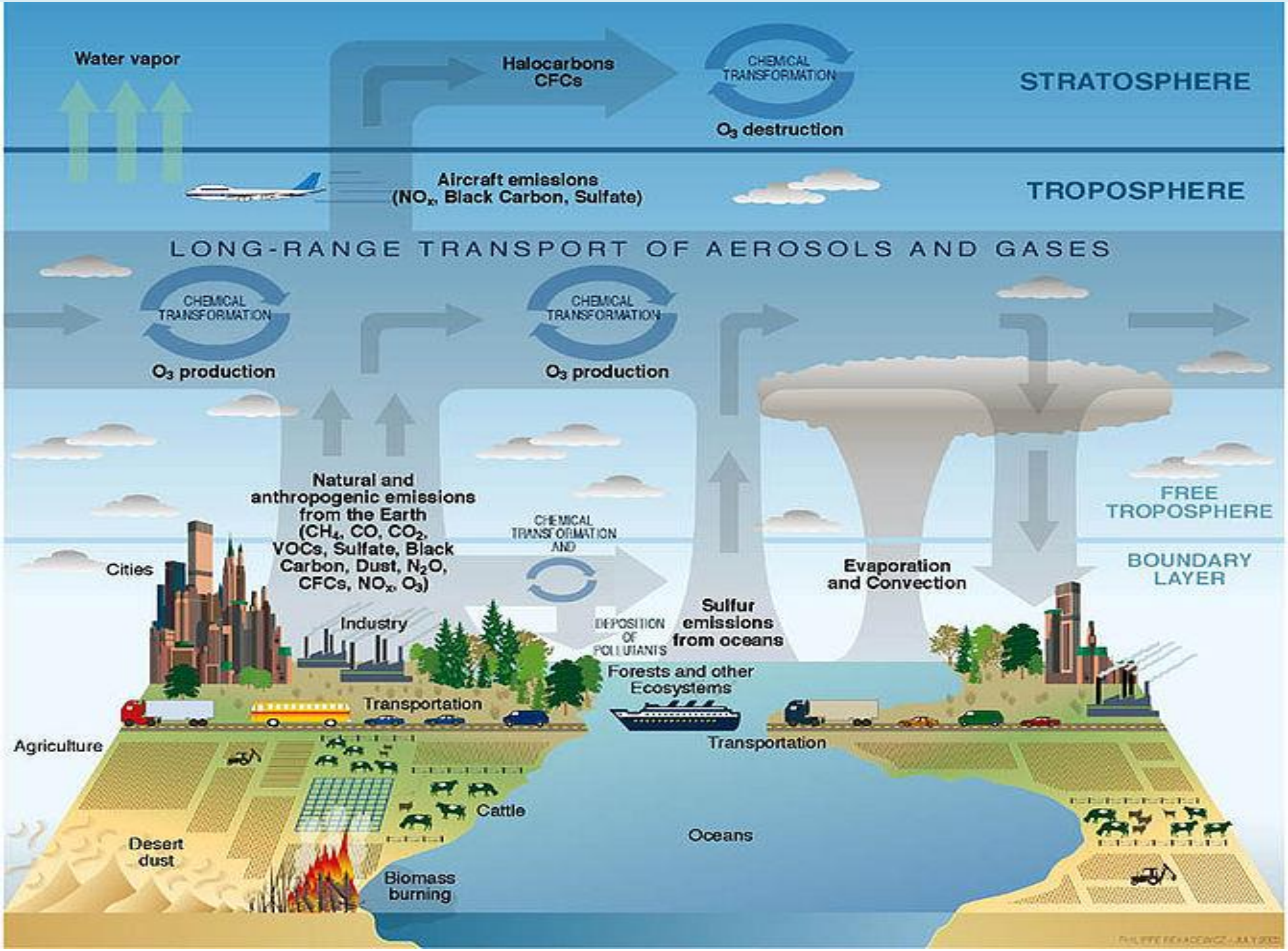
# The (complex) composition-climate system:



Source: US Climate Change Science Program.

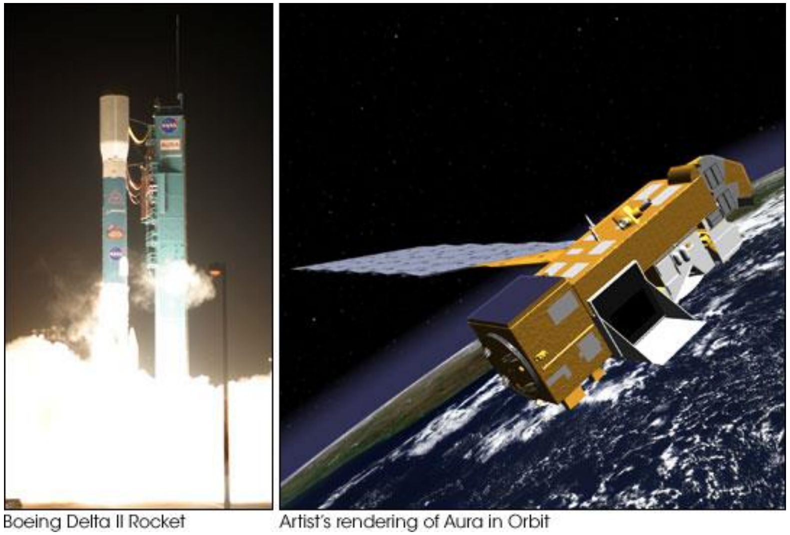
# Recent advances

**Models:** • ***Chemistry-climate models*** are climate models with atmospheric composition (gases, aerosols) “on top”.

• They have advanced a lot in the last 2-3 decades, but they can improve even more.

**Satellites:** ***Observations of atmospheric constituents*** have produced a wealth of data (e.g. NASA A-Train), especially in the last decade.

*Discover supercomputer*



*Aura satellite*

# Mass balance (continuity) equation for a gas/aerosol constituent

$$\frac{\partial n}{\partial t} = -\nabla \bullet (n\mathbf{U}) + \cancel{D\nabla^2 n} + P - L$$

Small in trop/strat

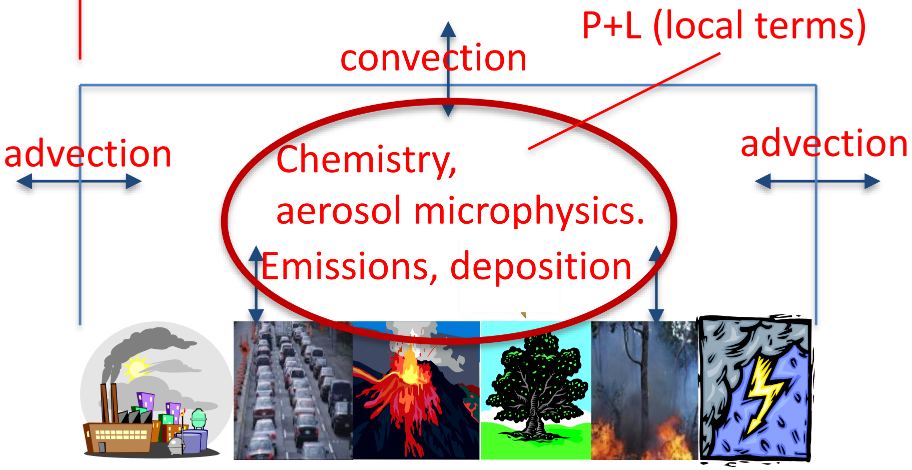
Local loss term: Chemical loss, wet and dry deposition, microphysics (in kg m$^{-3}$ s$^{-1}$).

Change of concentration of constituent with time (in molec. m$^{-3}$ s$^{-1}$).

Flux divergence due to transport (advection/convection). **U** is the wind velocity vector (m s$^{-1}$).

Flux divergence due to molecular diffusion. *D* is the molecular diffusion coefficient (m$^2$ s$^{-1}$).

Local production term: Emission, chemical production, microphysics (in kg m$^{-3}$ s$^{-1}$).



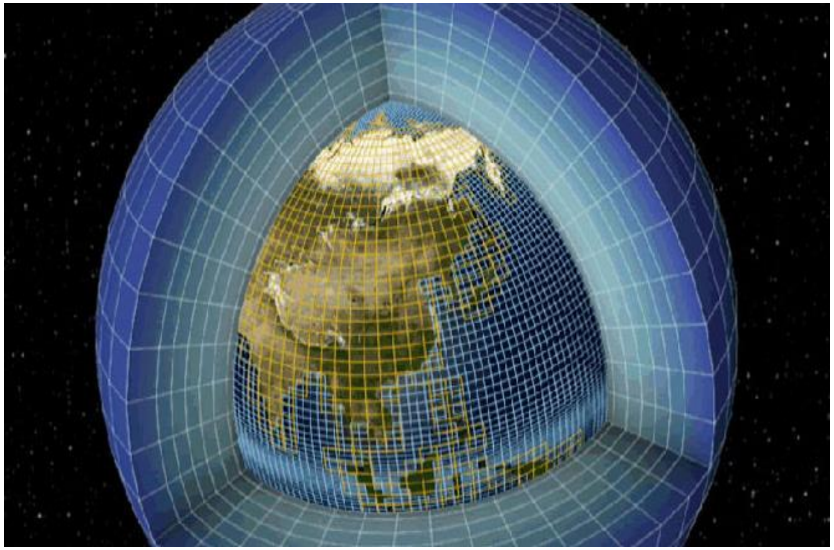
- This equation is for number concentration, but equivalent equations can be written for mass, mass concentration etc.

# Discretisation of mass balance equation in space

## (useful for global modelling)

- First order PDE in space and time. Need initial concentration and boundary conditions (i.e. fluxes at surface, top-of-the-atmosphere).

- Global models have 3D domain with finite number of gridboxes. Typical global models: horizontal resolution of ~100km, vertical of ~1km -> total of ~$10^6$ gridboxes. Equation then solved for *all* gridboxes.



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- Chemical transport models (CTMs): use external meteorological data as input; simulate the aerosols/gases.

- General circulation models (GCMs): simulate their own meteorology; use external aerosols gas forcings.

Composition-climate models (CCMs): **do both**.

# Discretisation of mass balance equation in time

- Split the equation into contributions from transport and local terms:

$$\frac{\partial n}{\partial t} = \left[\frac{\partial n}{\partial t}\right]_{TRANSPORT} + \left[\frac{\partial n}{\partial t}\right]_{LOCAL}$$

Advection+convection = $-\nabla \bullet (n\mathbf{U})$

Emissions, chemistry, deposition etc (*P-L*). If several species, then for species *i* we have $P_i(\mathbf{n})-L_i(\mathbf{n})$, where **n** a vector of concentrations of all species on which *i* depends.

- Use a transport operator and a local operator to decouple the two terms in finite difference form (assumed TRA and LOC are decoupled - can swap to test!):

$$n(t_0+\Delta t) = (\mathbf{LOC})\bullet(\mathbf{TRA})(n(t_0))$$

- Can split further (TRA to $\text{TRA}_x$, $\text{TRA}_y$, $\text{TRA}_z$, or LOC to chemistry, microphysics, emissions, deposition operators).

# Photolysis rate calculation

- For a given molecule A being photolyzed ($A + h\nu \rightarrow B + C$):

$$J_A(T) = \int \sigma_A(\lambda)\, \varphi_A(\lambda)\, F(\lambda) d\lambda \quad (s^{-1})$$

→ $\sigma_A(\lambda)$ : Absorption cross section (probability of a photon to be absorbed).

→ $\varphi_A(\lambda)$ : Quantum yield (number of molecules photolyzed per photon absorbed).

→ $F(\lambda)$ : Solar actinic flux (radiative flux from all directions).

- When photolysis rate multiplied by concentration -> gives loss rate of constituent (mass loss per unit time).
- Generally rate of reaction: $r = k(T)[A]^m[B]^n$, ($k$=reaction rate constant).

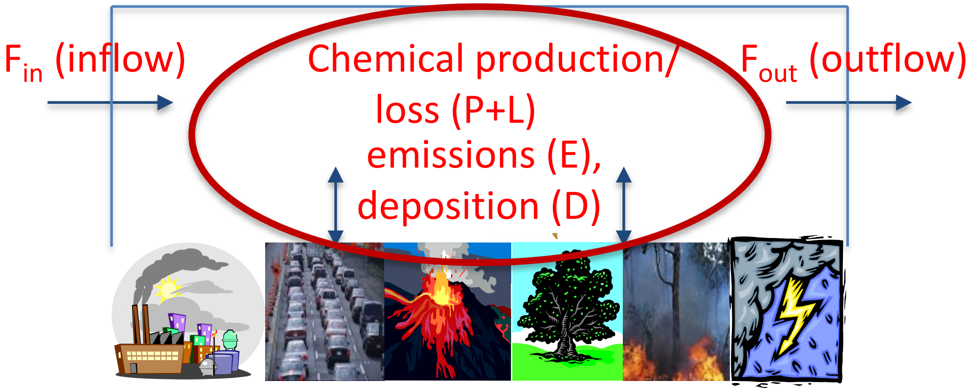
# Lifetimes of constituents

- The rate at which a chemical species A (with concentration *[A]*) is lost from the atmosphere is characterised by its *e*-folding lifetime $\tau_A$.
- It is the time required by a gas to decrease to 1/e its original concentration due to chemical reaction. Lifetimes are independent of emission/production rates.
- For example, for photolysis reaction: $\tau_A = \frac{1}{J_A} = \frac{[A]}{d[A]/dt}$
- If concentrations of a species are determined by multiple processes (1, 2,…, n), the overall lifetime is:

$$\tau_A = \frac{1}{\frac{1}{\tau_{A1}} + \frac{1}{\tau_{A2}} + \ldots + \frac{1}{\tau_{An}}}$$

# Simple one-box models (*0-dimensional*)

- Helpful for quickly testing hypotheses. Also OK for modelling WMGHGs (not very inhomogeneous in space).
- Consider gas (no microphysics) with mass *m*:



$F_{in}$ (inflow)

Chemical production/ loss (P+L) emissions (E), deposition (D)

$F_{out}$ (outflow)

$$\frac{\partial m}{\partial t} = \sum \text{sources} - \sum \text{sinks} = F_{in} + E + P - F_{out} - L - D$$

Overall lifetime: $$\tau = \frac{m}{\sum \text{sinks}} = \frac{m}{F_{out} + L + D}$$

Overall loss rate constant (in $s^{-1}$): $k = 1/\tau = k_{out} + k_L + k_D$ (note: if the only loss process is photolysis, then $k_L = J$).

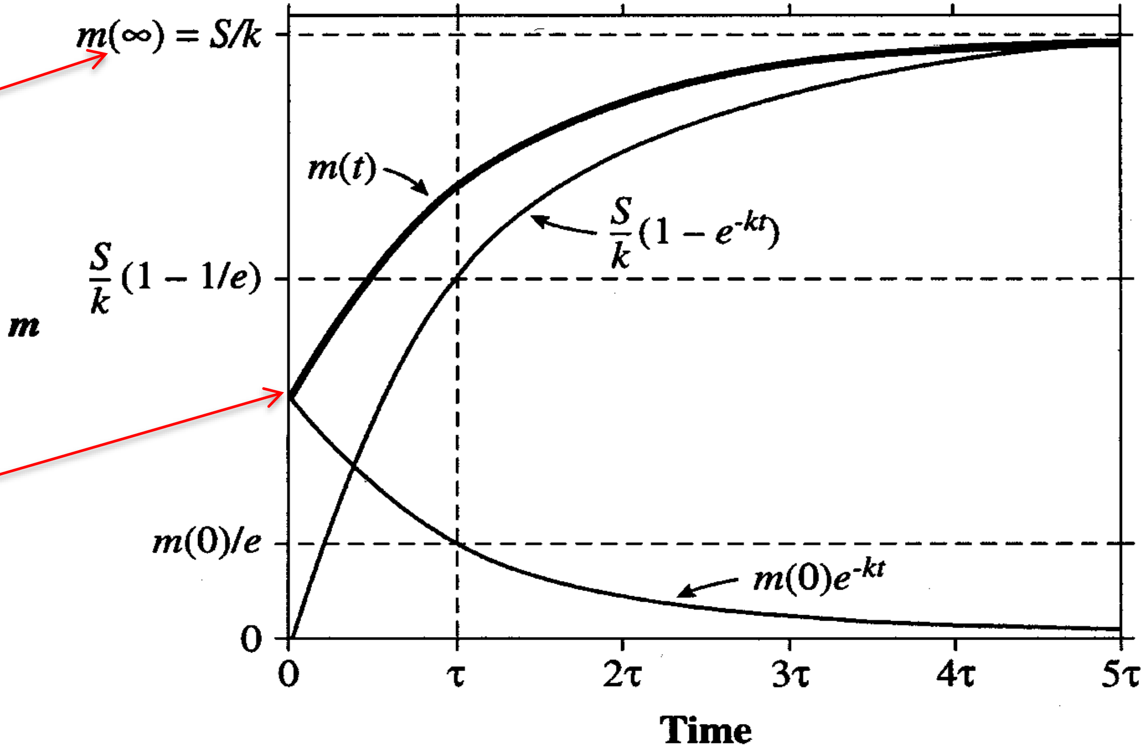
# Evolution of constituent mass in a box model

- Assume we have a constant known source *S* (emission, chemical, microphysical) and constant 1st order loss *L* (loss rate constant = *k*).

$$\frac{dm}{dt} = S - L = S - km \quad \Rightarrow \quad m(t) = m(0)e^{-kt} + \frac{S}{k}(1 - e^{-kt})$$

- Steady state when $dm/dt = 0$, i.e. abundance does not change with time.

- Takes about 2-3 lifetimes ($\tau$) to reach "quasi steady-state", though it depends on the initial conditions.



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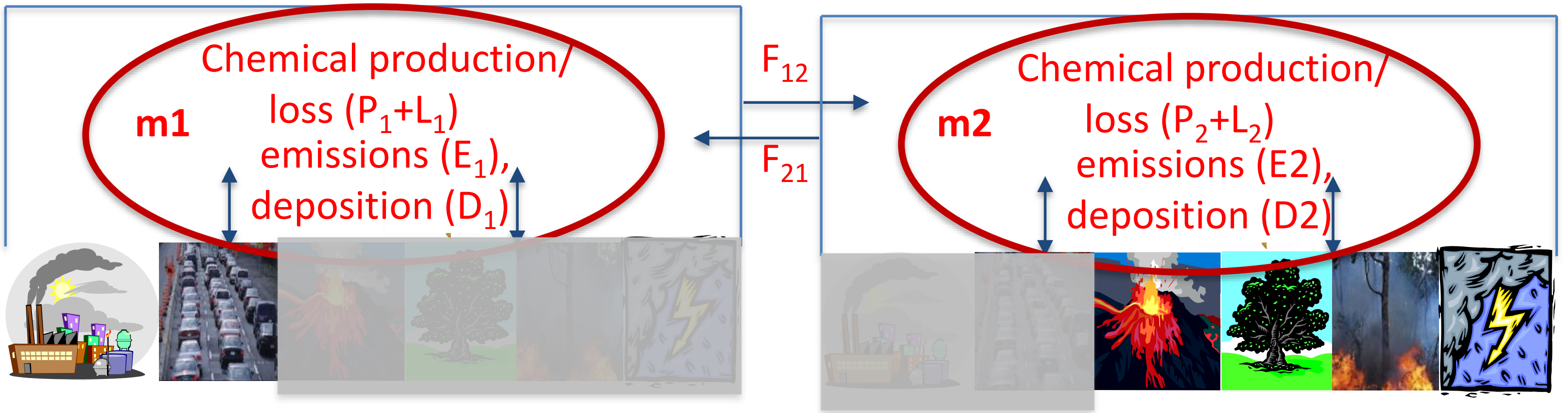
# Simple two-box model

- Useful if we have two distinct environments interacting

(e.g. boundary layer & free troposphere, Europe and the Sahara etc).



**m1**

Chemical production/
loss ($P_1$+$L_1$)
emissions ($E_1$),
deposition ($D_1$)

$F_{12}$

$F_{21}$

**m2**

Chemical production/
loss ($P_2$+$L_2$)
emissions (E2),
deposition (D2)

$$\frac{dm_1}{dt} = E_1 + P_1 - L_1 - D_1 - F_{12} + F_{21}$$

*(and similar for box 2)*

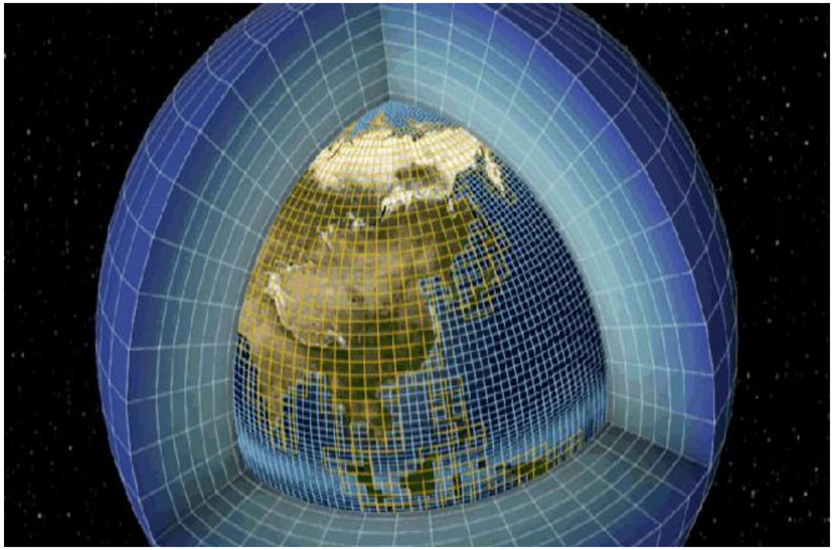
We may be given that some loss process is first order (e.g. the left to right transport flux). Then we can express $F_{12} = k_{F12}m_1$.

Note that if we are told that the system has reached steady state, we have two simple algebraic equations.

# Back to large-scale models

- First order PDE in space and time. Need initial concentration and boundary conditions (i.e. fluxes at surface, top-of-the-atmosphere).

- Global models have 3D domain with finite number of gridboxes. Typical global models: horizontal resolution of ~100km, vertical of ~1km -> total of ~$10^6$ gridboxes. Equation then solved for *all* gridboxes.



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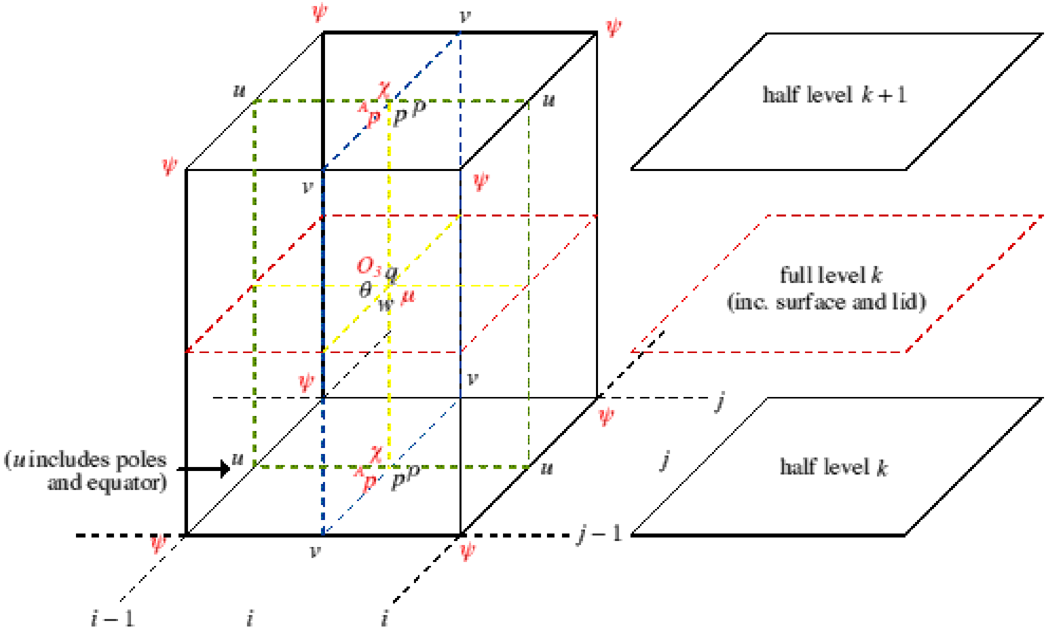


*http://www.met.reading.ac.uk/~ross/DARC/Grids.html*

# Back to large-scale models: Thermodynamic energy equation

$$\frac{\partial E}{\partial t} = -\nabla \bullet (\mathbf{U}E) + \rho_A \frac{\theta_V}{T_V} \frac{dQ}{dt}$$

Change of energy density with time in a gridbox (in J $m^{-3}$ $s^{-1}$).

Flux divergence for energy density due to transport. **U** is the wind velocity vector (m $s^{-1}$).

Heat production and loss terms ($\rho_A$ is the density of air, and $\vartheta_v/T_v$ are the virtual potential temperature and virtual temperature).
Includes diabatic heating/cooling by greenhouse gases/aerosols.

- It is also solved for each timestep in a GCM or a CCM. In the CCM "online" simulated gases/aerosols will be used for diabatic heating
- Simulated heating rates and temperatures are then fed back to the chemistry/aerosol "scheme" to influence atmospheric composition.

# Conservation of momentum (*Navier Stokes equation*)

$$\frac{\partial \mathbf{U}}{\partial t} = -(\mathbf{U} \bullet \nabla)\mathbf{U} + v\nabla^{2}\mathbf{U} - \frac{\nabla p}{\rho_{A}} + g$$

Change in air velocity in a gridbox (in m $s^{-2}$).

Advection term for **U**.

Changes due to diffusion.

Pressure-gradient & gravity terms, exerting local accelerations.

- Familiar? Analogous to the mass balance equation.
- Heating/cooling rates calculated from thermodynamic balance (previous) affect pressures, which are fed into this part of the model (dynamics) to calculate changes in wind velocities (i.e. circulation).
- Then circulation changes, together with other resulting meteorological changes that occur during the timestep, feed into the chemistry/aerosol scheme to affect constituent transport, reaction rates, wet deposition etc.
- Everything coupled (in a CCM)!

# Radiative transfer

$$dL_\nu = -L_\nu \beta^{ext} ds + J_\nu \beta^{ext} ds$$

Spectral radiance (W m$^{-2}$ sr$^{-1}$ (freq)$^{-1}$)

Extinction coefficient (m$^{-1}$)

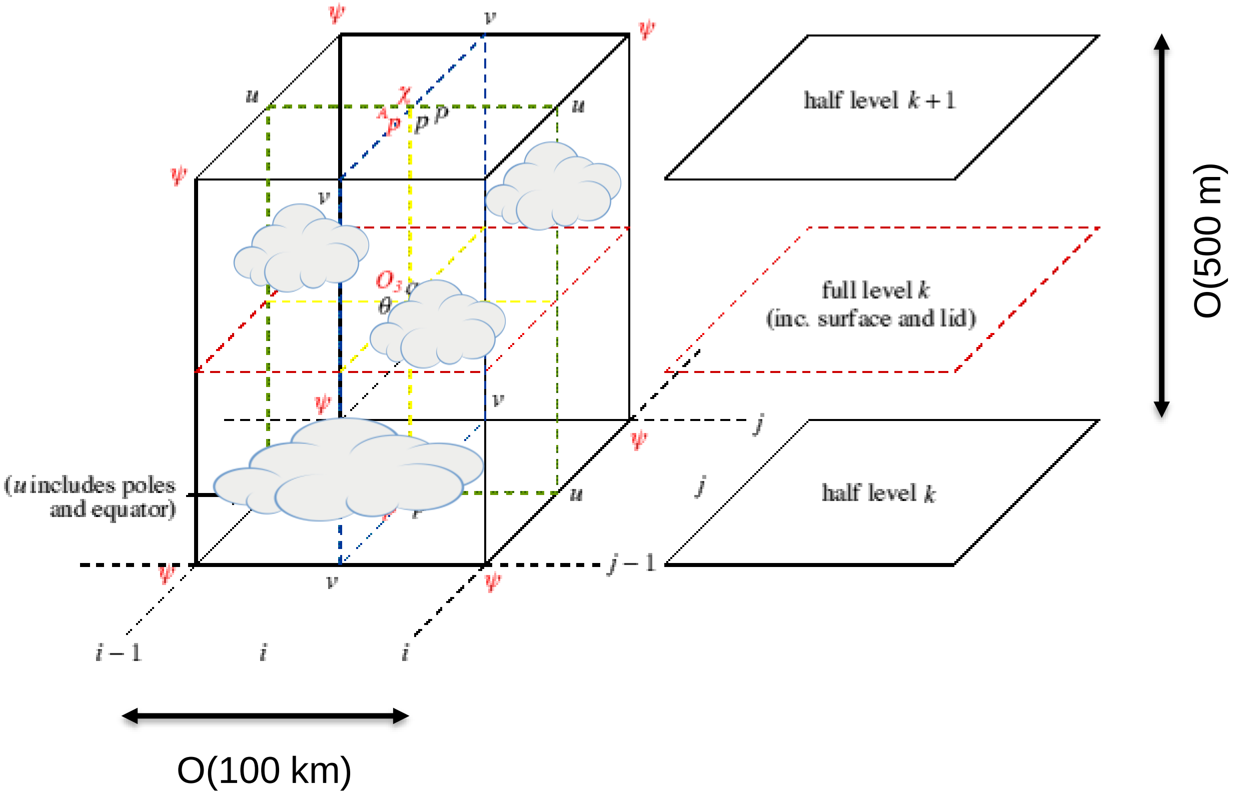
Source function

- Also needs to be discretized – in frequency and direction as well as space and time

- One of the source terms (dQ) in thermodynamic equation – typically represents one of the most computationally intensive components of a climate model

# Parameterisations for sub-grid processes

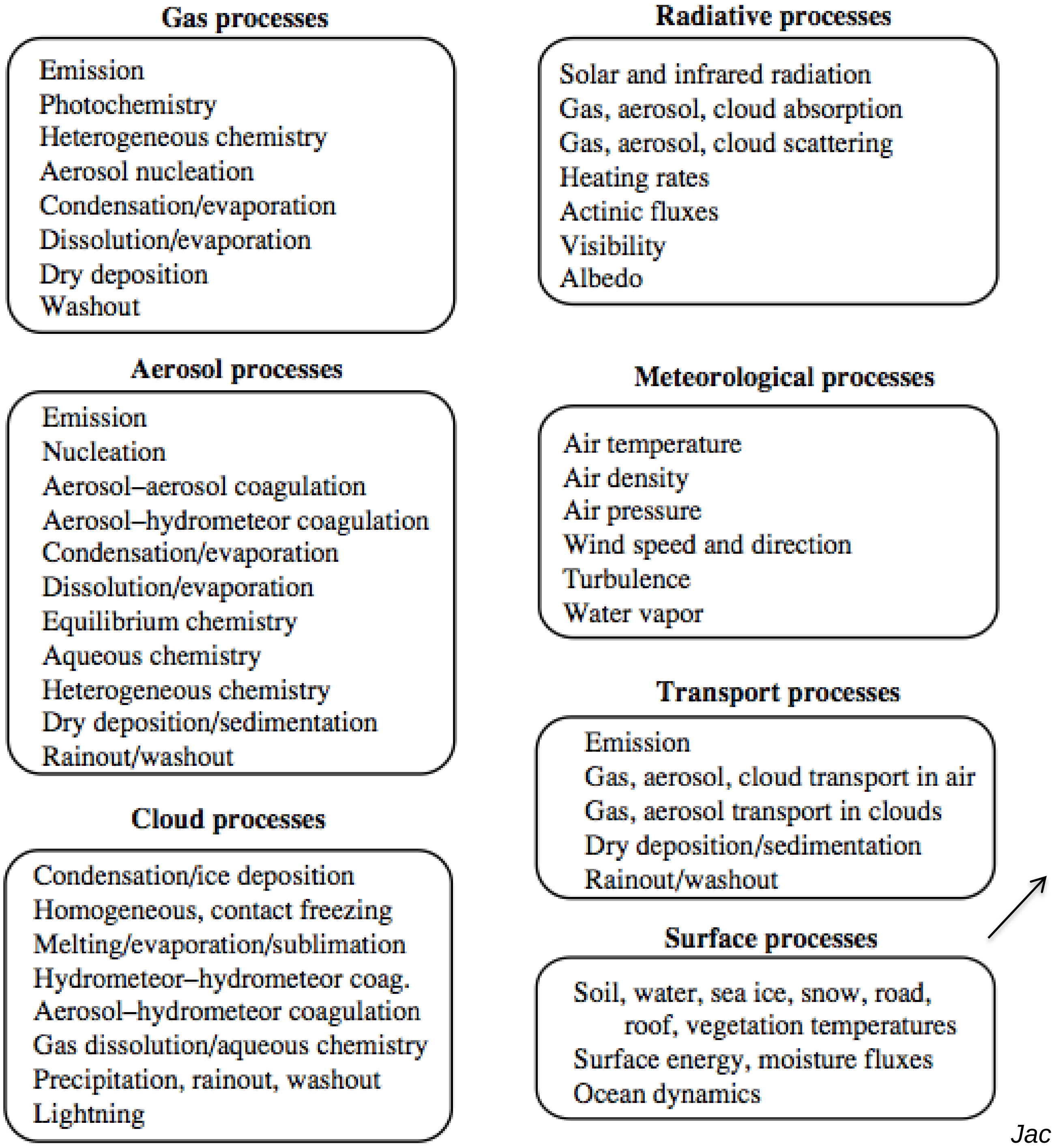
- As well as explicitly solving PDEs in discretised space/time, need to parameterise effects of un-resolved processes



Examples of processes that might be parameterised:

- Convection (O(10m))
- Cloud microphysics (O($10^{-6}$m))
- Gravity waves (O(100m))
- Snow/ice cover
- Wildfires
- Radiation

# Atmospheric processes simulated in a CCM



**Gas processes**

- Emission
- Photochemistry
- Heterogeneous chemistry
- Aerosol nucleation
- Condensation/evaporation
- Dissolution/evaporation
- Dry deposition
- Washout

**Aerosol processes**

- Emission
- Nucleation
- Aerosol–aerosol coagulation
- Aerosol–hydrometeor coagulation
- Condensation/evaporation
- Dissolution/evaporation
- Equilibrium chemistry
- Aqueous chemistry
- Heterogeneous chemistry
- Dry deposition/sedimentation
- Rainout/washout

**Cloud processes**

- Condensation/ice deposition
- Homogeneous, contact freezing
- Melting/evaporation/sublimation
- Hydrometeor–hydrometeor coag.
- Aerosol–hydrometeor coagulation
- Gas dissolution/aqueous chemistry
- Precipitation, rainout, washout
- Lightning

**Radiative processes**

- Solar and infrared radiation
- Gas, aerosol, cloud absorption
- Gas, aerosol, cloud scattering
- Heating rates
- Actinic fluxes
- Visibility
- Albedo

**Meteorological processes**

- Air temperature
- Air density
- Air pressure
- Wind speed and direction
- Turbulence
- Water vapor

**Transport processes**

- Emission
- Gas, aerosol, cloud transport in air
- Gas, aerosol transport in clouds
- Dry deposition/sedimentation
- Rainout/washout

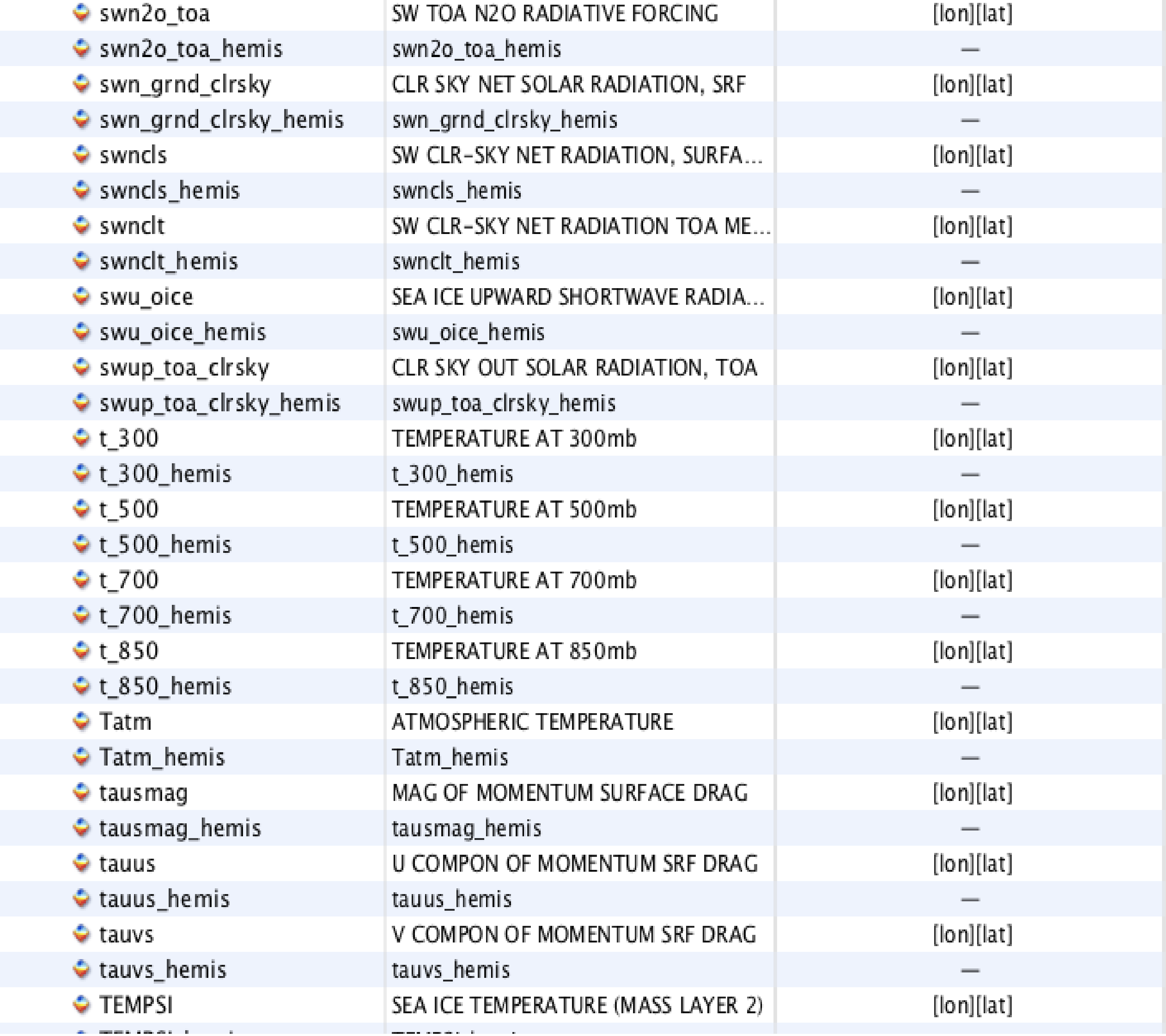
**Surface processes**

- Soil, water, sea ice, snow, road, roof, vegetation temperatures
- Surface energy, moisture fluxes
- Ocean dynamics

Surface processes not strictly atmospheric, but can influence atmosphere. In Earth system models, the biosphere is simulated simultaneously, i.e. vegetation type, growth, and emissions depend on simulated climate.

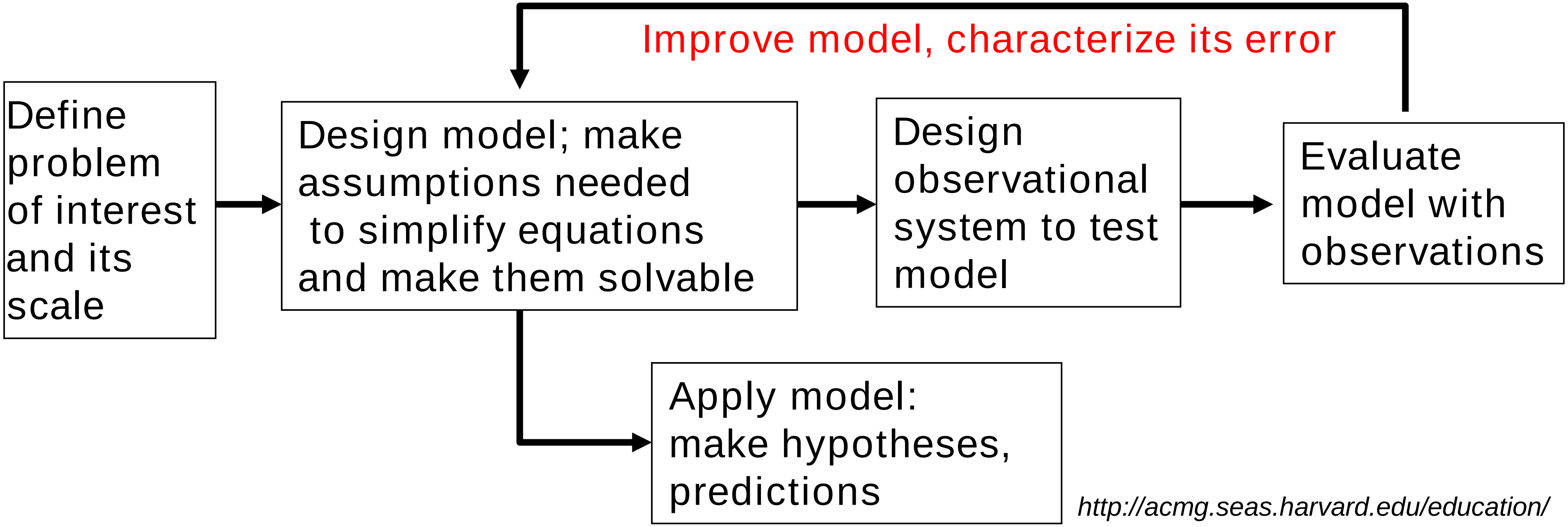
*Jacobson (2005)*

**Example: Screenshot of NASA GISS model output**



| | | |
|---|---|---|
| swn2o_toa | SW TOA N2O RADIATIVE FORCING | [lon][lat] |
| swn2o_toa_hemis | swn2o_toa_hemis | — |
| swn_grnd_clrsky | CLR SKY NET SOLAR RADIATION, SRF | [lon][lat] |
| swn_grnd_clrsky_hemis | swn_grnd_clrsky_hemis | — |
| swncls | SW CLR-SKY NET RADIATION, SURFA... | [lon][lat] |
| swncls_hemis | swncls_hemis | — |
| swnclt | SW CLR-SKY NET RADIATION TOA ME... | [lon][lat] |
| swnclt_hemis | swnclt_hemis | — |
| swu_oice | SEA ICE UPWARD SHORTWAVE RADIA... | [lon][lat] |
| swu_oice_hemis | swu_oice_hemis | — |
| swup_toa_clrsky | CLR SKY OUT SOLAR RADIATION, TOA | [lon][lat] |
| swup_toa_clrsky_hemis | swup_toa_clrsky_hemis | — |
| t_300 | TEMPERATURE AT 300mb | [lon][lat] |
| t_300_hemis | t_300_hemis | — |
| t_500 | TEMPERATURE AT 500mb | [lon][lat] |
| t_500_hemis | t_500_hemis | — |
| t_700 | TEMPERATURE AT 700mb | [lon][lat] |
| t_700_hemis | t_700_hemis | — |
| t_850 | TEMPERATURE AT 850mb | [lon][lat] |
| t_850_hemis | t_850_hemis | — |
| Tatm | ATMOSPHERIC TEMPERATURE | [lon][lat] |
| Tatm_hemis | Tatm_hemis | — |
| tausmag | MAG OF MOMENTUM SURFACE DRAG | [lon][lat] |
| tausmag_hemis | tausmag_hemis | — |
| tauus | U COMPON OF MOMENTUM SRF DRAG | [lon][lat] |
| tauus_hemis | tauus_hemis | — |
| tauvs | V COMPON OF MOMENTUM SRF DRAG | [lon][lat] |
| tauvs_hemis | tauvs_hemis | — |
| TEMPSI | SEA ICE TEMPERATURE (MASS LAYER 2) | [lon][lat] |

# How to use a model



Improve model, characterize its error

Define problem of interest and its scale

Design model; make assumptions needed to simplify equations and make them solvable

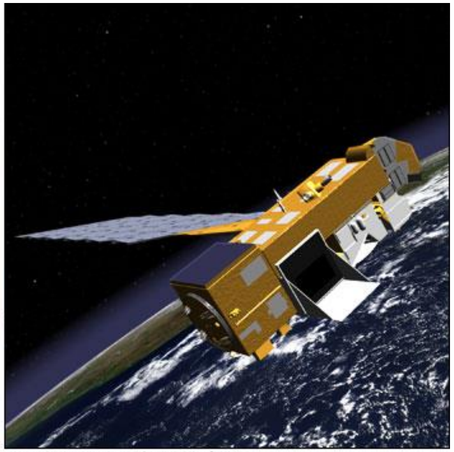
Design observational system to test model

Evaluate model with observations

Apply model: make hypotheses, predictions

*http://acmg.seas.harvard.edu/education/*

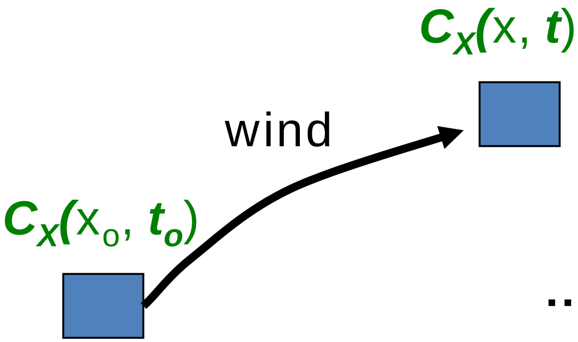
Boeing Delta II Rocket



Artist's rendering of Aura in Orbit

Need to be in constant dialogue.

# Lagrangian model: Follow air parcel moving with wind

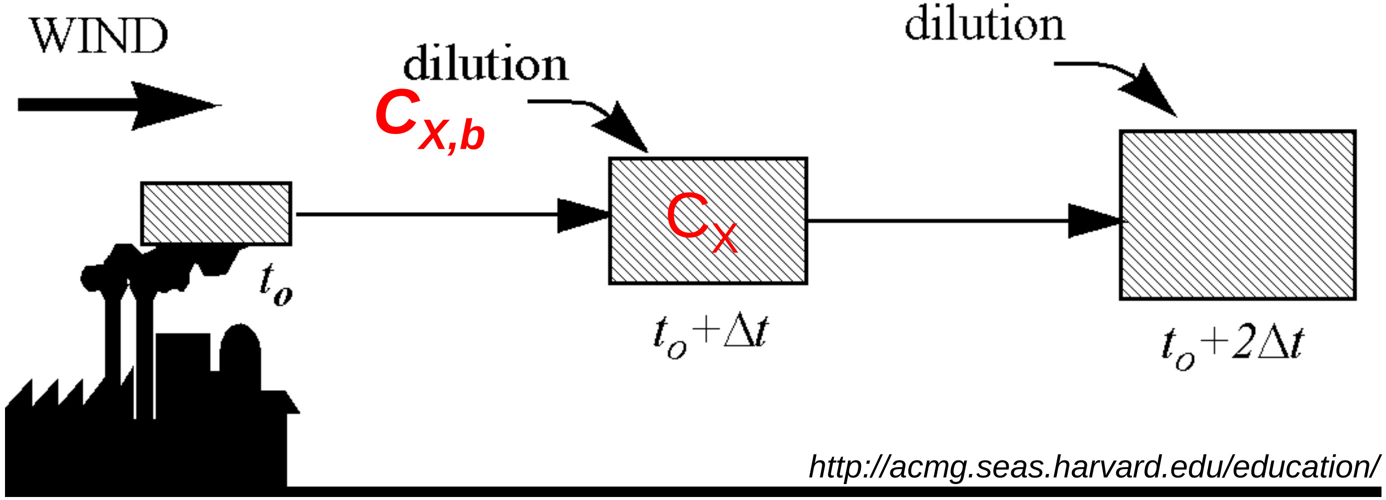


In the moving box (***C*** is the concentration),

$$\frac{dC_X}{dt} = E + P - L - D$$

**…no transport terms! (they're implicit in the trajectory)**

Application to the chemical evolution of an isolated pollution plume:

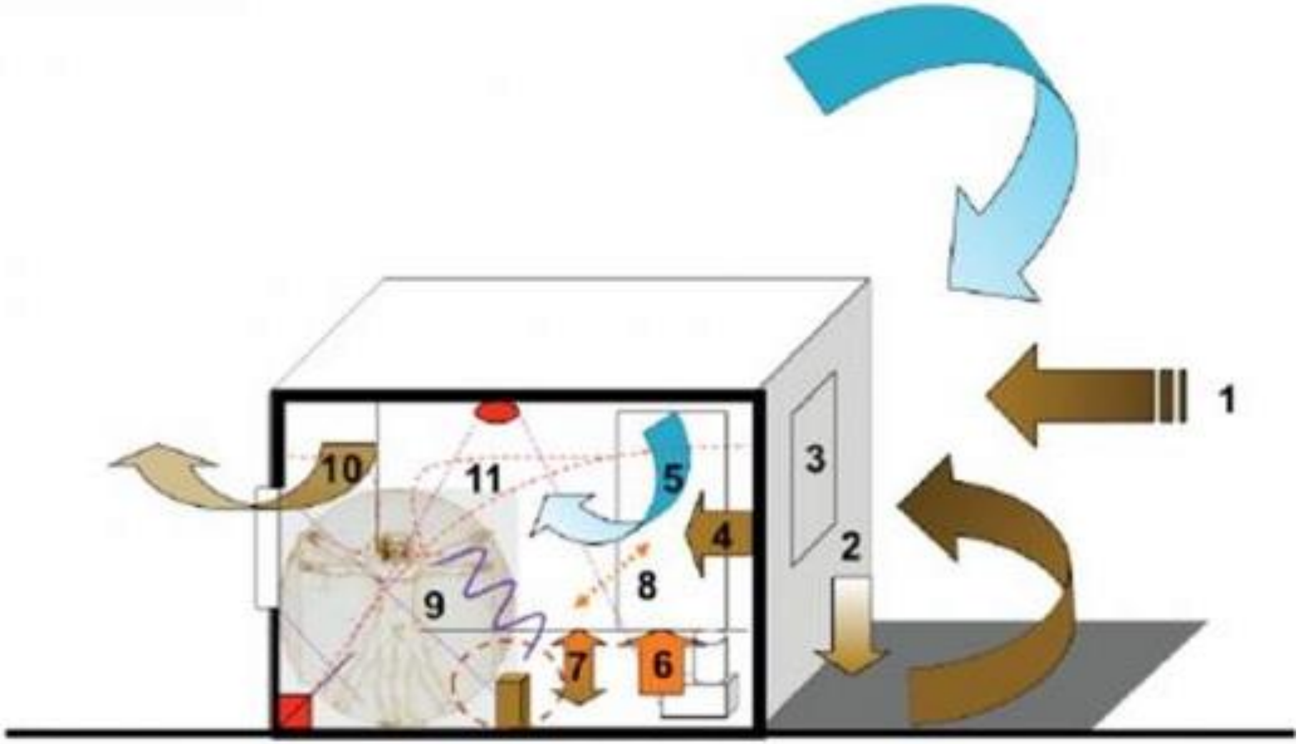


*http://acmg.seas.harvard.edu/education/*

In pollution plume,

$$\frac{dC_X}{dt} = E + P - L - D - k_{dilution}(C_X - C_{X,b})$$

# Even indoor air pollution models!



1. Levels of outdoor-PM and its distributions
2. Penetration loss of outdoor-PM concentrations
3. Building characteristics
4. Outdoor-PM indoors gain through natural ventilation and infiltration
5. Outdoor clean air through natural ventilation
6. Levels of indoor-PM from indoor sources
7. Deposition loss and re-suspension of PM
8. Indoor-PM concentrations loss and gain through other rooms and/or indoor passageways
9. Human/animal presence and activity
10. Indoor-PM loss through natural ventilation and exfiltration
11. Interaction of and between pollutants (i.e. formation, phase change, coagulation)

- In many ways similar to what we saw earlier.

- Atmospheric models share several of their principles/characteristics, from the (very) local to the global scale.

# Summary

- Showed and discussed the mass balance equation for atmospheric constituents in a model.

- Discussed one-box and two-box models.

- Presented basic thermodynamic and dynamic equations in models, and mentioned their interactions.

- Gave a summary of how models are typically used.

- Briefly mentioned Lagrangian and indoor air quality models.