



The University of Edinburgh

Atmospheric Modelling of Greenhouse Gases [GHGs]

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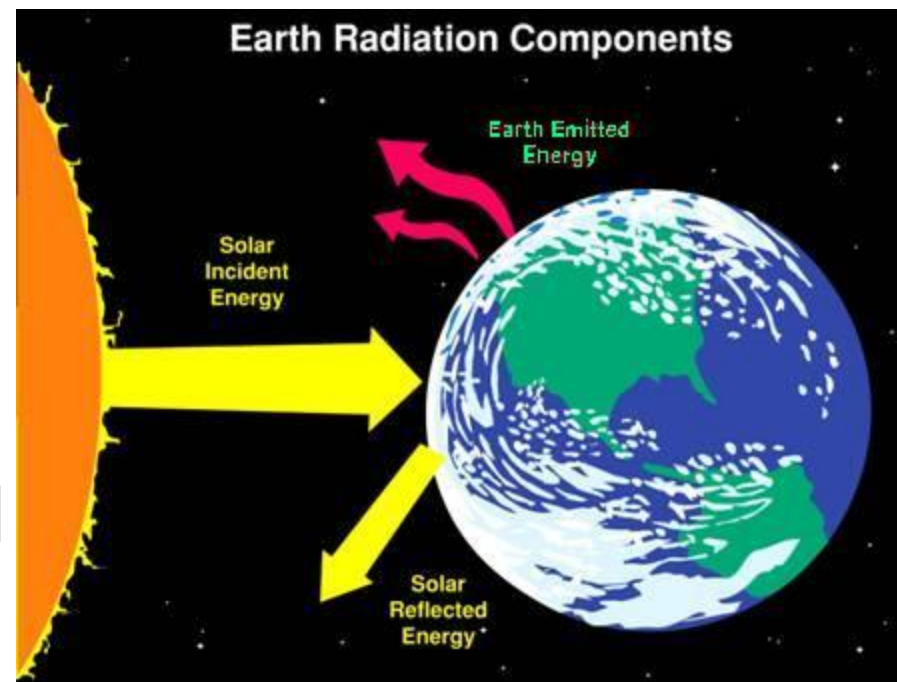
Overview

- **Motivation:** why do GHGs matter?
- **Measurements:** what do measurements tell us about the behaviour of GHGs
- **Modelling:** What is GHG modelling and what can it tell us?

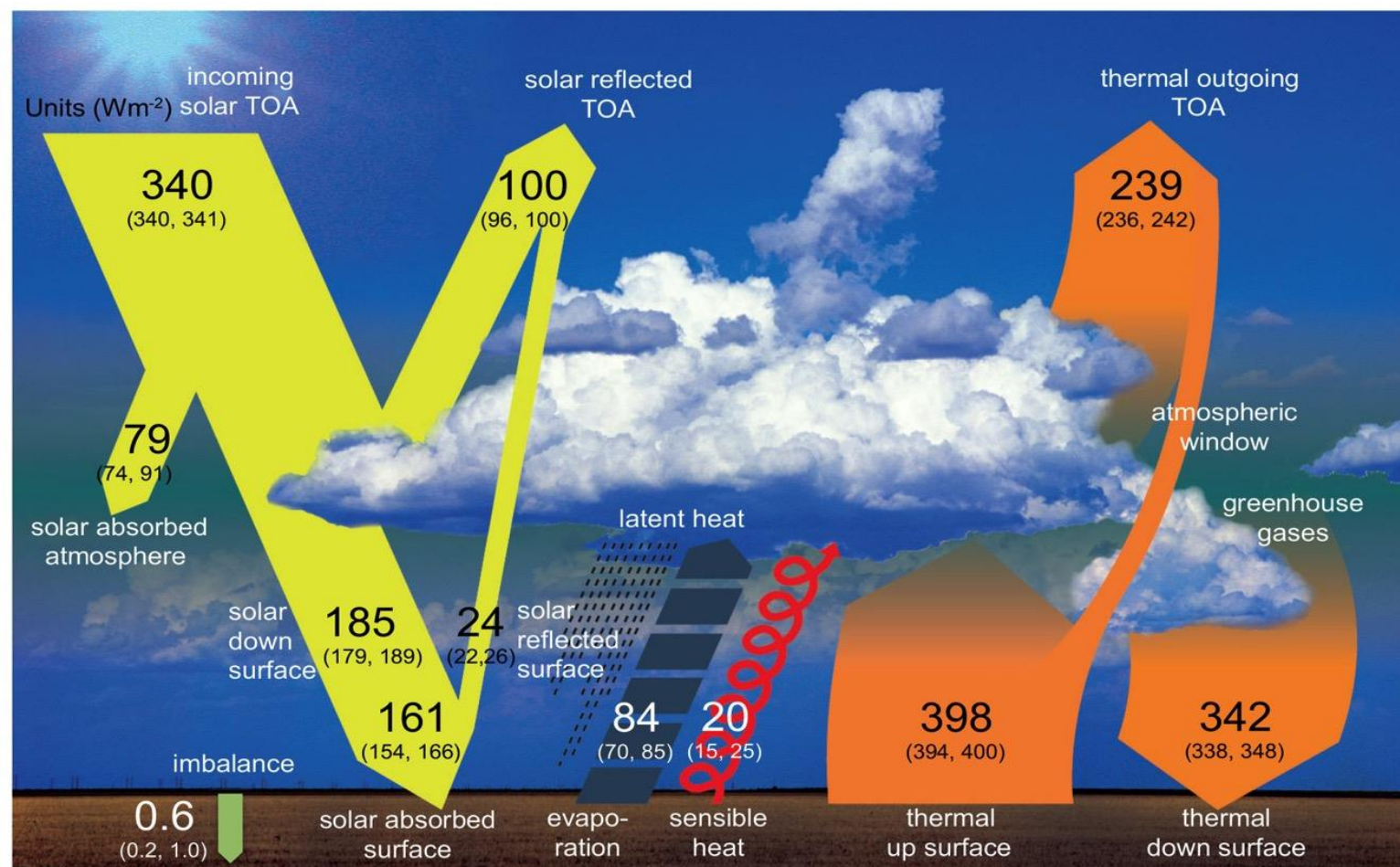
Mostly CO₂, some CH₄ and general trace gas modelling

Radiation balance of the Earth

- Earth *must* emit as much energy as it receives from the sun
- Some is reflected, rest is adsorbed
- For **Mars**, this well-predicts the temperature
 - But it suggests **Earth** would have average temp of -18C
 - It's warmer! (15C)

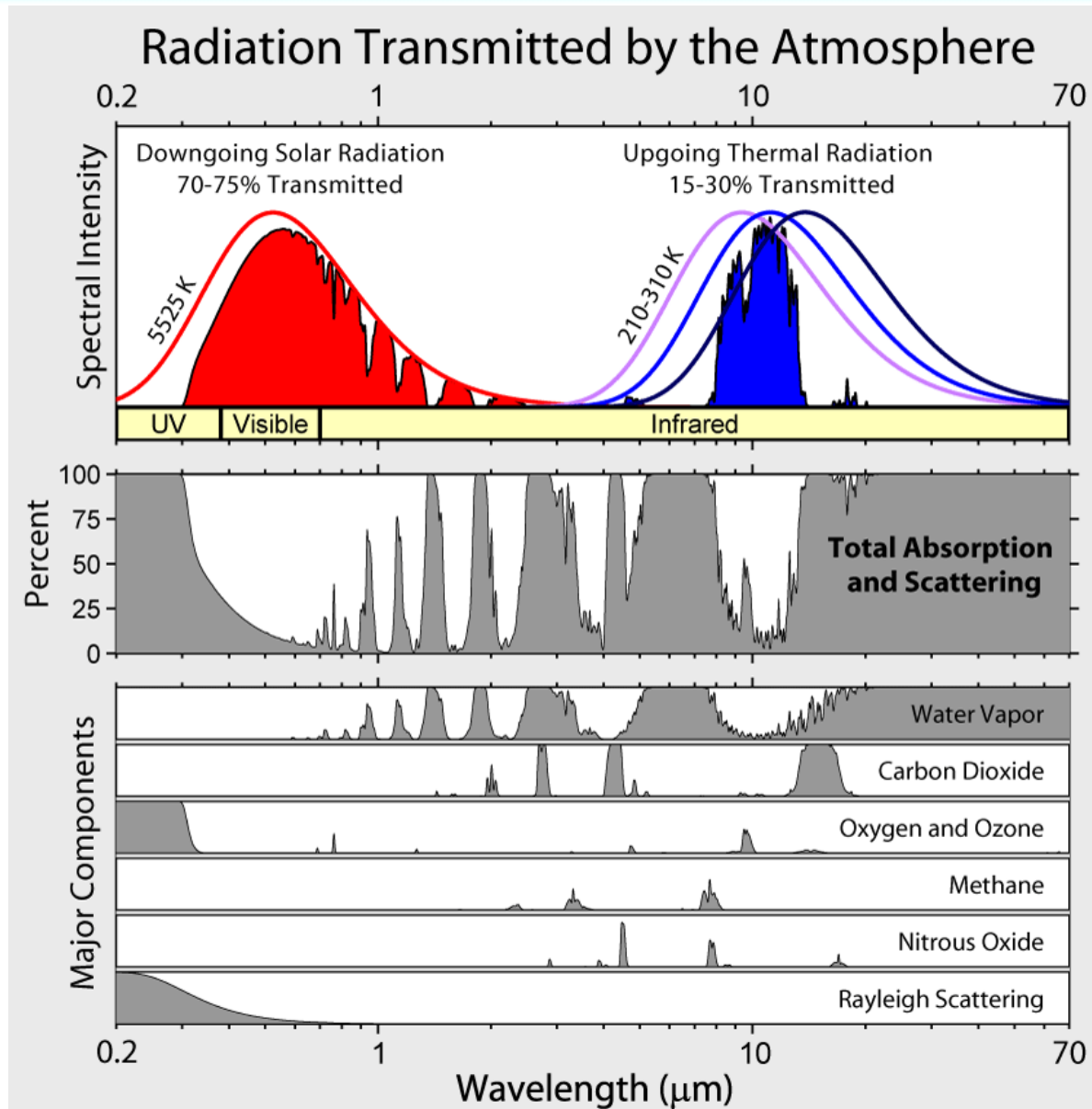


Radiation balance of the Earth



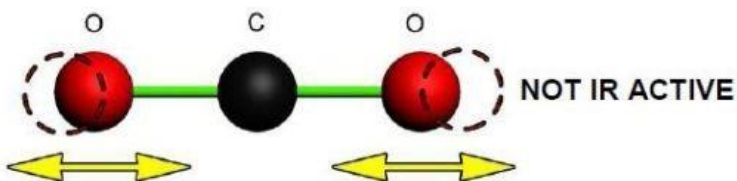
Radiation balance of the Earth

- Earth is colder than the sun
- Different wavelengths of radiation
- Different gases adsorb the radiation coming in as going out!
 - GHGs let radiation in, but block it leaving

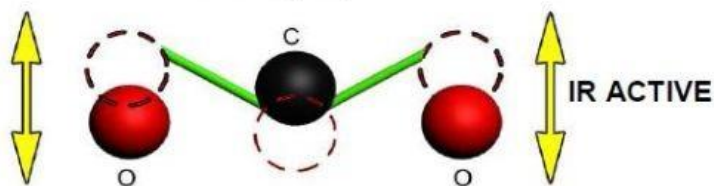


Why do some gases adsorb in the IR and not others?

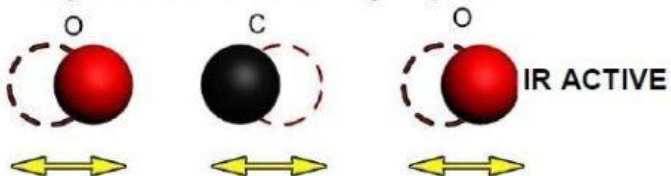
Symmetric Stretching No Dipole



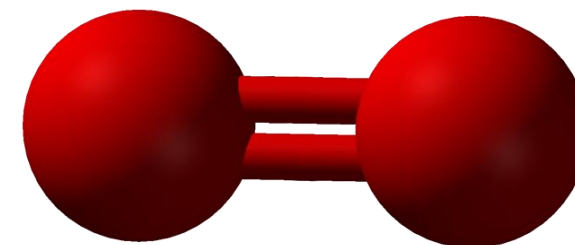
Bending Dipole



Asymmetric Stretching Dipole



- *IR active* if vibration changes the electrostatic dipole moment of the molecule.
- Two different ways of vibrating a CO₂ molecule do this
- Impossible to do this for O₂, N₂.



Measuring GHGs

- It should come as a surprise that we have only measured GHGs since the late 1950s.
- The link between GHGs and climate is now well established so that GHGs are a political issue.
- Consequently, we are only just getting to grips with issues that should have been addressed decades ago.

Measuring Atmospheric CO₂

- Best, longest term record (1950s) is from the Mauna Loa observatory in Hawaii
- Charles Keeling discovered:
 - A seasonal cycle
 - Long-term increase

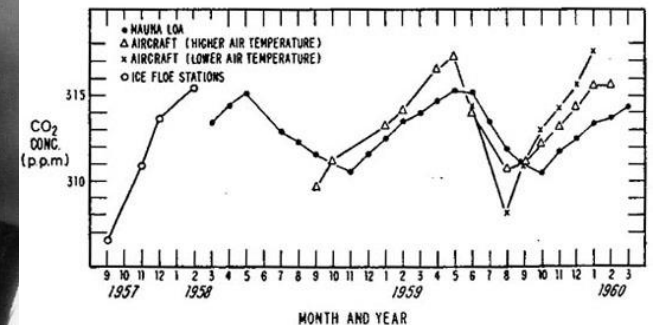
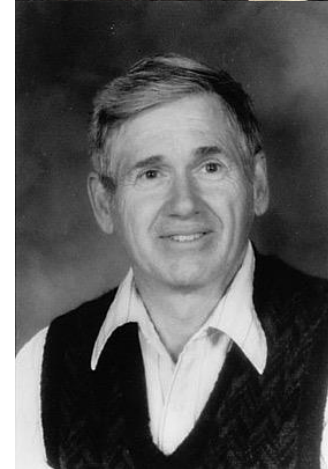
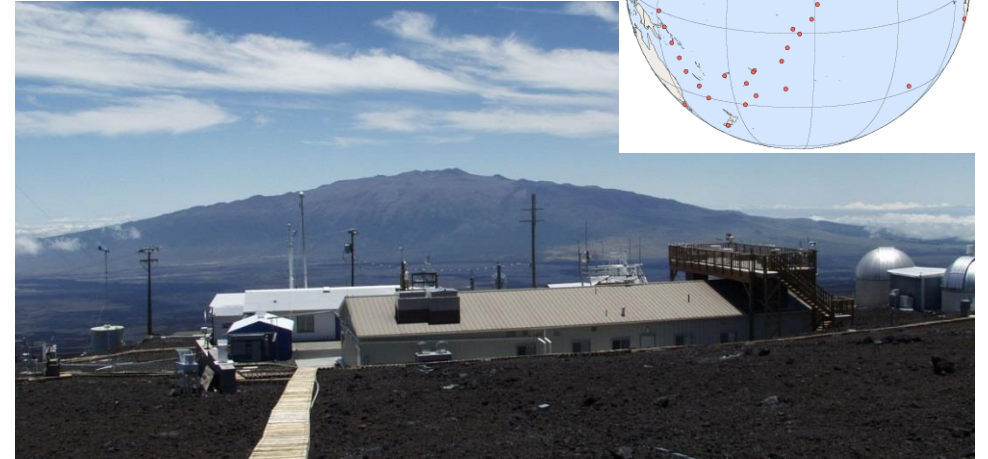
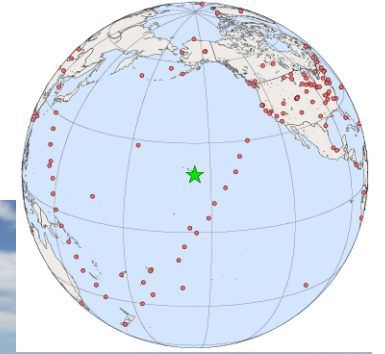
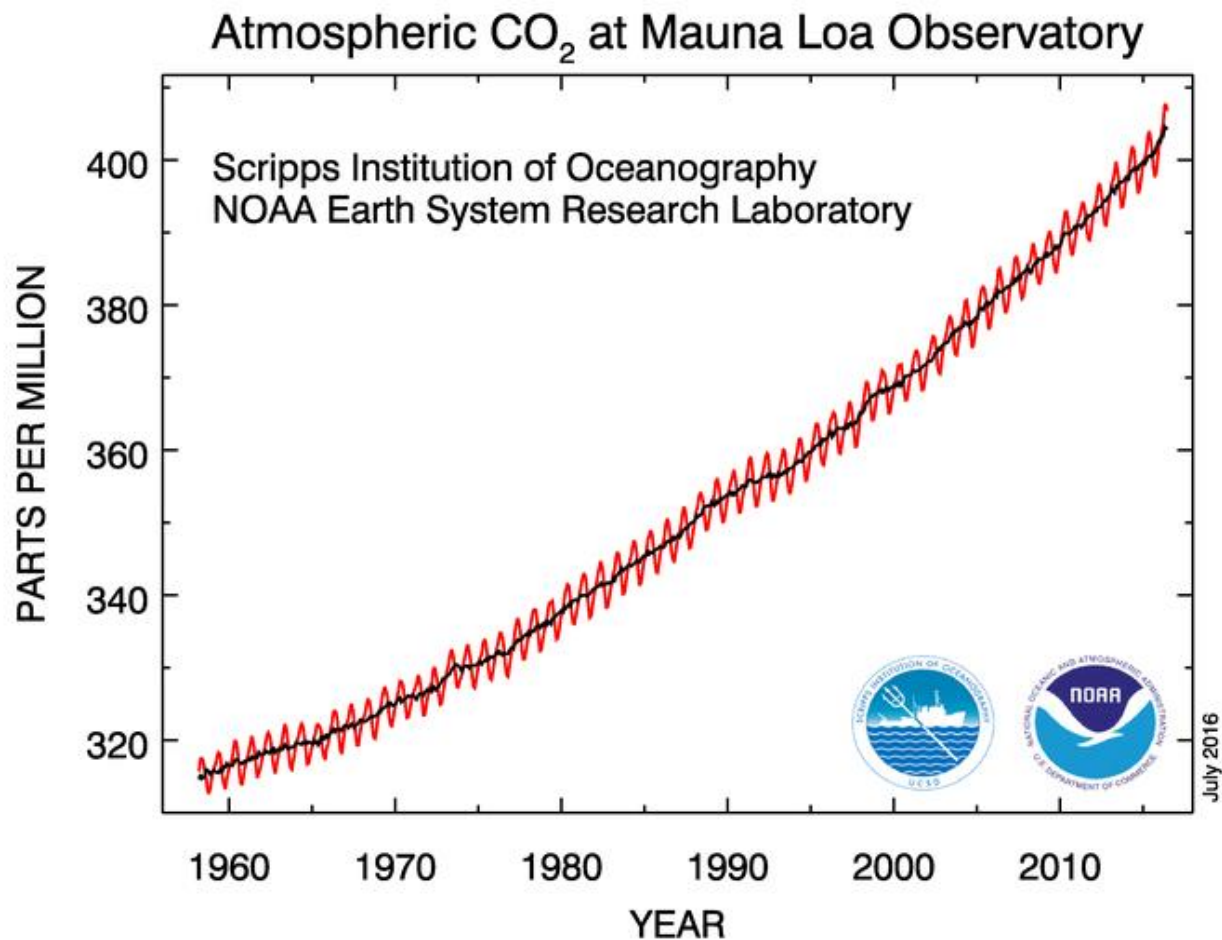


Fig. 1. Variation in concentration of atmospheric carbon dioxide in the Northern Hemisphere.

Tellus XII (1960), 2

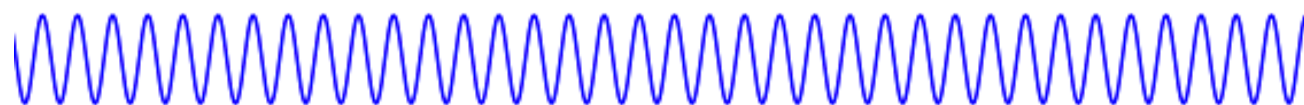
Measuring Atmospheric CO₂

- A zeroth order model:
 - An annual linear increase (fossil fuel combustion) superimposed with a sinusoid (land and ocean biosphere)

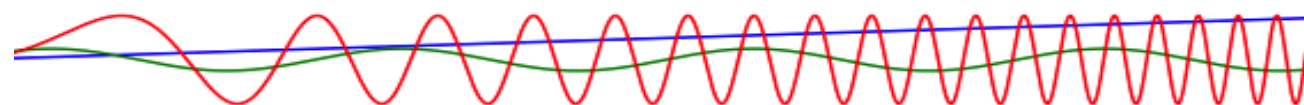
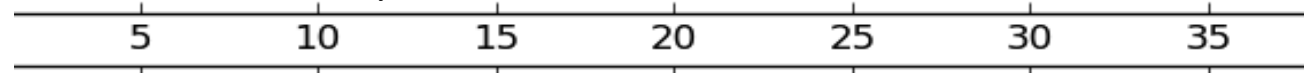


Superimposed signatures

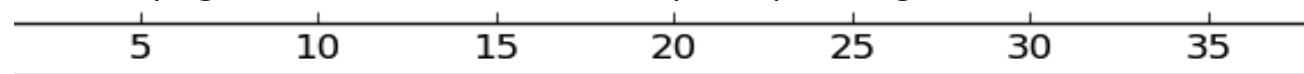
GHG concentration [unit]



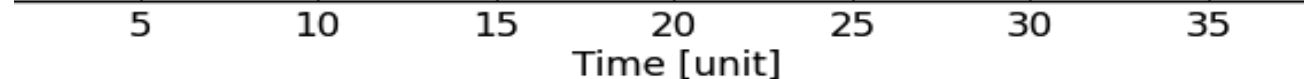
Invariant seasonal cycle



Anthropogenic and natural factors superimpose signatures

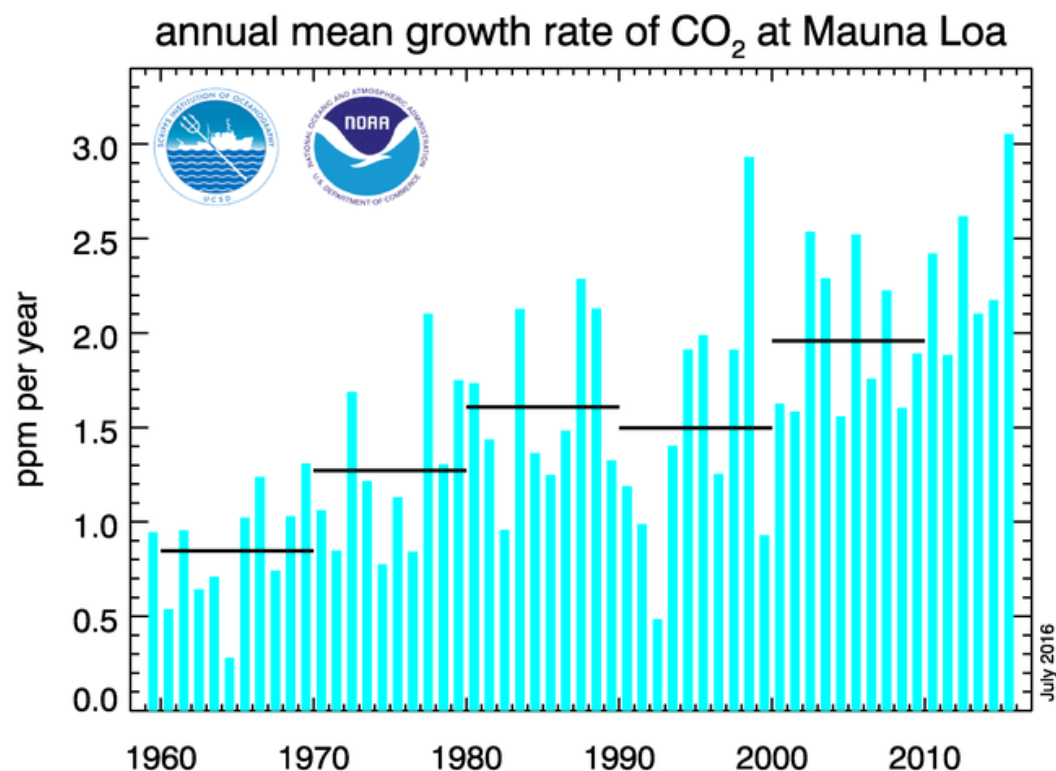


What we are left with: a complex observed variation



Time [unit]

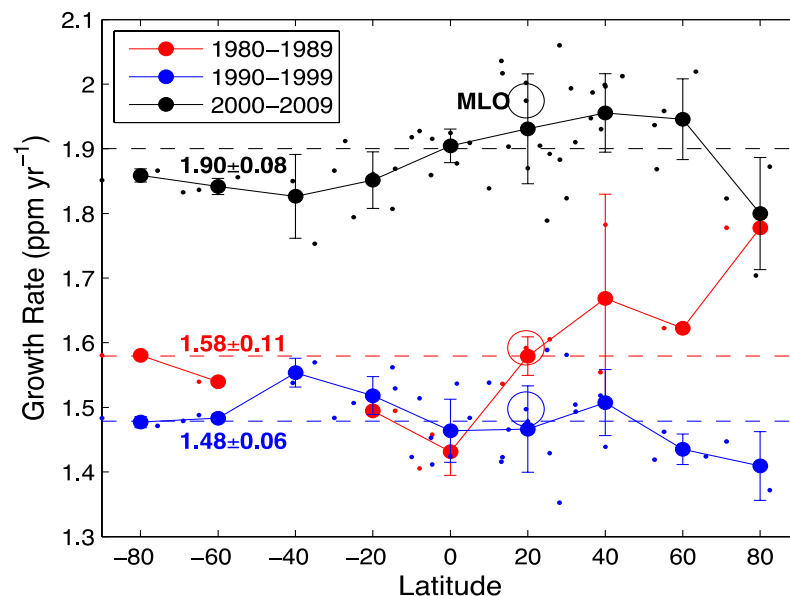
Year-on-year rise of atmospheric CO₂



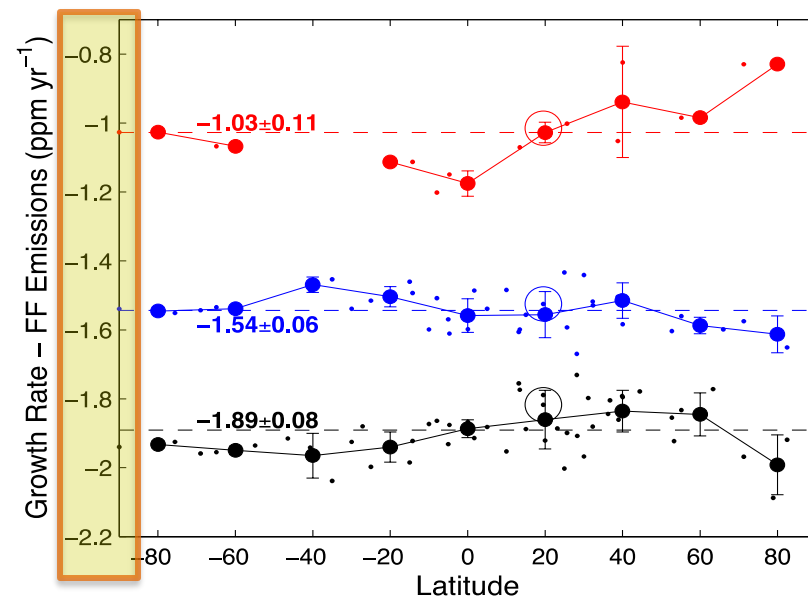
- Every year the average mixing ratio of CO₂ increases
- However this is *less* than what we'd expect from adding up all the carbon we burn

Year-on-year rise of atmospheric CO₂

Net Carbon Flux to Atmosphere



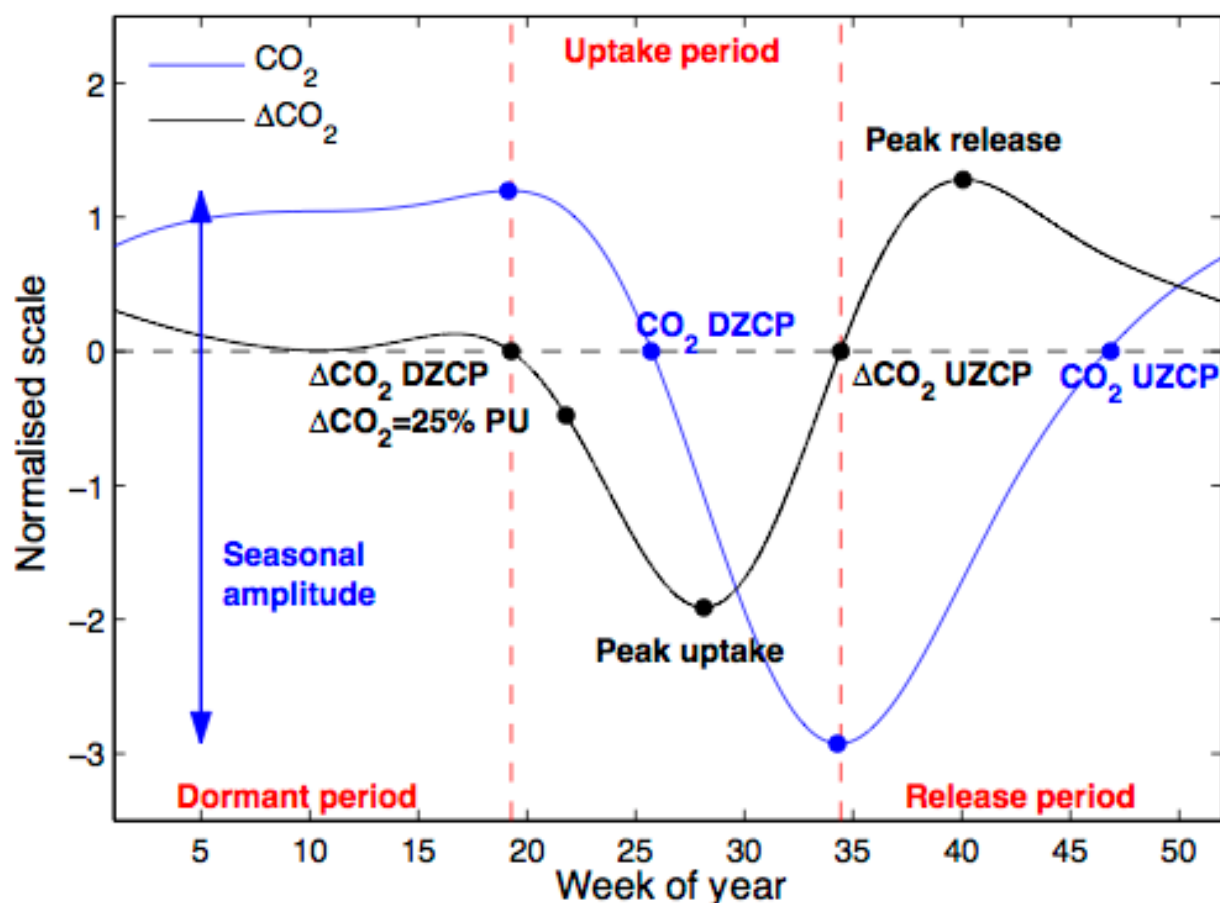
Net Natural Carbon Flux to atmosphere (growth rate – FF emissions)



Barlow et al, 2015

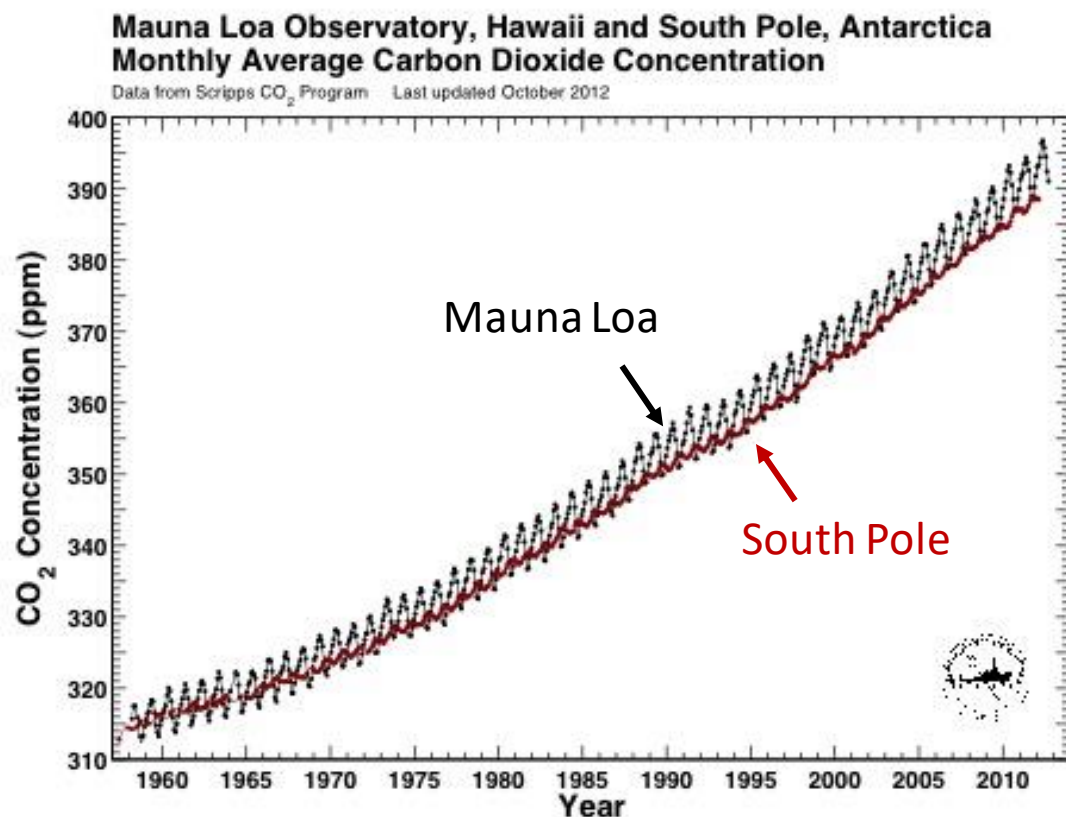
Over the past 50 years approximately $44.1 \pm 14.4\%$ of emitted CO₂ (inc. fossil fuel and LUC) has stayed in the atmosphere: the natural biosphere appears to respond to increasing atmospheric CO₂.

Seasonality of atmospheric CO₂



- CO₂ taken out of atmosphere during (Northern Hemisphere) Spring/summer by plants (biosphere)
- In autumn this reverses.

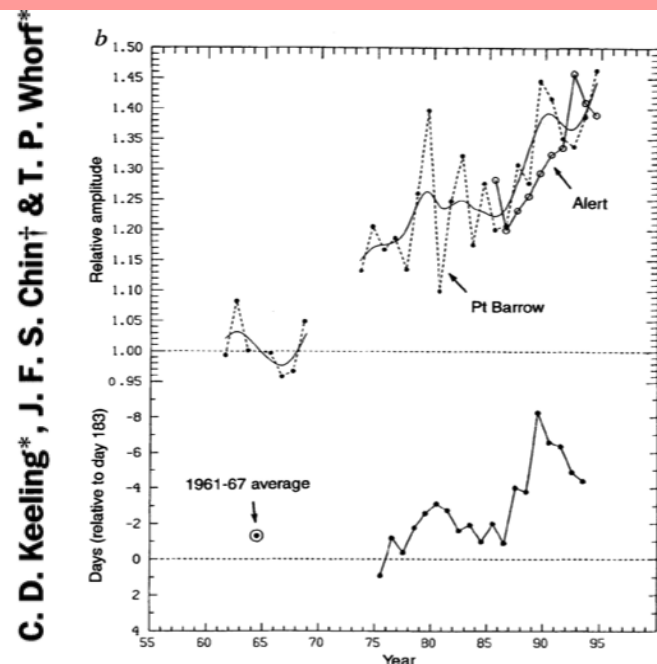
Seasonality of atmospheric CO₂



- Same happens in Southern Hemisphere (6 months out of phase), but less intense as there's less biomass.

Changes in seasonality of atmospheric CO₂

Greater seasonal amplitude



plant activity⁶. Here we report that the annual amplitude of the seasonal CO₂ cycle has increased by 20%, as measured in Hawaii, and by 40% in the Arctic, since the early 1960s. These increases are accompanied by phase advances of about 7 days during the declining phase of the cycle, suggesting a lengthening of the growing season. In addition, the annual amplitudes show maxima which appear to reflect a sensitivity to global warming episodes that peaked in 1981 and 1990. We propose that the amplitude increases reflect increasing assimilation of CO₂ by land plants in response to climate changes accompanying recent rapid increases in temperature.

Earlier Spring

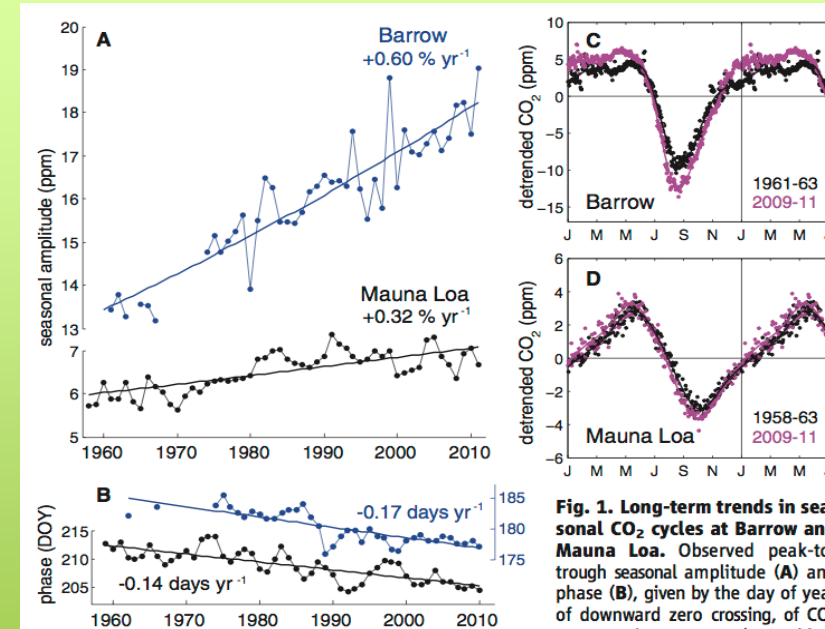
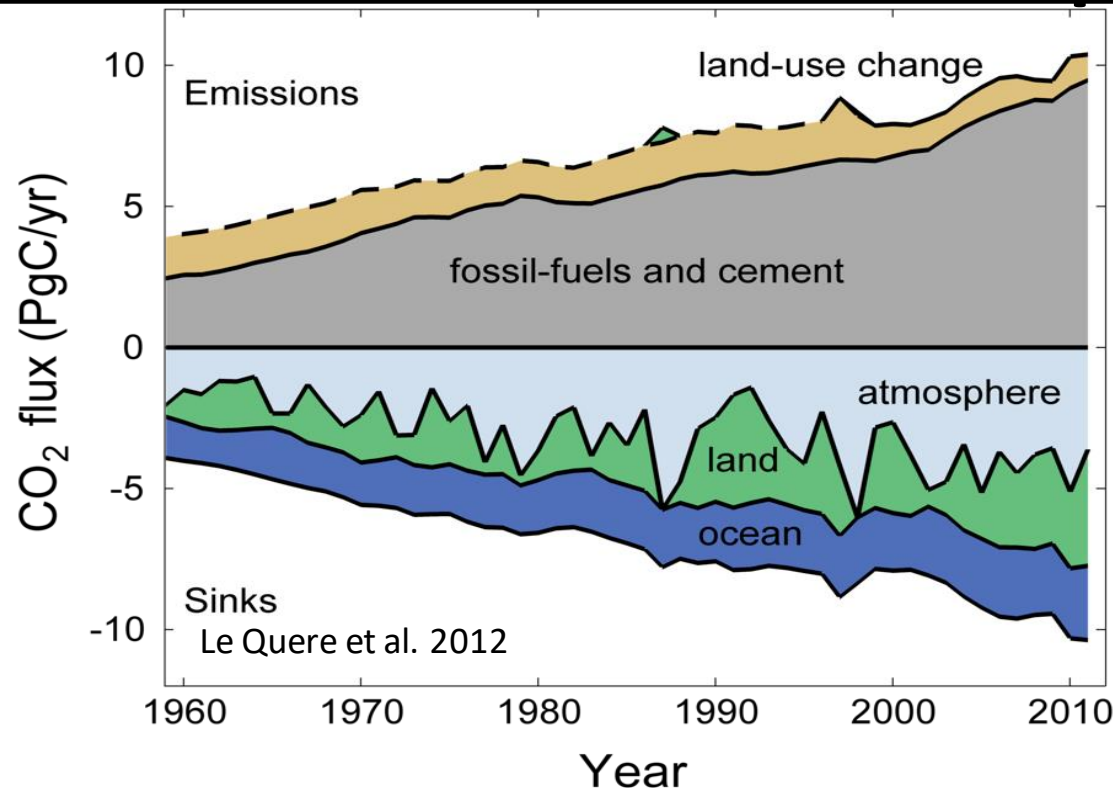


Fig. 1. Long-term trends in seasonal CO₂ cycles at Barrow and Mauna Loa. Observed peak-to-trough seasonal amplitude (**A**) and phase (**B**), given by the day of year of downward zero crossing, of CO₂ concentration at Barrow (71°N, blue) and Mauna Loa (20°N, black) measured by the Scripps CO₂ Program (7, 8) and the NOAA Global Monitoring Division (9). Growth rate of amplitude is given in percentage change per year, with 1 SD uncertainty of ±0.05 to 0.07% year⁻¹. Seasonal CO₂ cycles observed at Barrow (**C**) and Mauna Loa (**D**) for the 1961 to 1963 or 1958 to 1963 and 2009 to 2011 time periods. The first 6 months of the year are repeated.

Graven et al, 2013

Sources and sinks of atmospheric CO₂



2003-2012 Sources (PgC/yr)

- LUC: 0.8 ± 0.5 (9%)
- FF: 8.6 ± 0.4 (91%)

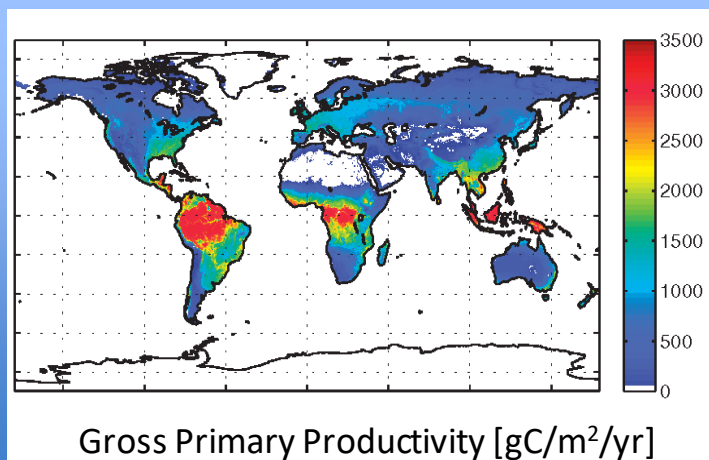
2003-2012 Sinks (PgC/yr)

- Atmosphere: 4.3 ± 0.1 (45%)
- Ocean: 2.6 ± 0.5 (27%)
- Land: 2.6 ± 0.8 PgC/yr (28%)
(land estimate residual)

- ⊙ What natural processes absorb half of the CO₂ emitted by human activities?
- ⊙ Why does the amount of CO₂ absorbed change from year to year?
- ⊙ Will this change in the future, as the climate changes?

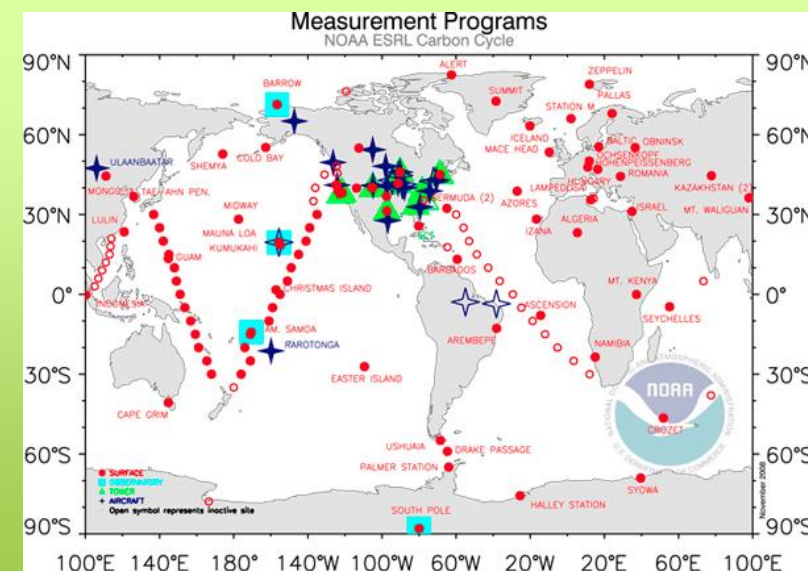
How do we know what we know?

Beer et al, 2010



Highest CO₂ emitting power plants in the world

carma.org



Outcome: For CO₂ we have an incomplete understanding of regional fluxes.
Situation worse for CH₄ and N₂O.

Models

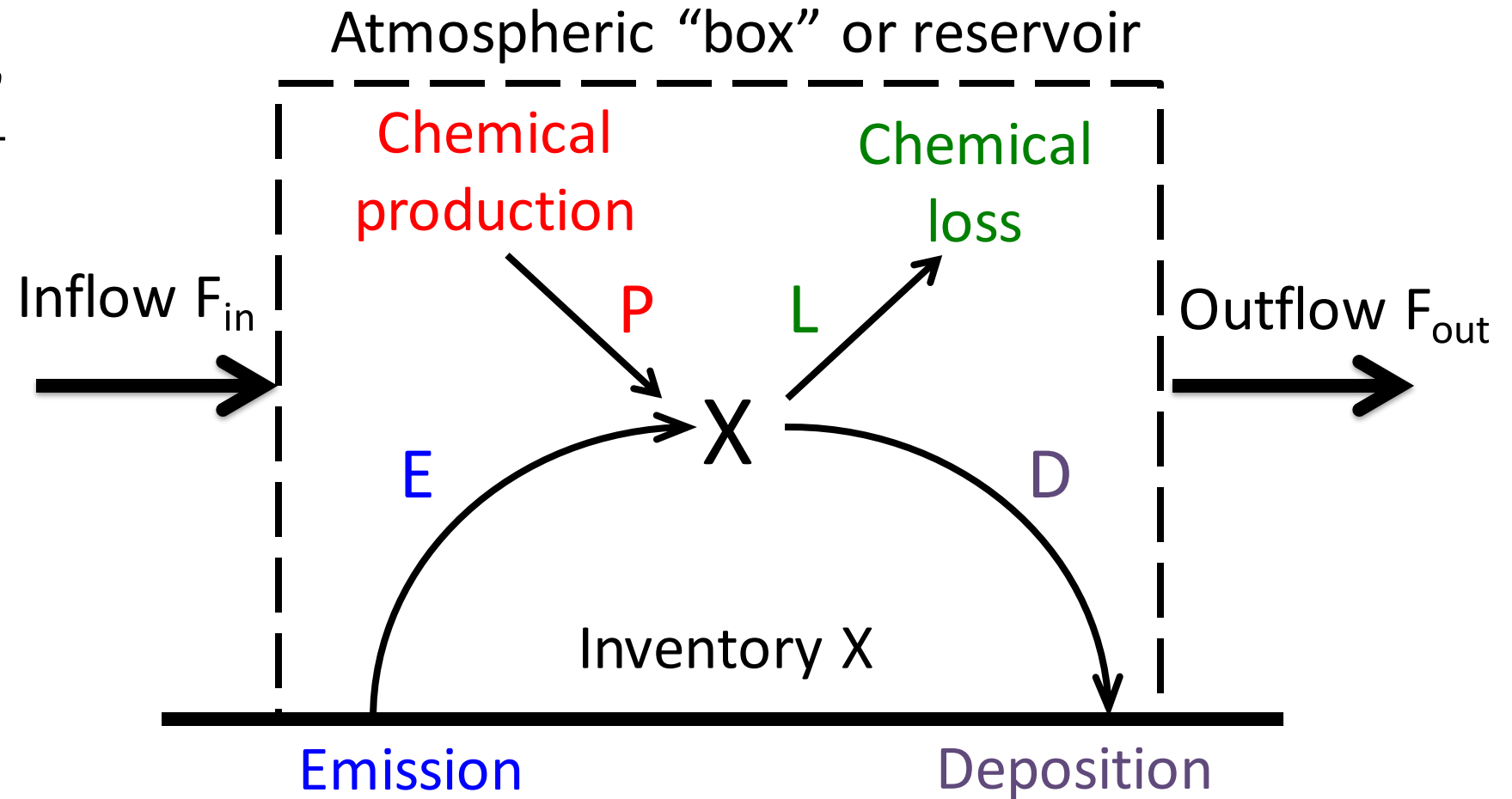
- One definition:
 - *A model is a framework (typically mathematical) that tests scientific understanding through its ability to explain data.*
 - *It should be sufficiently simple that it can, in principle, be rejected (and refined) with data.*
 - *A predictive capability is developed through this refinement process.*

Interesting articles:

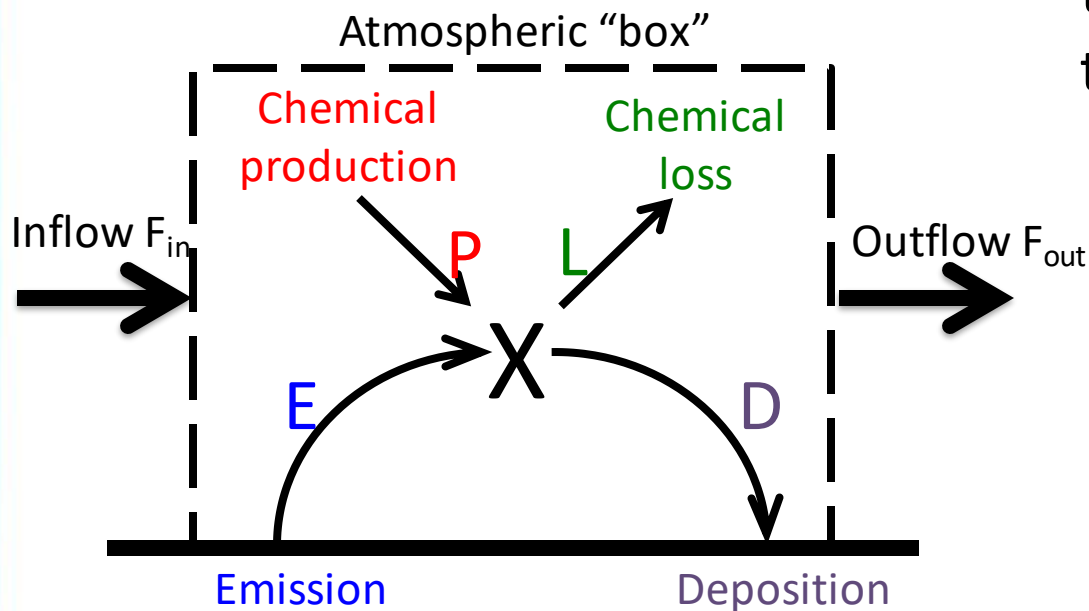
DOI: <http://dx.doi.org/10.1175/BAMS-D-13-00080.1>

DOI: <http://dx.doi.org/10.1016/j.cell.2008.07.033>

A “box model”



“Lifetime” of a molecule



The lifetime t of X in the box: average time that a molecule of X remains in that box.

$$t = \frac{m}{F_{out} + L + D}$$

← Mass of X (kg)

Losses (kg.s⁻¹)

Often called the *residence time* when the loss is a physical process (e.g., F_{out} or D)

“Lifetime of a molecule”

We’re often interested in the *relative importance* of each loss term

Fraction f

removed by
export out of
the box

$$f = \frac{F_{out}}{F_{out} + L + D}$$

Sink-specific

lifetimes, e.g.,
lifetime against
export

$$t_{out} = \frac{m}{F_{out}}$$

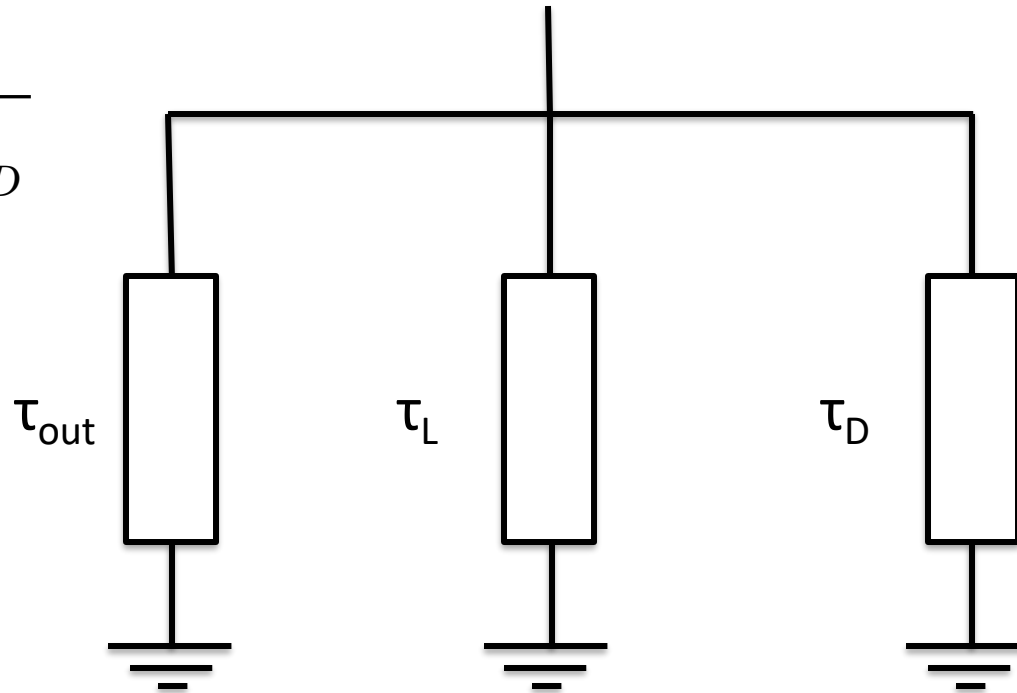
Total lifetime is calculated in parallel:

$$\frac{1}{t} = \frac{1}{t_{out}} + \frac{1}{t_L} + \frac{1}{t_D}$$

These are considered *first order losses*: the more you have the more you can lose.

Resistor model for losses

$$\frac{1}{t} = \frac{1}{t_{out}} + \frac{1}{t_L} + \frac{1}{t_D}$$



Chemical lifetime

Consider a first-order chemical loss for X with rate constant k_c

Chemical loss rate is: $L = k_c m$

$$\tau_c = \frac{m}{L} = \frac{m}{k_c m} = \frac{1}{k_c} \quad \longrightarrow \quad k_c = \frac{1}{\tau_c} \quad t_c = \frac{m}{L} = \frac{1}{k_c}$$

Generalise!

$$F_{out} + L + D = (k_{out}m + k_L m + k_D m) = k_{all}m$$

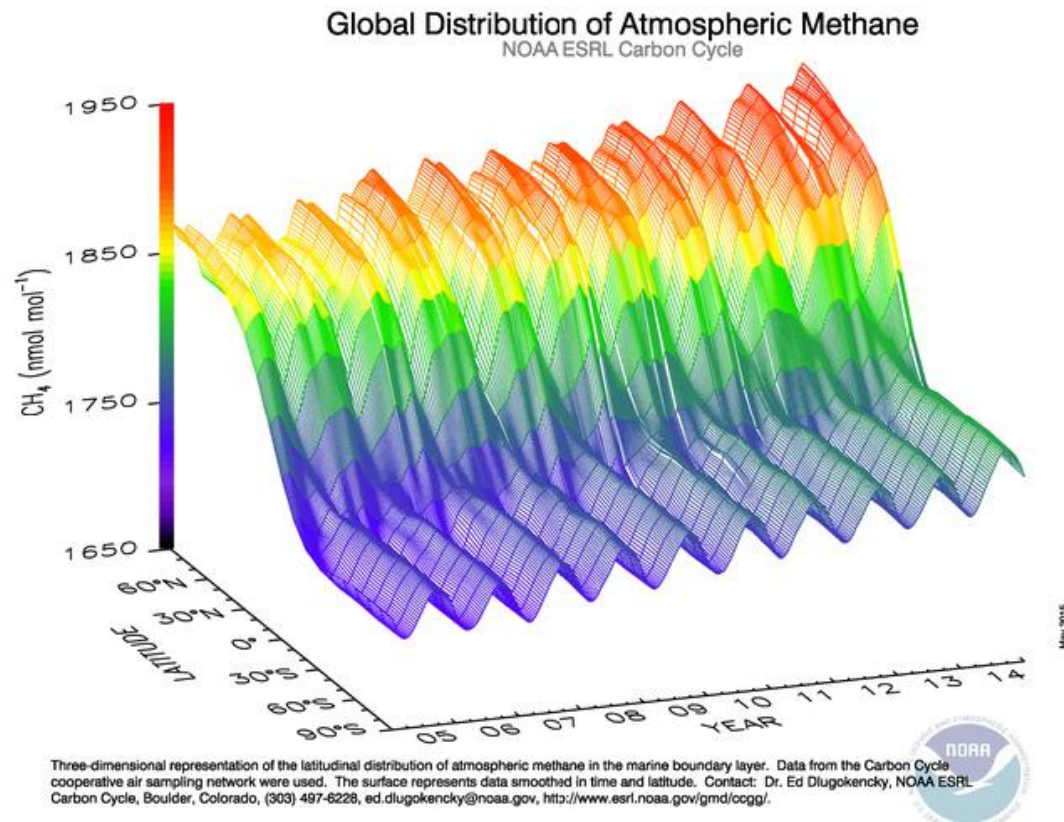
$$\tau_{all} = \frac{1}{k_{all}}$$

(k_{all} , τ_{all} normal written as simply k , τ)

Lifetime of atmospheric CH₄

- Lifetime against sinks include:
 - Hydroxyl radical (OH): 9.6 years
 - Soils: 160 years
 - Stratospheric sinks: 120 years
- These sinks are acting in parallel
- Net lifetime = $\frac{1}{\frac{1}{9.6} + \frac{1}{160} + \frac{1}{120}} = 8.4$ years.
- Much shorter than CO₂, resulting in larger inter-hemispheric gradients

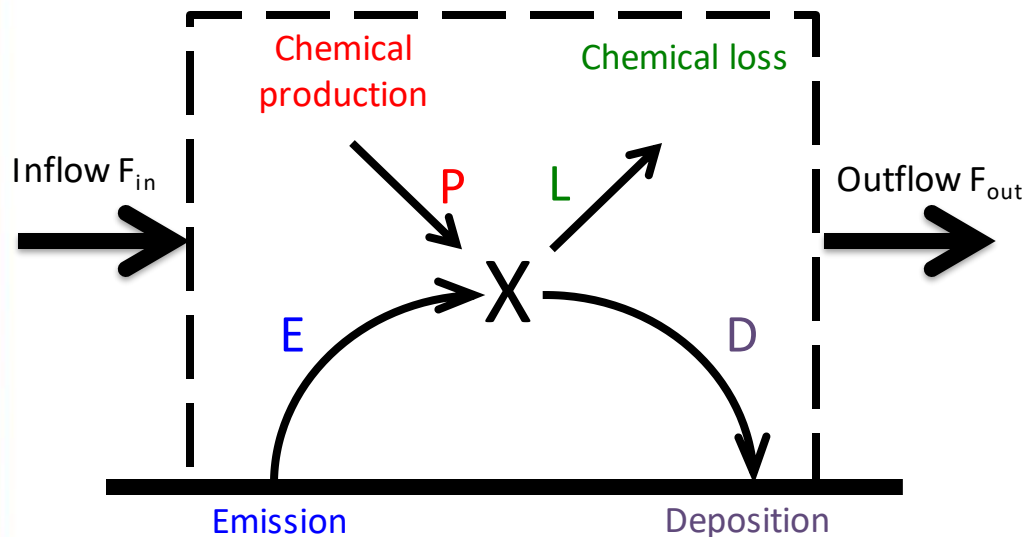
Mixing ratios of atmospheric CH₄



- The “magic carpet”
- More production of CH₄ in northern hemisphere.
- Losses greatest in summers

Mass balance

What is the rate of change of the mass of X in the box?



$$\begin{aligned} \frac{dm}{dt} &= \sum \text{sources} - \sum \text{sinks} \\ &= (F_{in} + E + P) - (F_{out} + L + D) \\ &= S - km \end{aligned}$$

Where overall source rate $S = F_{in} + E + P$

Mass balance

$$\frac{dm}{dt} = S - km$$



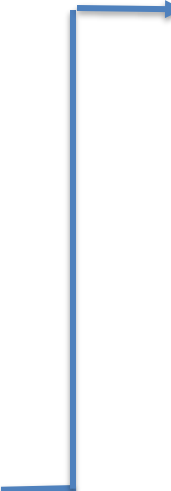
$$\frac{dm}{S - km} = dt$$



$$\left(-\frac{1}{k}\right) \ln(S - km) \Big|_0^T = t \Big|_0^T$$



$$\left(-\frac{1}{k}\right) \ln\left(\frac{S - km(T)}{S - km(0)}\right) = T$$


$$m(T) = m(0)e^{-kT} + \frac{S}{k}(1 - e^{-kT})$$

Mass balance

$$m(T) = m(0)e^{-kT} + \frac{S}{k}(1 - e^{-kT})$$

If $T = 0$

$$m = m(0)$$

Initial
conditions

transition

If $T = \text{"very large"}$

$$m = \frac{S}{k}$$

Steady-state,
Gains = losses

Mass balance

$$m(T) = m(0)e^{-kT} + \frac{S}{k}(1 - e^{-kT})$$



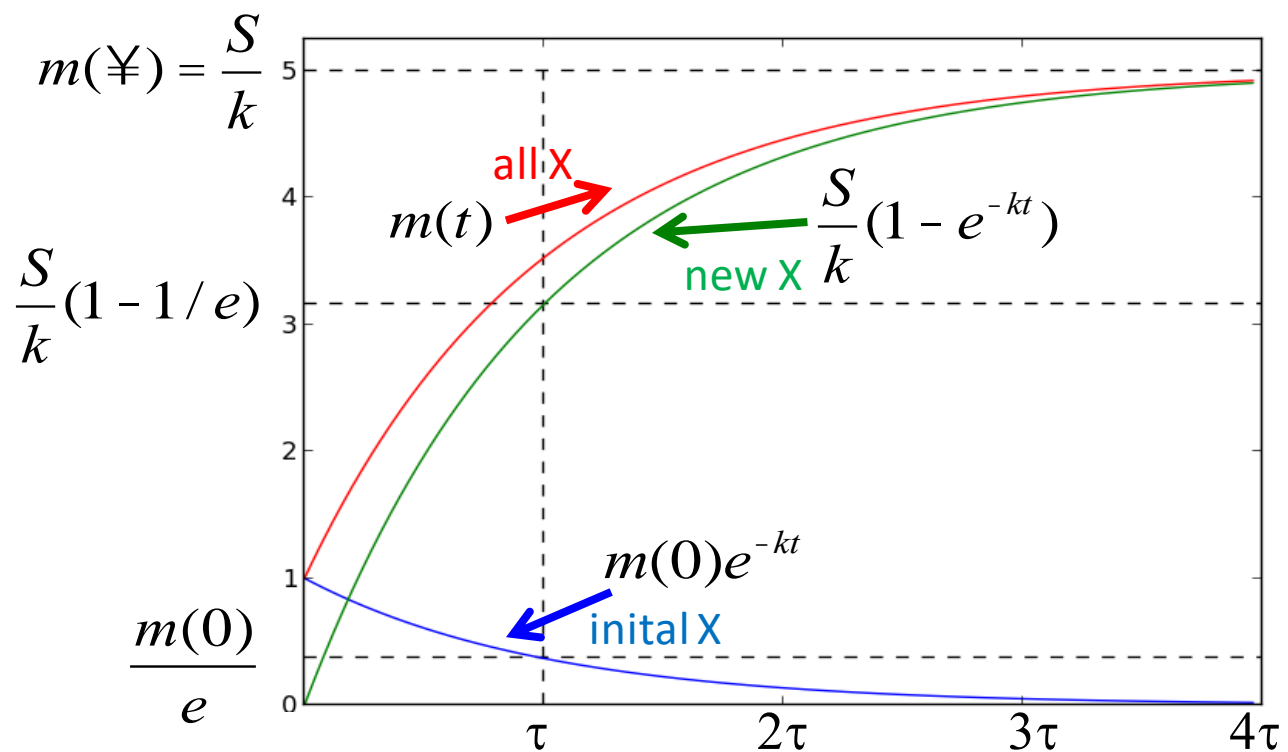
If $T = 1/k = \tau$

$$m = m(0)e^{-1} + \frac{S}{k}(1 - e^{-1})$$

- the first term has decayed to 37% and the second term has reached 63% of its final value...
- τ is a useful *characteristic time* sometimes called the **e-folding lifetime**

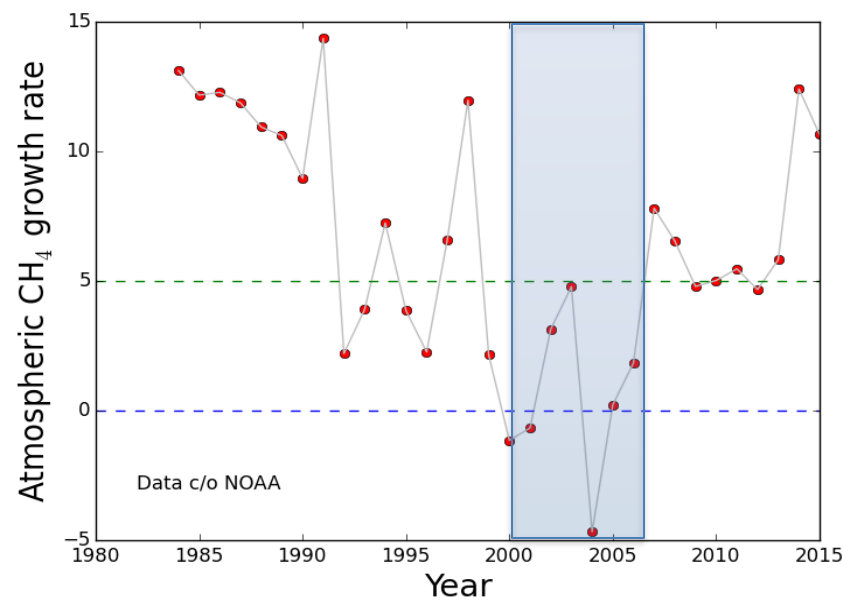
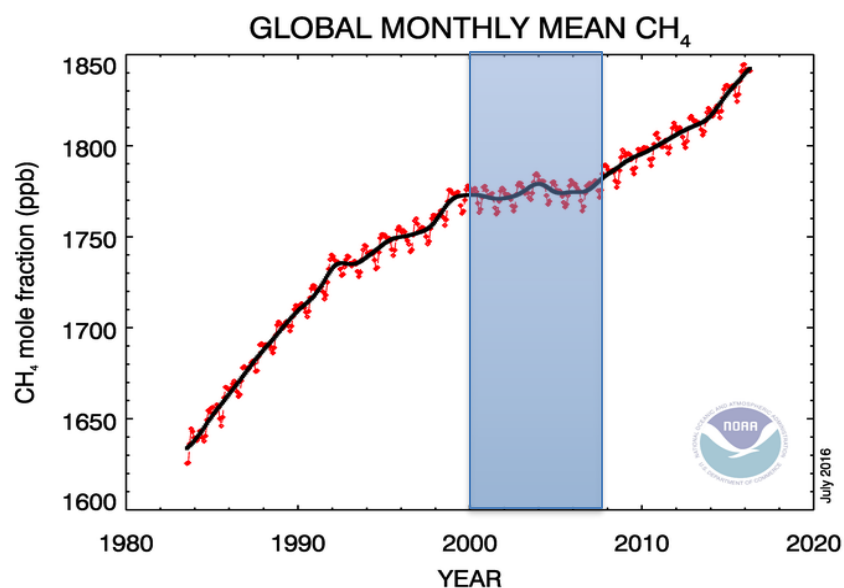
Mass balance

$$m(t) = m(0)e^{-kt} + \frac{S}{k}(1 - e^{-kt})$$



- On time scales $\gg \tau$ steady state can be assumed
 - e.g. For OH, $\tau < \text{second}$, so measurements basically tell us the current S/k balance
- If mass stable, suggests sources=sinks

Mass balance of CH₄ on earth



- $dC/dt \approx 0$ does NOT mean that sources are not still active. It means that $P \approx L$.
- For CH₄ we do not know with certainty why the growth rate slowed down in 2000 or why it resumed after 2007.

Moving beyond the box model

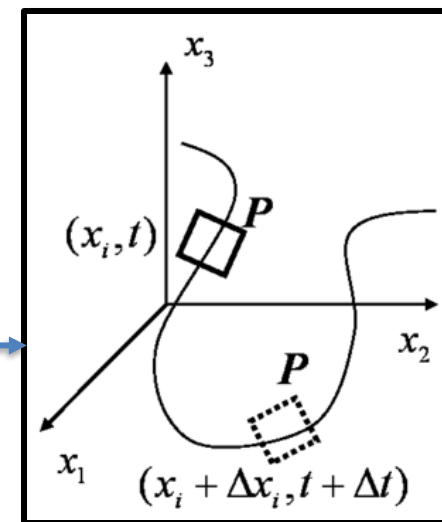
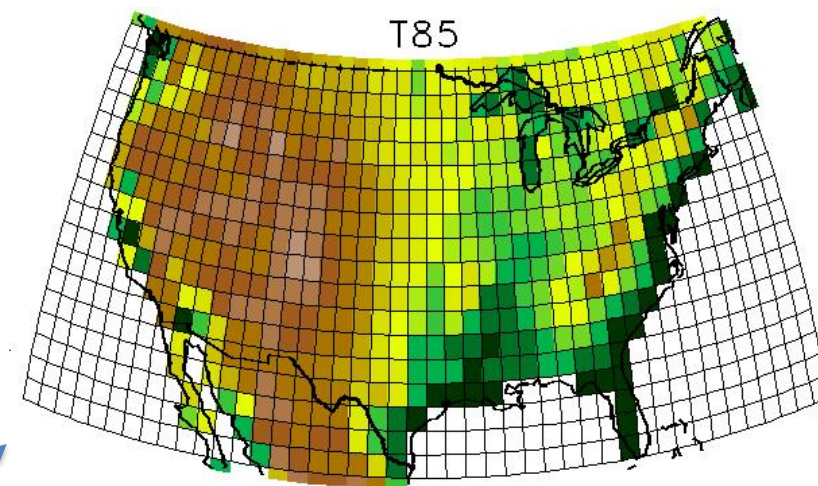
- Broadly, there are two types of atmospheric models:
 - **Eularian** models have a **fixed grid** of multiple boxes. In time, air (and it's components!) moves from box to box.
 - **Lagrangian** models have boxes that move in space, following a parcel of air.

Moving beyond the box model

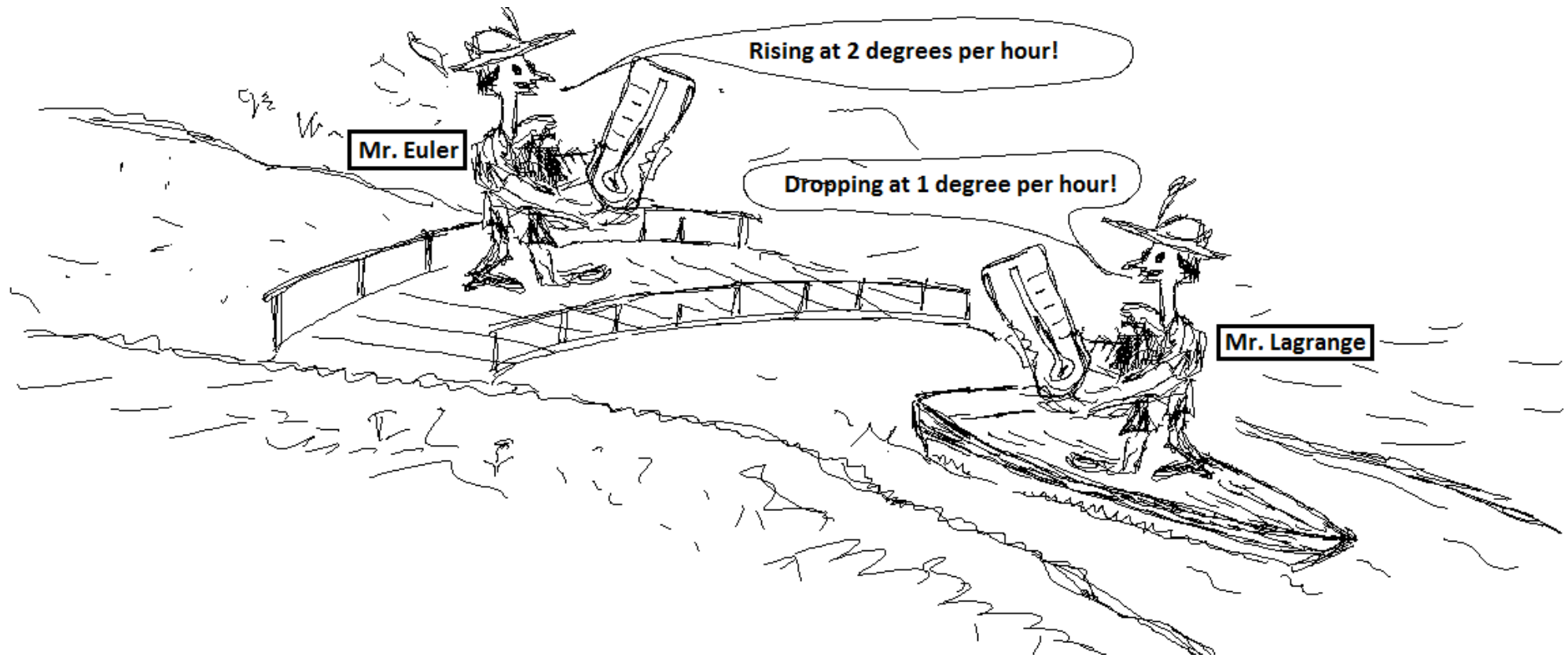
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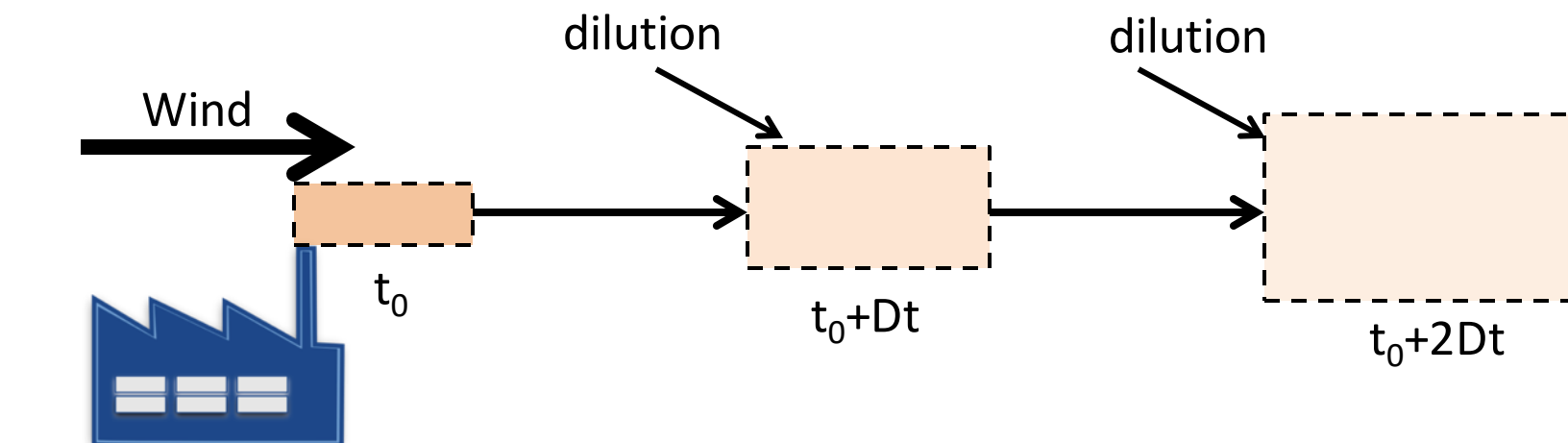


Lagrangian vs. Eulerian



Puff model

Follow a volume of air (usually an interesting one!), and include terms in the model to account for dilution from the surrounding air as it travels downwind.

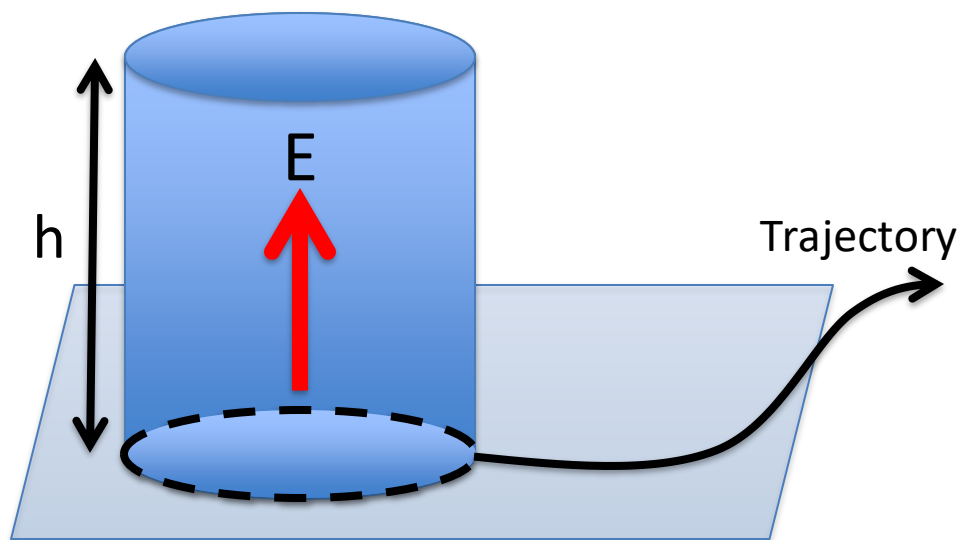


Mass balance equation same as the box model but given in terms of concentration rather than mass so the size of the puff is kept arbitrary.

$$\frac{d}{dt}[X] = E + P - L - D - k_{dil}([X] - [X]_b) \quad k_{dil} \text{ (/s) is a dilution rate constant}$$

- Used to follow evolution of isolated pollution plume (e.g., landfill).

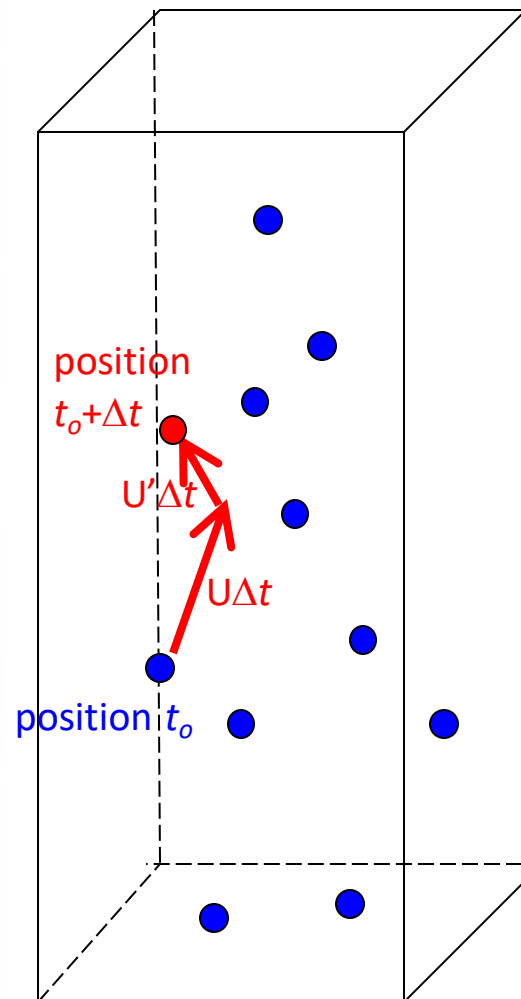
Column model



$$\frac{d}{dt}[X] = \frac{E}{h} + P - L - D$$

- Column is “blown” across the surface, picking up flux E of species (in units $\text{kg.m}^{-2}.\text{s}^{-1}$)
- Assume well mixed over height h (in m).
 - This height might vary over time/space
 - More sophisticated models may have multiple layers with interchange
- Frequently used to simulate air pollution over and downwind of cities.

Lagrangian



- Transport large number of points with trajectories from input meteorological data base (U) + random turbulent component (U') over time steps Δt
- Points have mass but no volume
- Determine local concentrations as the number of points within a given volume

Lagrangian pros and cons

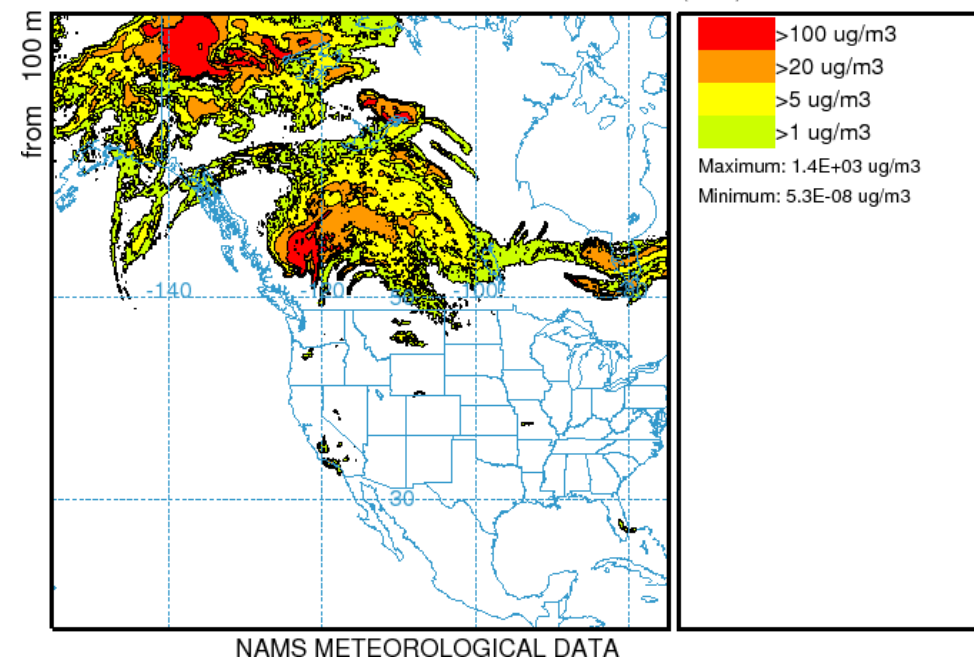
- **PROS over Eulerian models:**
 - no Courant number restrictions (restriction on time step length required for good results)
 - no numerical diffusion/dispersion
 - easily track air parcel histories
 - invertible with respect to time
- **CONS:**
 - need very large # points for statistics
 - inhomogeneous representation of domain
 - convection is poorly represented
 - nonlinear chemistry is problematic

ARL/NESDIS EXPERIMENTAL SMOKE FORECAST

Air Concentration (ug/m³) Layer Average 0 m and 5000 m

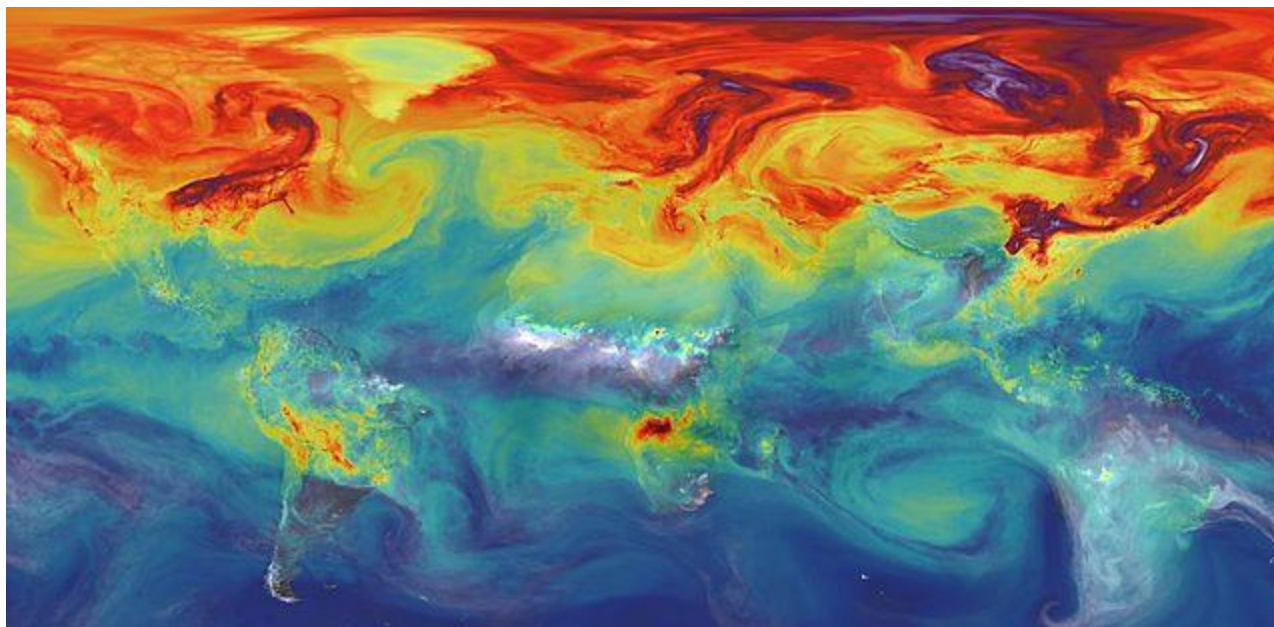
Integrated from 0600 15 Jul to 0700 15 Jul 17 (UTC)

PM25 Release started at 0600 15 Jul 17 (UTC)



Going global...

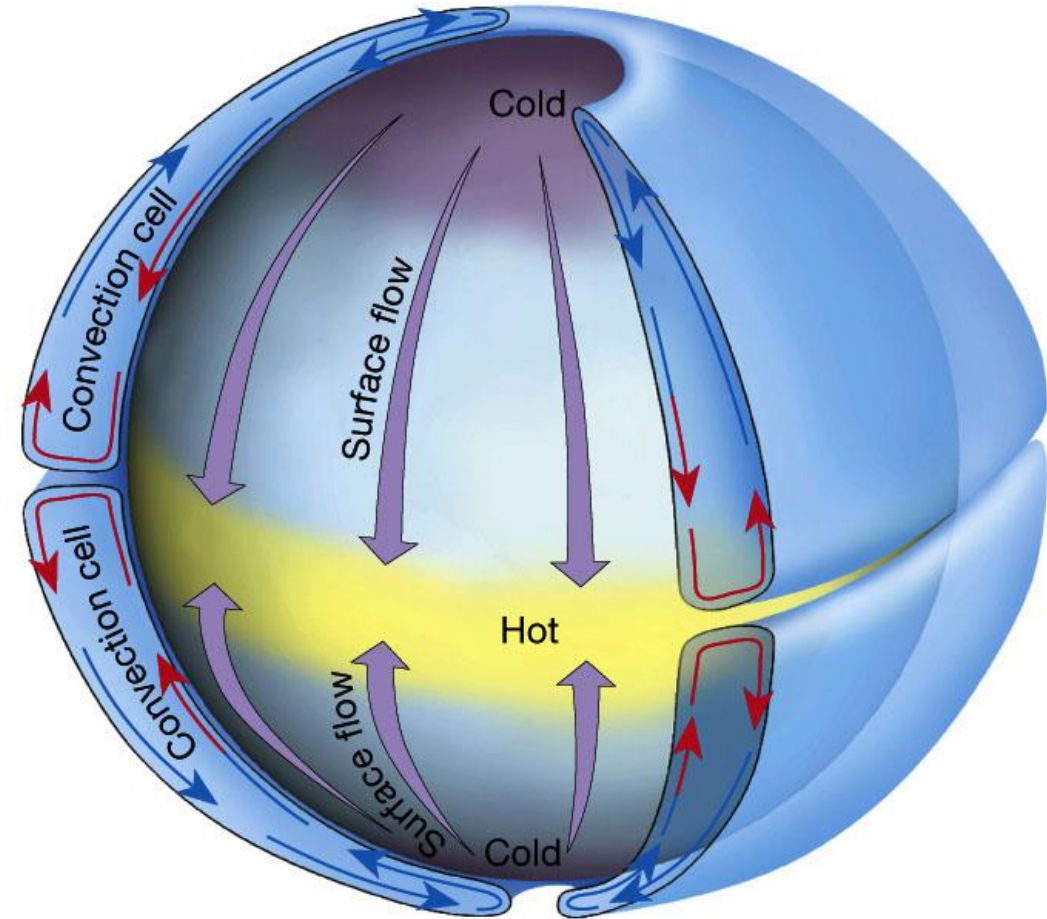
- With computers doing the maths, we can do reasonable simulations of the atmospheric chemistry of large regions, or even the whole world!



NASA simulation of carbon dioxide mixing ratios

Atmospheric motion

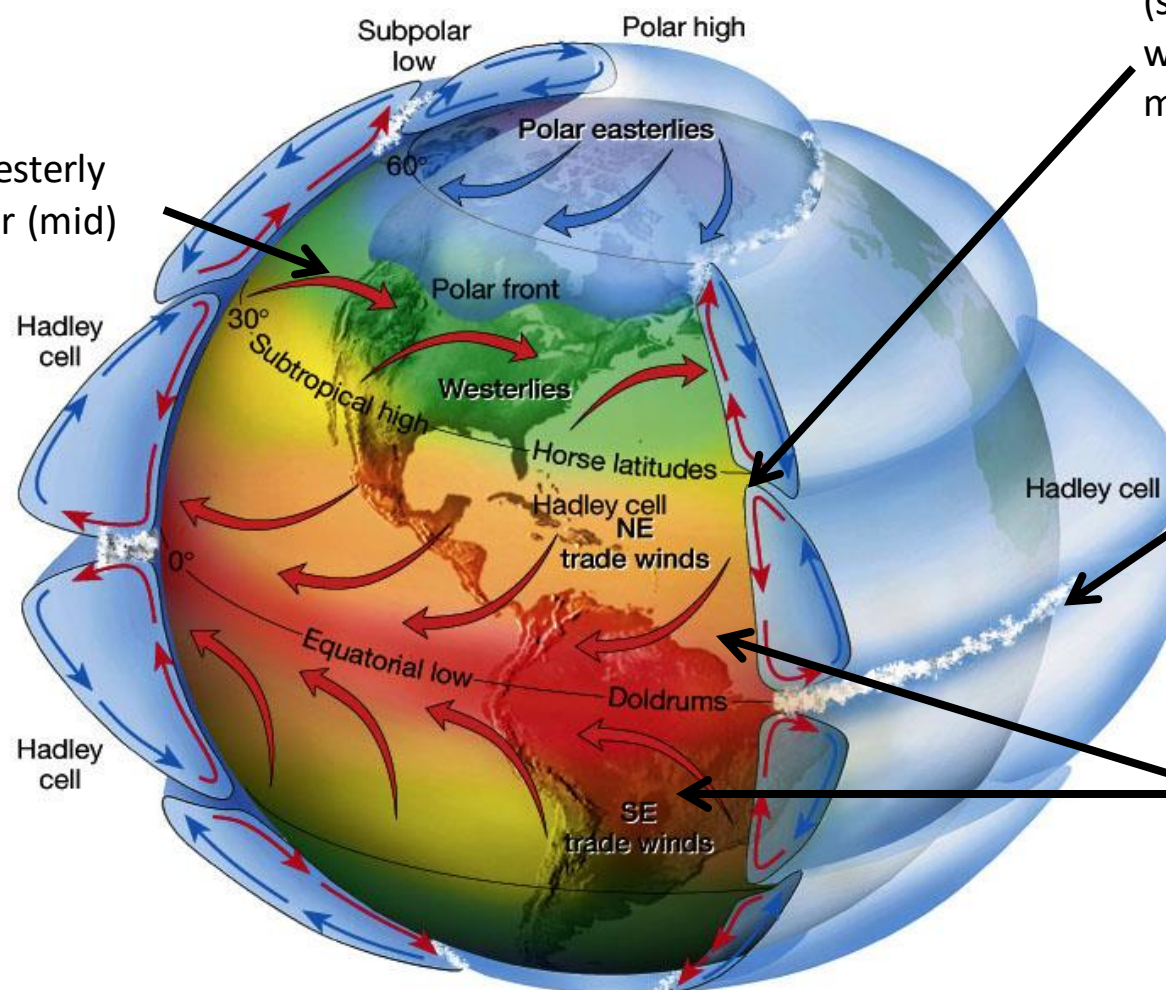
- If the earth didn't rotate, the equator being hotter than the poles would be the main driving force.



Non-rotating earth

Atmospheric motion

Wind shift to a westerly direction at higher (mid) latitudes.

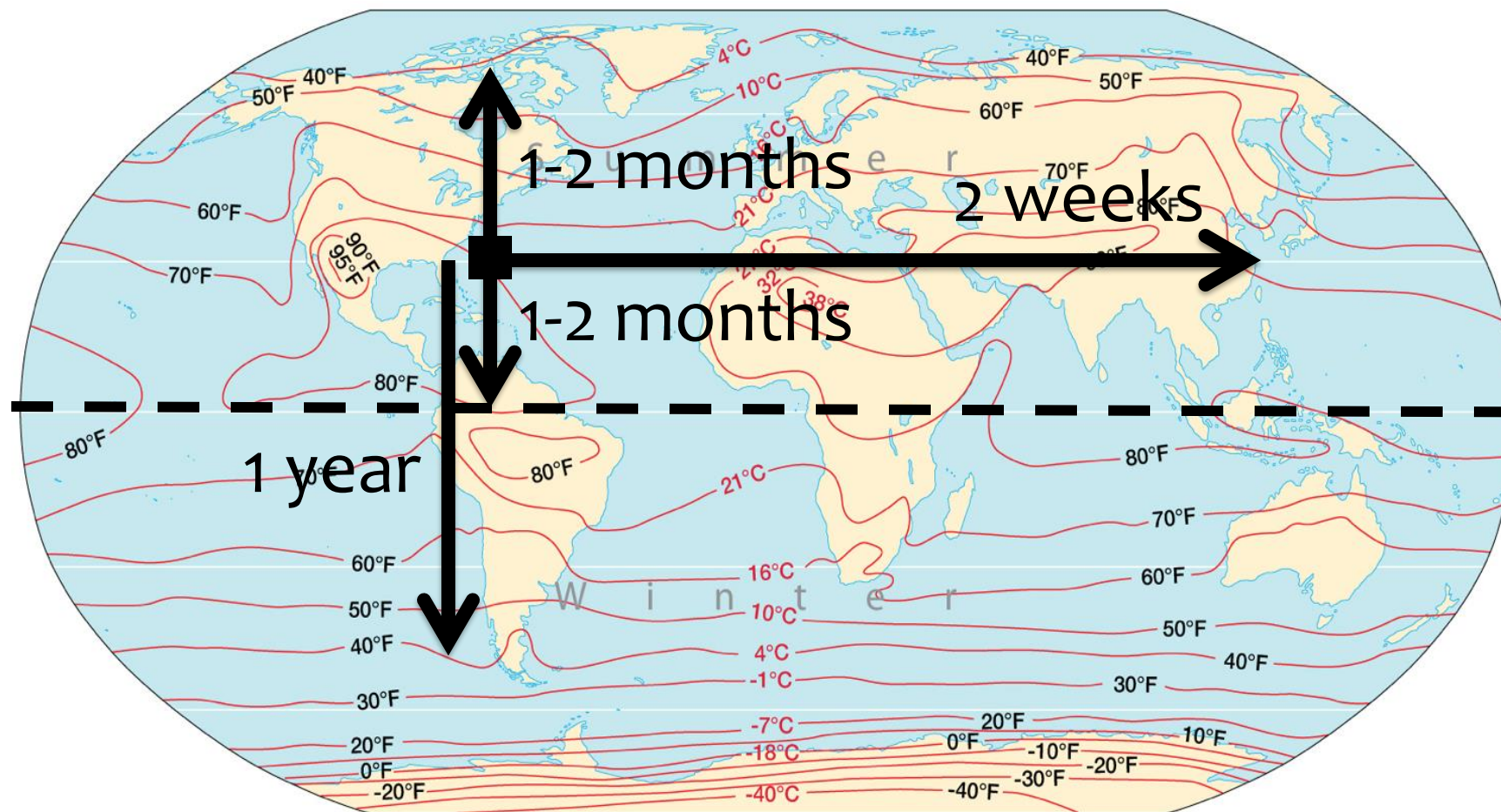


Approx 30°N and 30°S are regions of high pressure (subtropical anticyclones). This is where we find most of the major deserts.

Inter-tropical convergence zone (ITCZ): persistent convergence of air and associated rain and clouds. O(100s km) thick.

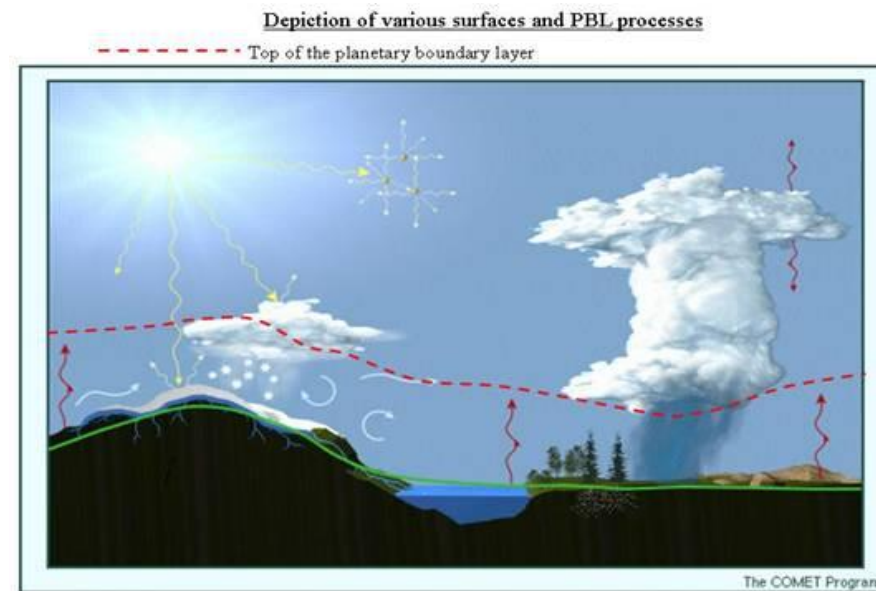
From ITCZ to 20-30° is the tropical easterlies (trade winds).

Horizontal transport



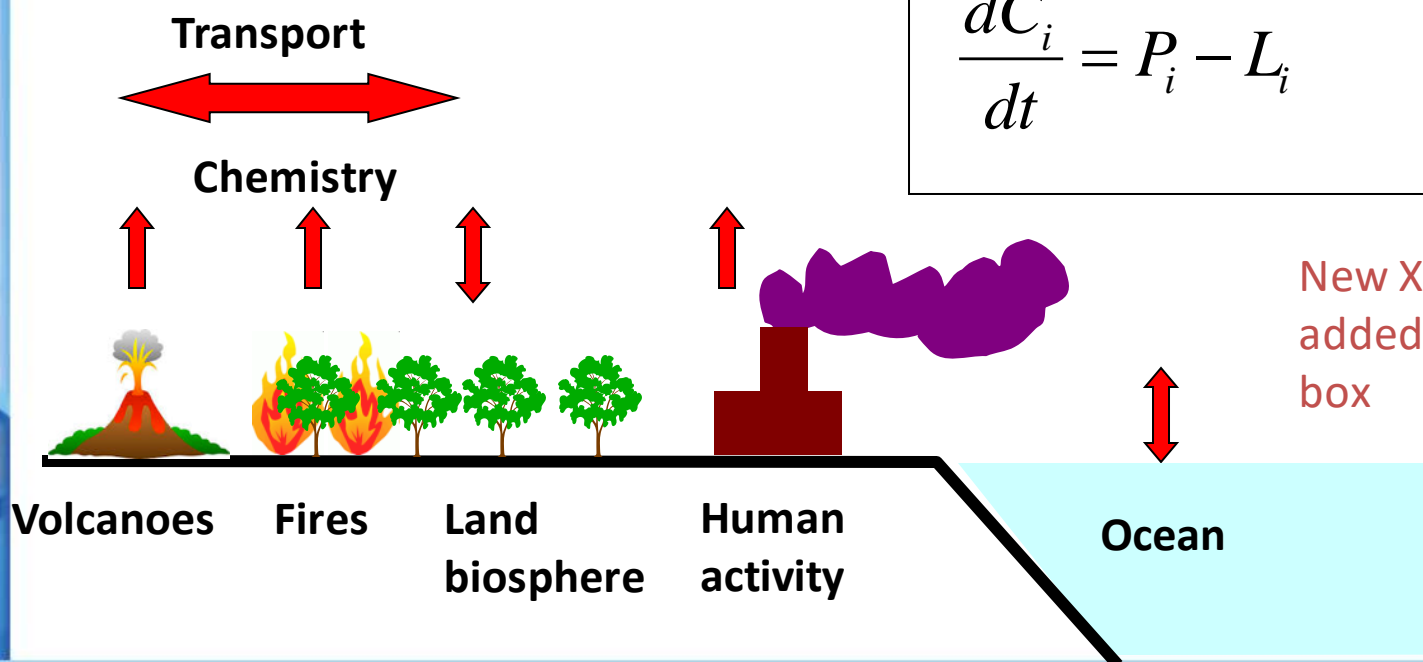
Vertical transport

- Vertical transport due to horizontal divergence or convergence is 1mm-1cm per s (cf 1-10 m/s for horizontal).
- Timescales from surface to tropopause about 3 months.
- Local buoyancy can result in faster transport, e.g. fires
- Boundary layer mixing can be very fast
- Models typically assume BL mixing is instantaneous



Modelling in 4D

Solve continuity equation for mixing ratios $C_i(\mathbf{x}, t)$



Eulerian form:

$$\frac{\partial C_i}{\partial t} = -\mathbf{U} \cdot \nabla C_i + P_i - L_i$$

Lagrangian form:

$$\frac{dC_i}{dt} = P_i - L_i$$

Movement to/from other boxes which might have more/less X

\mathbf{U} = wind vector

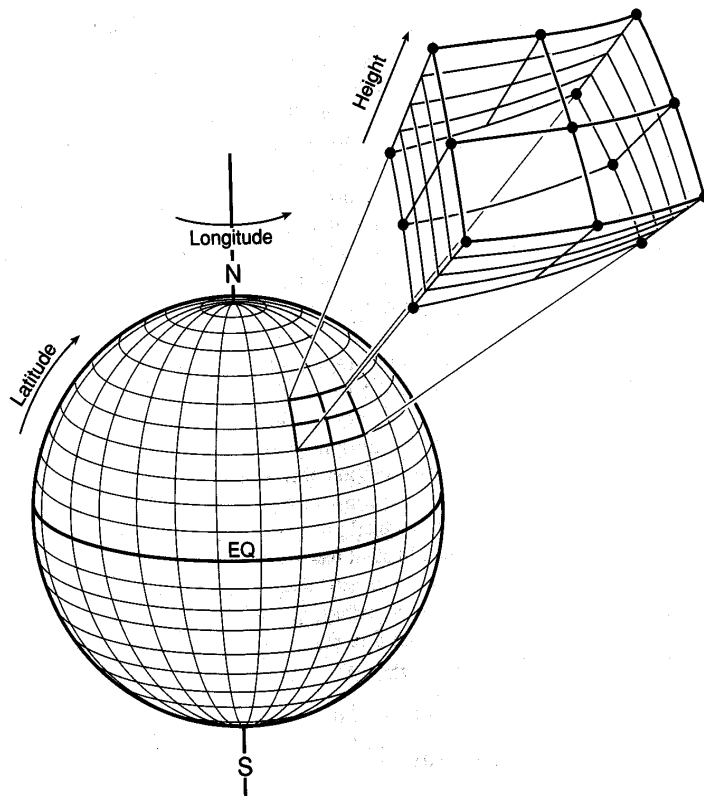
P_i = local source of chemical i

L_i = local sink

New X added/created in box

X removed/destroyed in box

Modelling in 4D



- Solve continuity equation for individual gridboxes
- MANY calculations
 - More if smaller boxes (for more detailed results) wanted.
 - Current global models have a horizontal resolution of $\sim 0.25^\circ$ (~ 25 km) and a vertical resolution of 100s m.

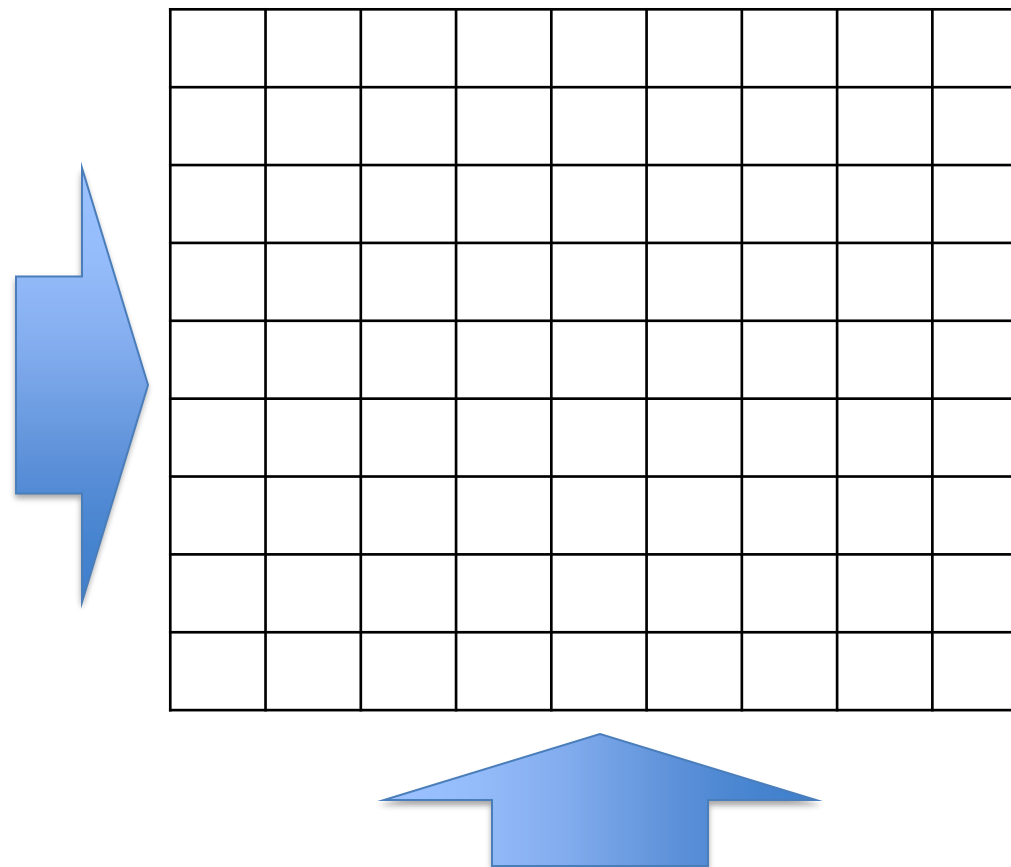
© Chemical Transport Models (CTMs) use external meteorological data as input
© General Circulation Models (GCMs) compute their own meteorological fields

Time steps

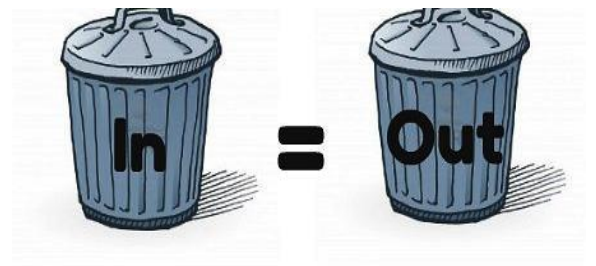
- Models divide time into discrete time steps
- Calculate changes in modelled parameters from one time step to next
 - “Temporal discretization”
- As with space, shorter time steps can give more detailed results and higher performance, but require more computational resources.

Boundary conditions

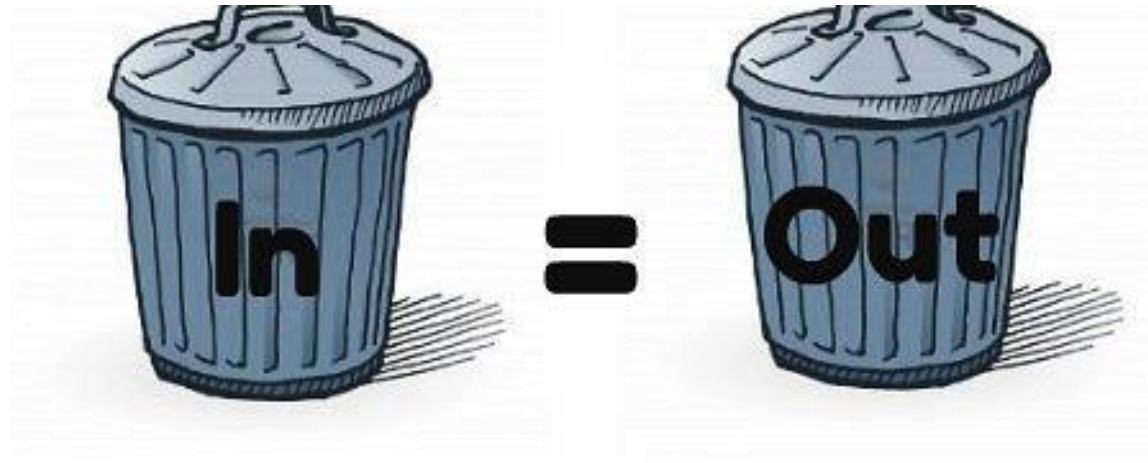
- For a regional grid, can't ignore winds blow in air from outside the model domain
- Need boundary conditions
 - From another model
 - A decent guess!



Flux inventories



Garbage in, garbage out



A model is only as good as its inputs!



Movie

- <https://svs.gsfc.nasa.gov/11719>

Interactive exercise

- Python-based exercise
 - Code provided, no prior experience needed!
- Model of e-folding lifetimes
- Simple balances of sources and sinks
- Models vs. real world data
- Source apportionment in a 3D model
- Basics of inverse modelling