Global Climate Models for Chemistry and Aerosol

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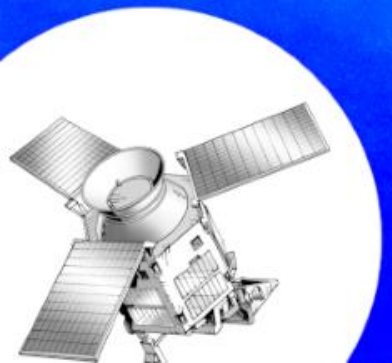
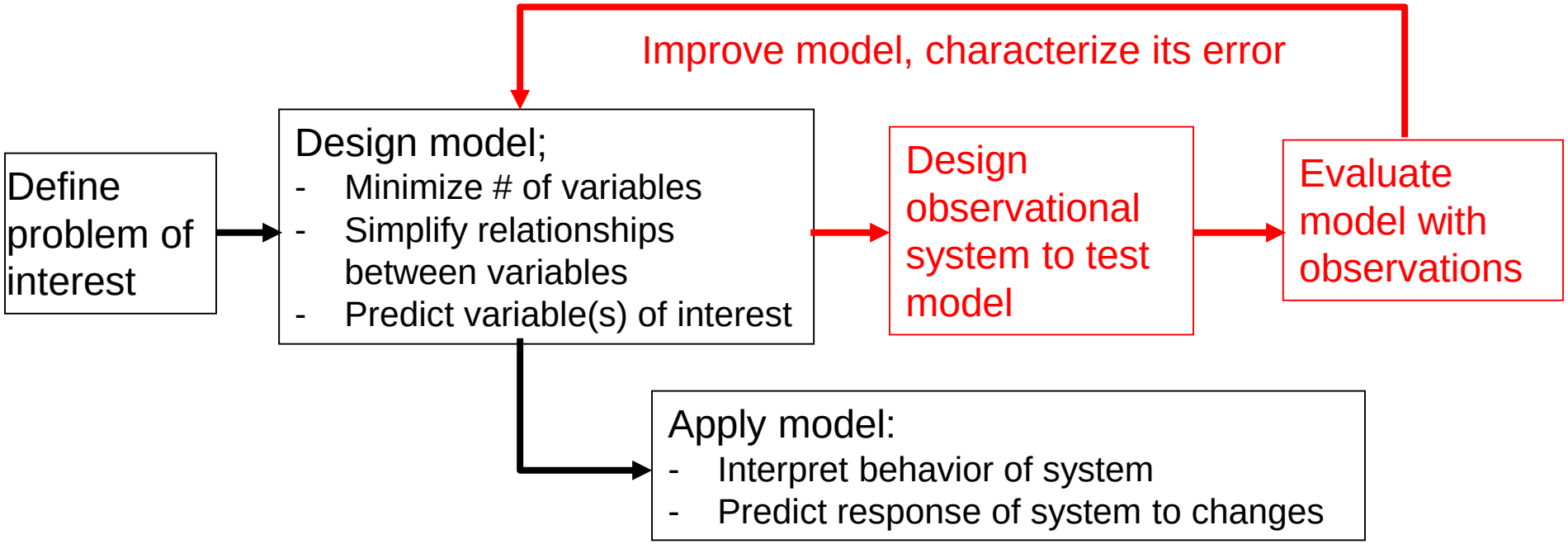


Copernicus Europe's eyes on Earth
ECMWF
Atmosphere Monitoring Service atmosphere.copernicus.eu
EUMETSAT
esa

What is a model?

- A representation of a system that we want to study
- Can vary in level of complexity and resolution
- For atmospheric transport models: governed by equations to ensure that mass, energy, and momentum are conserved
- Can include various chemical reactions
- Usually requires simplified representation of some complex processes: *parameterization*

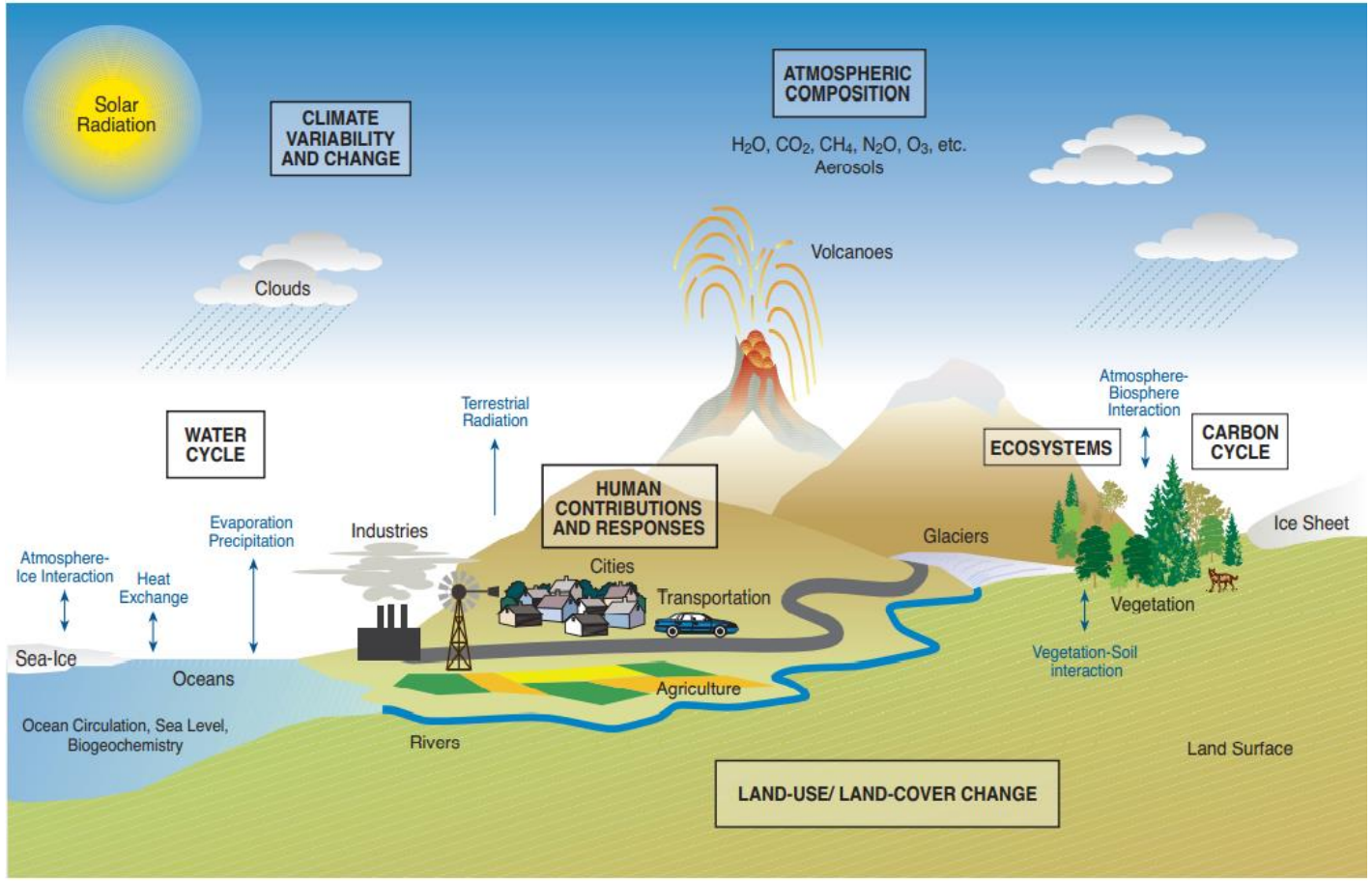
A simplified representation of a complex system enabling prediction of the system behavior within acceptable error



Some classes of large-scale atmospheric models:

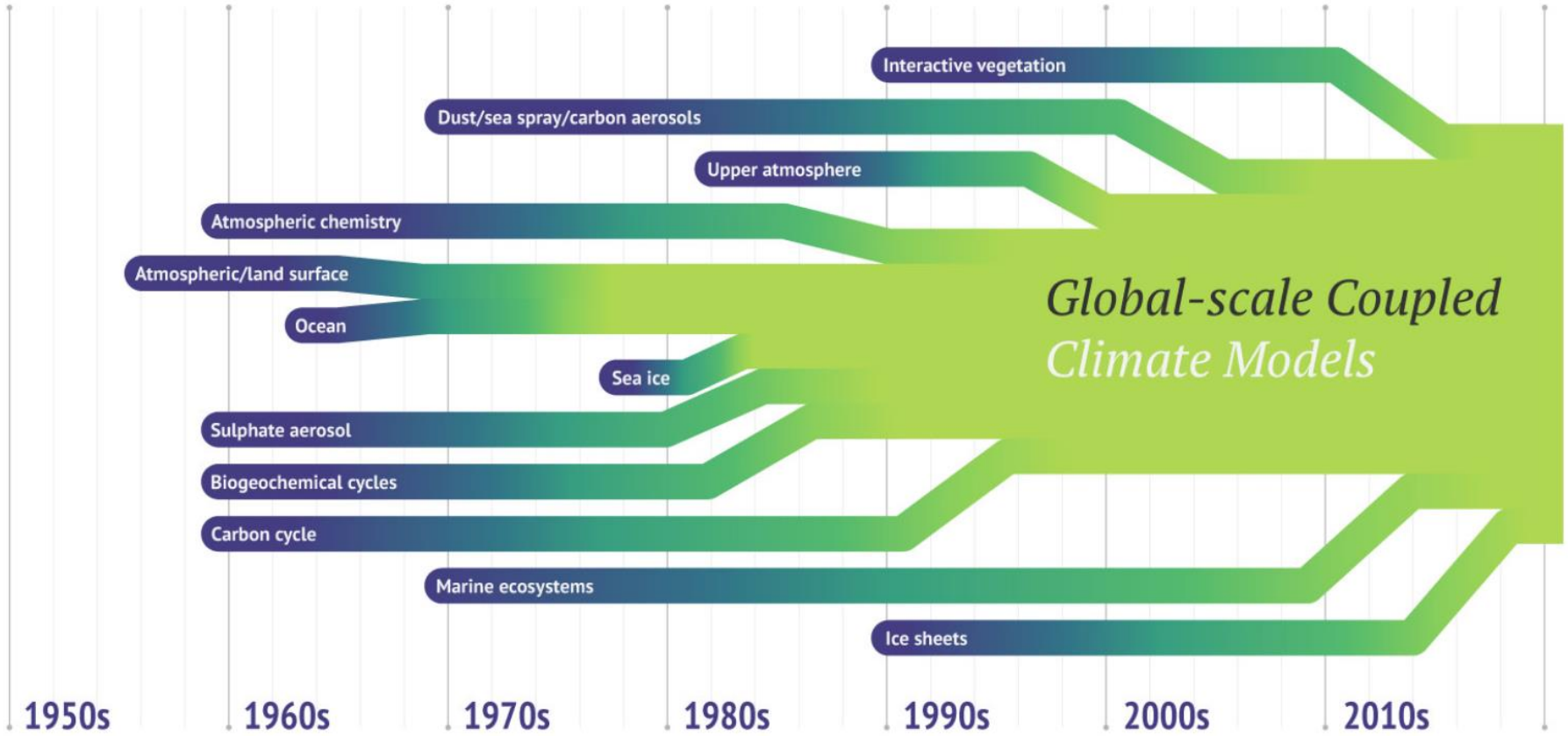
- Numerical weather prediction (NWP) models: simulate their own meteorology based on initial conditions from observations: need full model physics, often neglect chemistry entirely
- Chemical transport models (offline): use external meteorological data as input and simulate tracer transport and chemistry (aerosols and gases)
- General circulation models (GCMs): simulate their own meteorology (traditionally at lower resolution), use external forcings (gases, aerosols, radiation…)
- Chemistry climate models: simulate their own meteorology and tracers, given different scenarios (*Representative Concentration Pathways*)
- Earth system models (ESMs): includes interactions between the oceans and land biosphere, etc.

Which components do we need to model the climate?



Strategic Plan for the U.S. Climate Change Science Program, Fig. 2-5

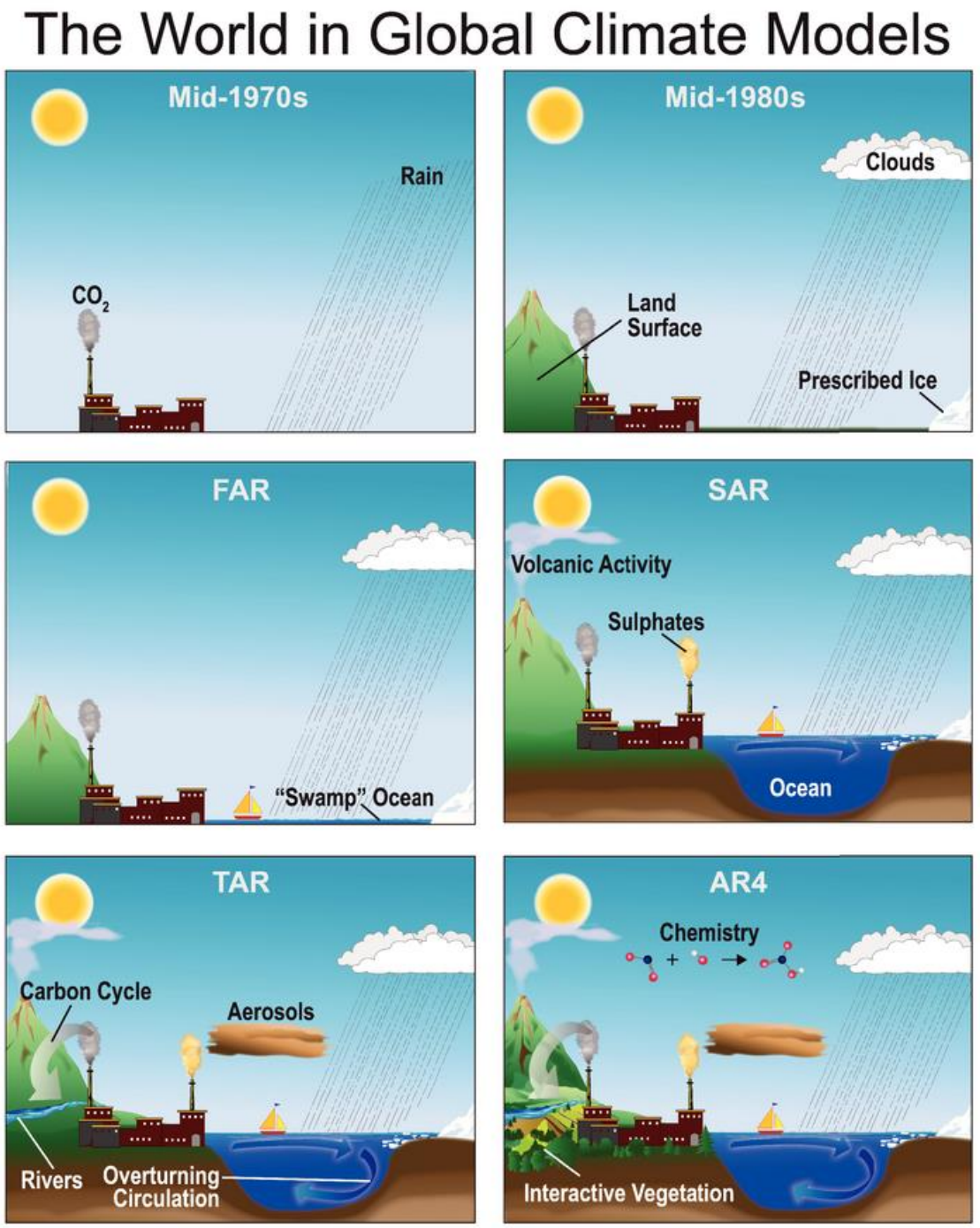
Climate models have been increasing in complexity over time…



Note: There were some very simplified models before the dates mentioned.

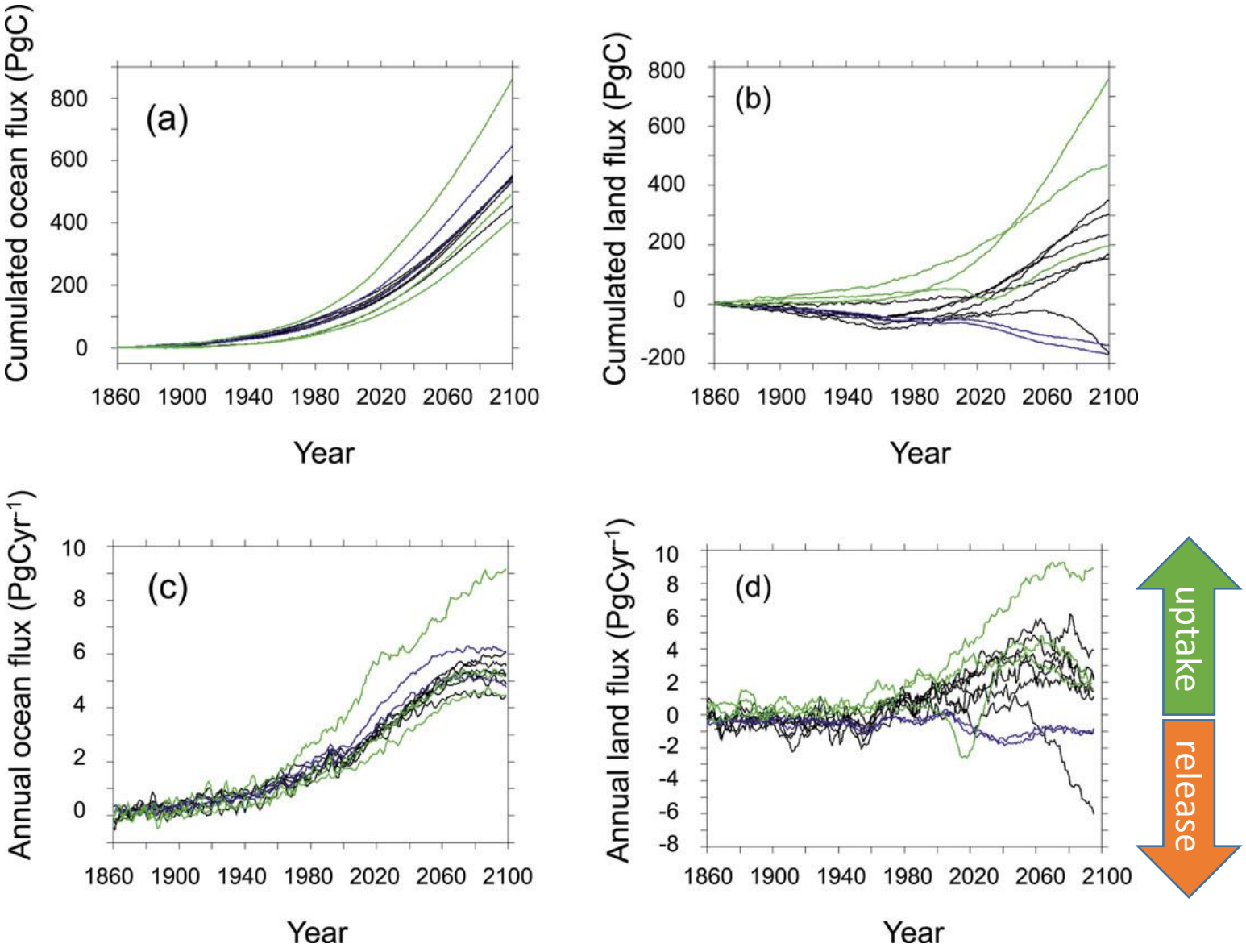
CarbonBrief
CLEAR ON CLIMATE

Climate models have been increasing in complexity over time…



Source: IPCC AR4, Fig 1.2

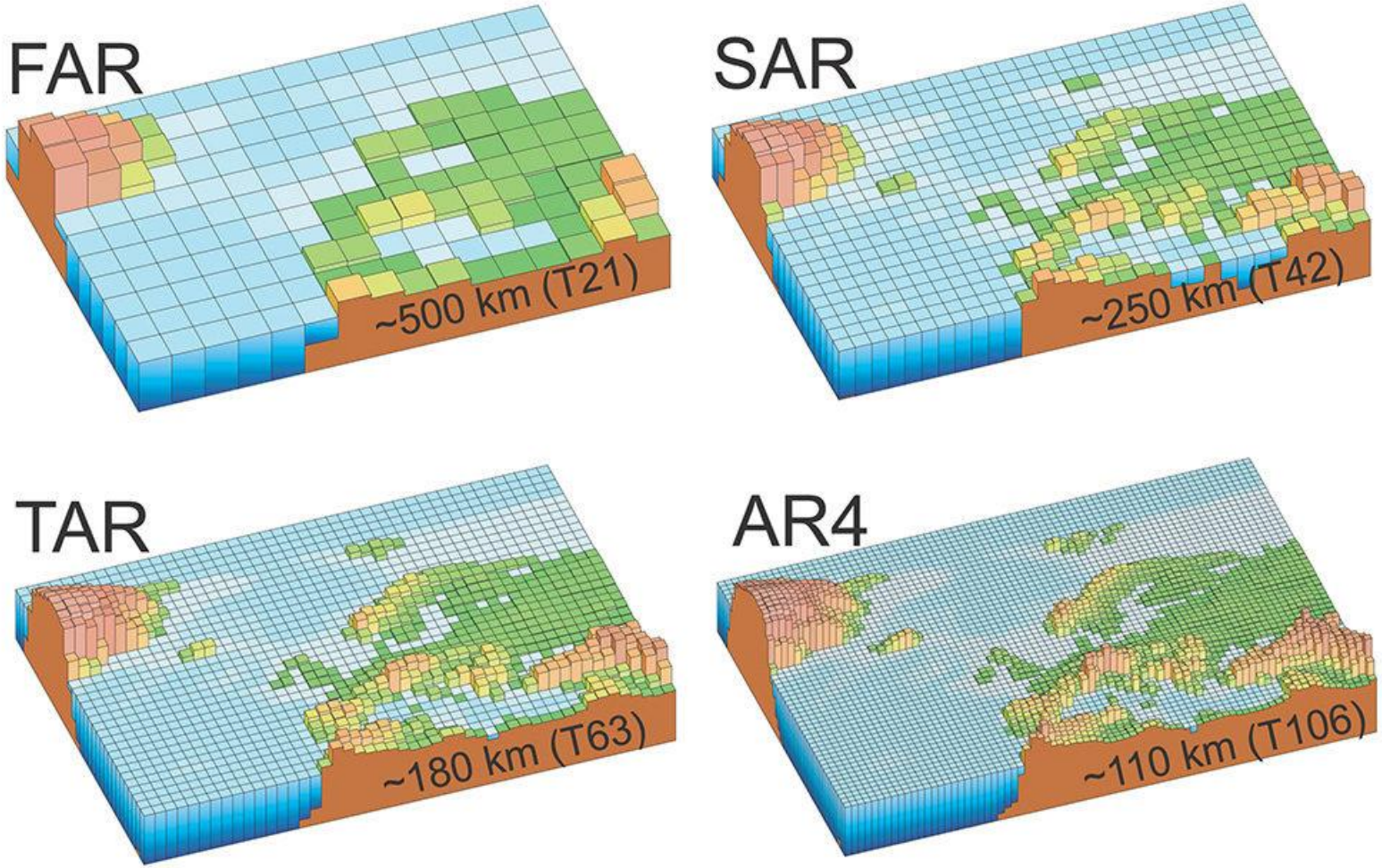
…which does not always lead to clearer answers!



Uncertainties in carbon-climate feedback are relevant to climate prediction, and a significant source of uncertainty in projections.

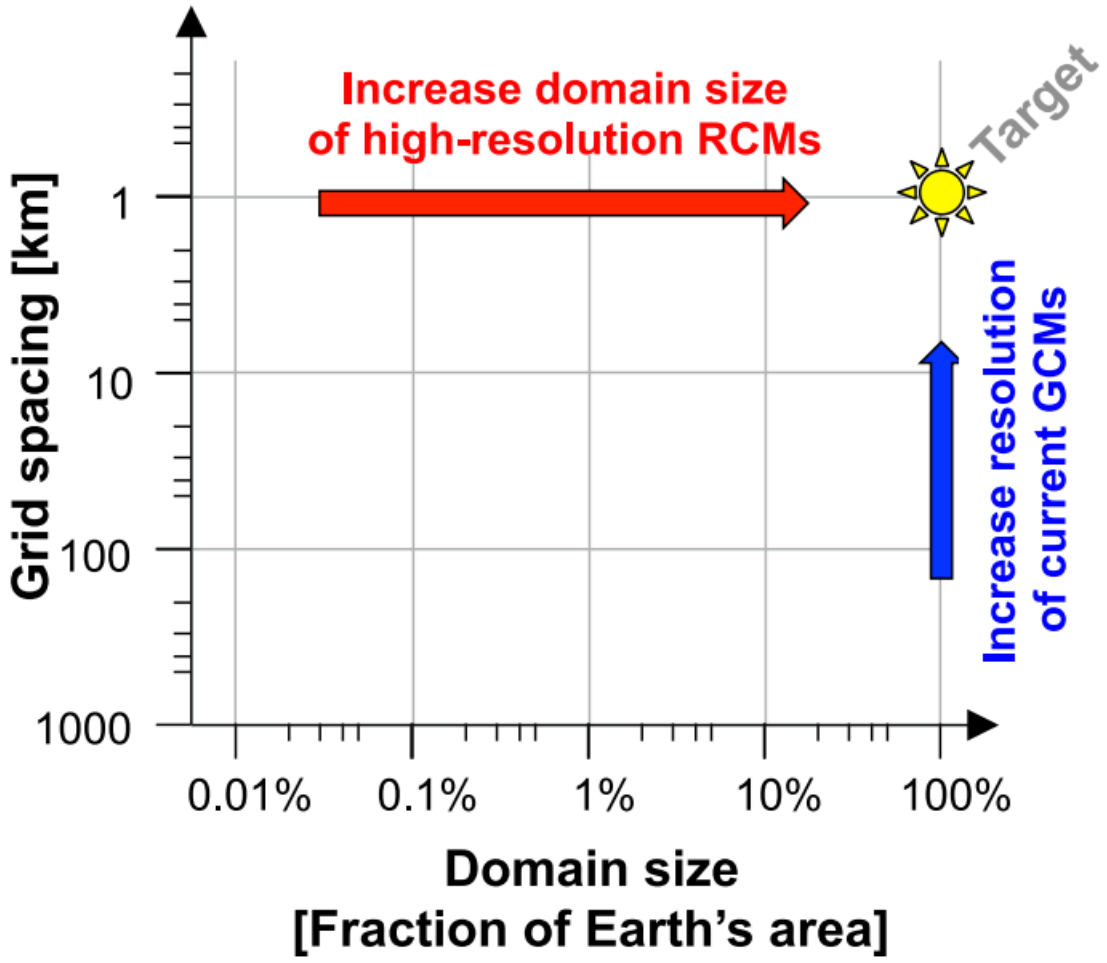
Friedlingstein et al., BAMS, 2014

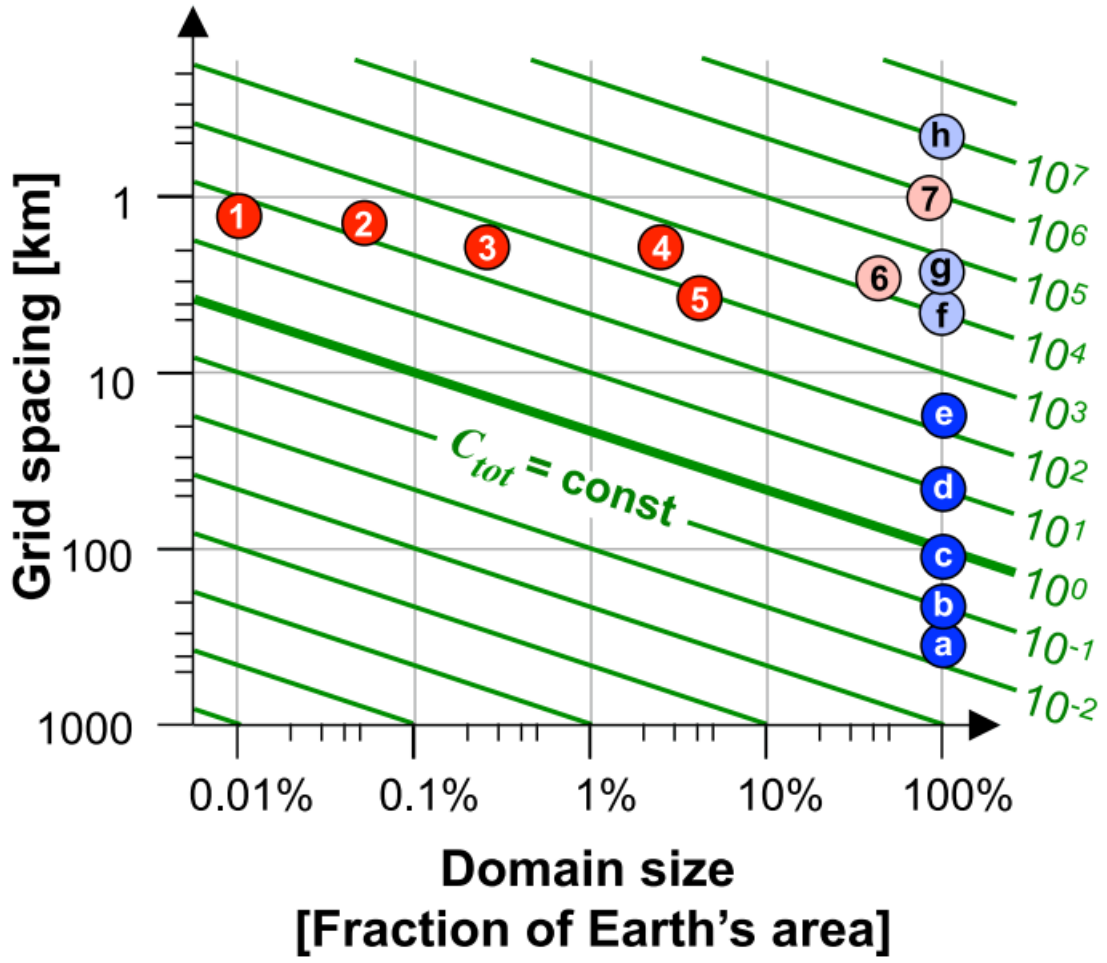
Resolution has been increasing as well!



Source: IPCC AR4, Fig 1.2

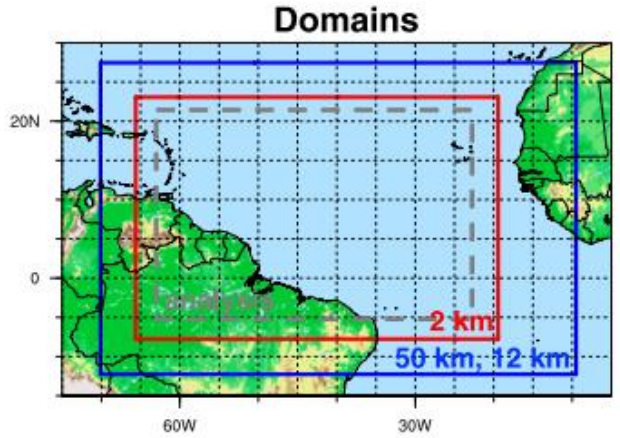
And the resolution keeps increasing!

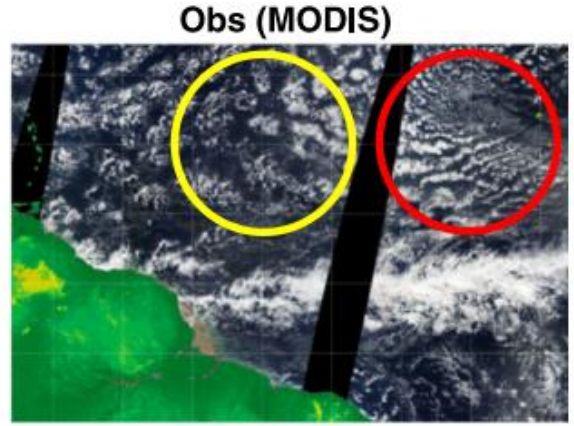


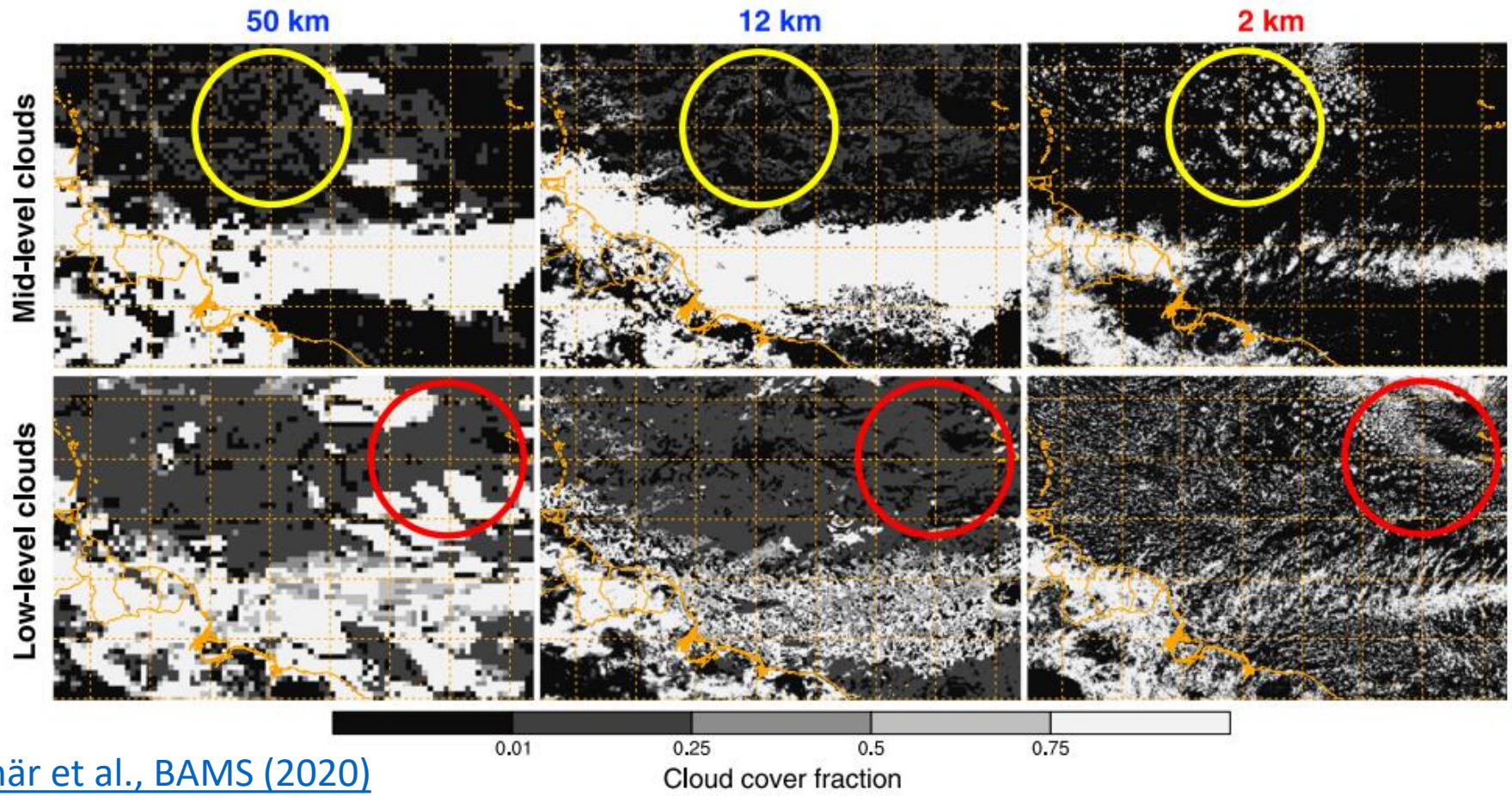


Kilometer-scale climate models, Schär et al., BAMS (2020)

Why does resolution matter for physics?





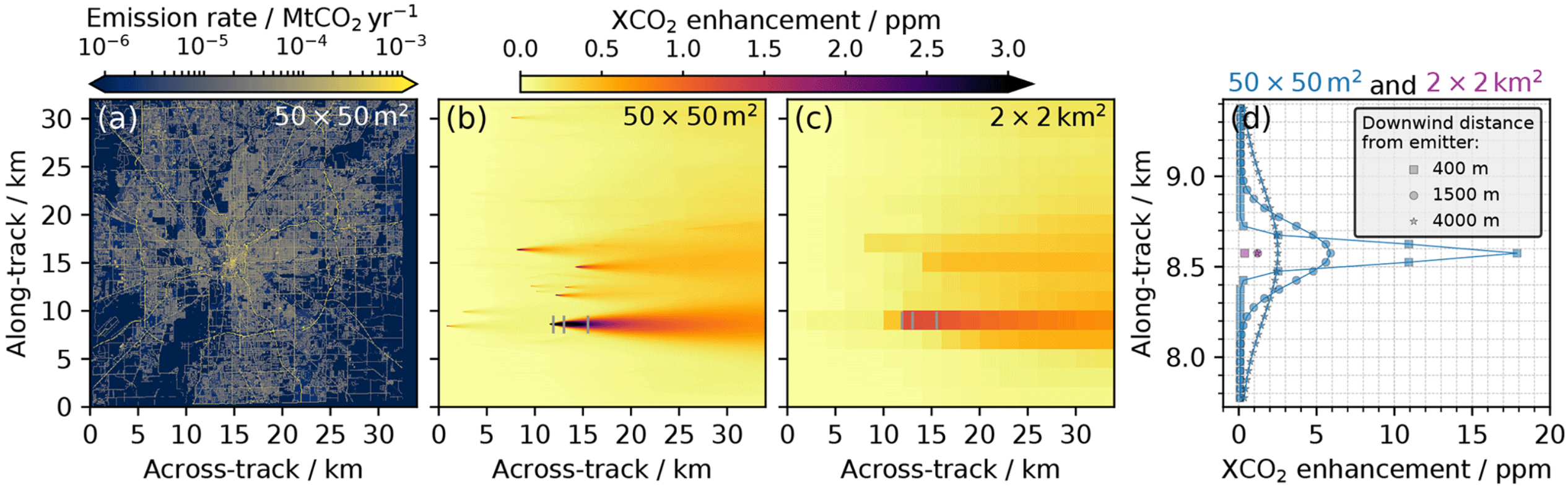


[Kilometer-scale climate models, Schär et al., BAMS (2020)]

Why does resolution matter for physics?

- Higher resolution models (~ 1 km) allow for convection to be resolved, rather than based on parameterizations
- Even higher resolution models (~ 10 m) allow for turbulent processes to be resolved (Large Eddy Simulations)

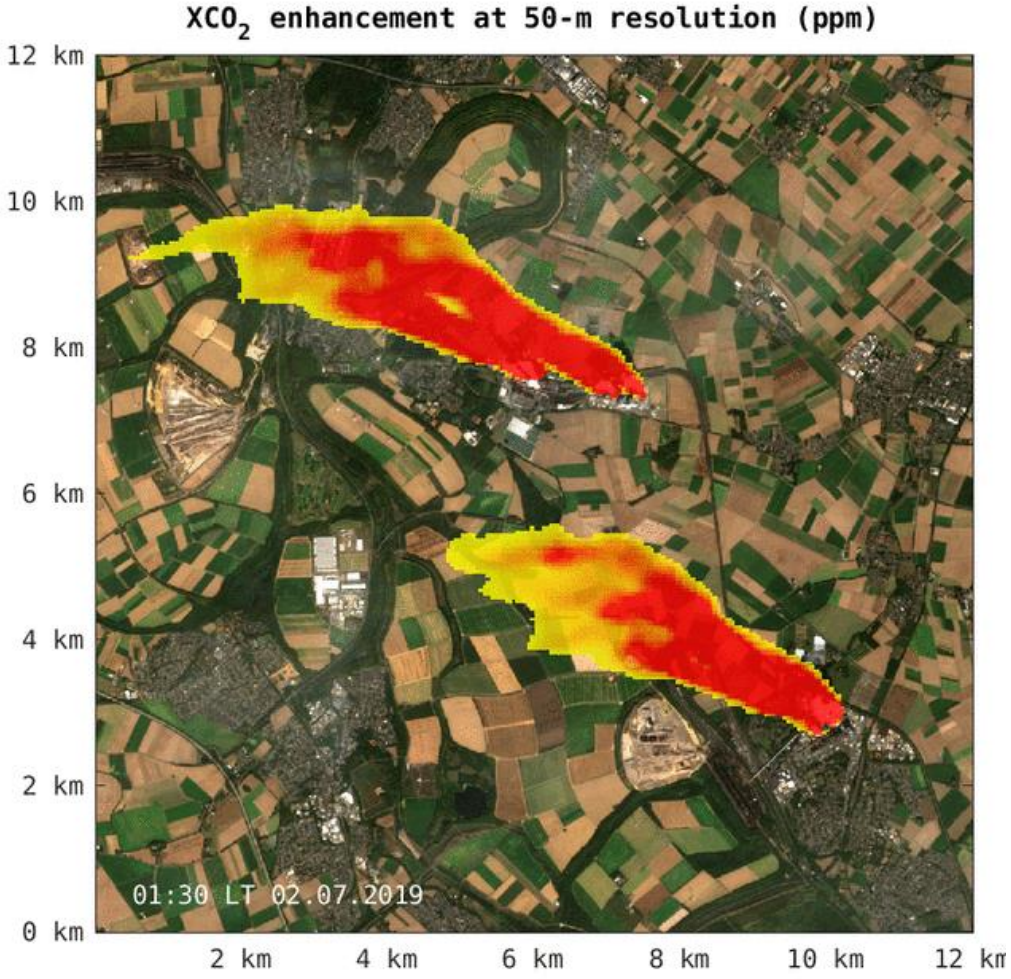
Why does resolution matter for tracers?

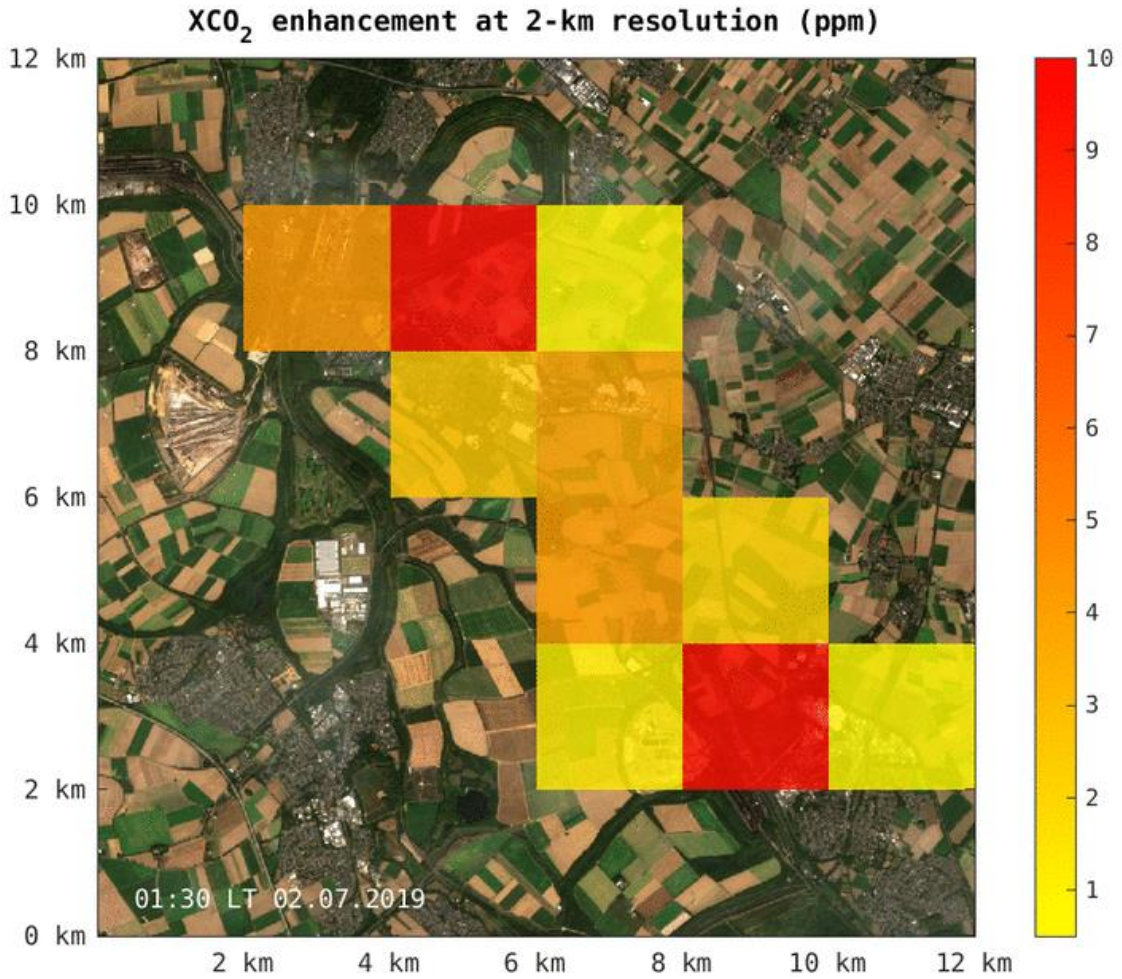


Also critical for chemistry: reactions are calculated based on concentrations!

Strandgren et al., AMT, 2020

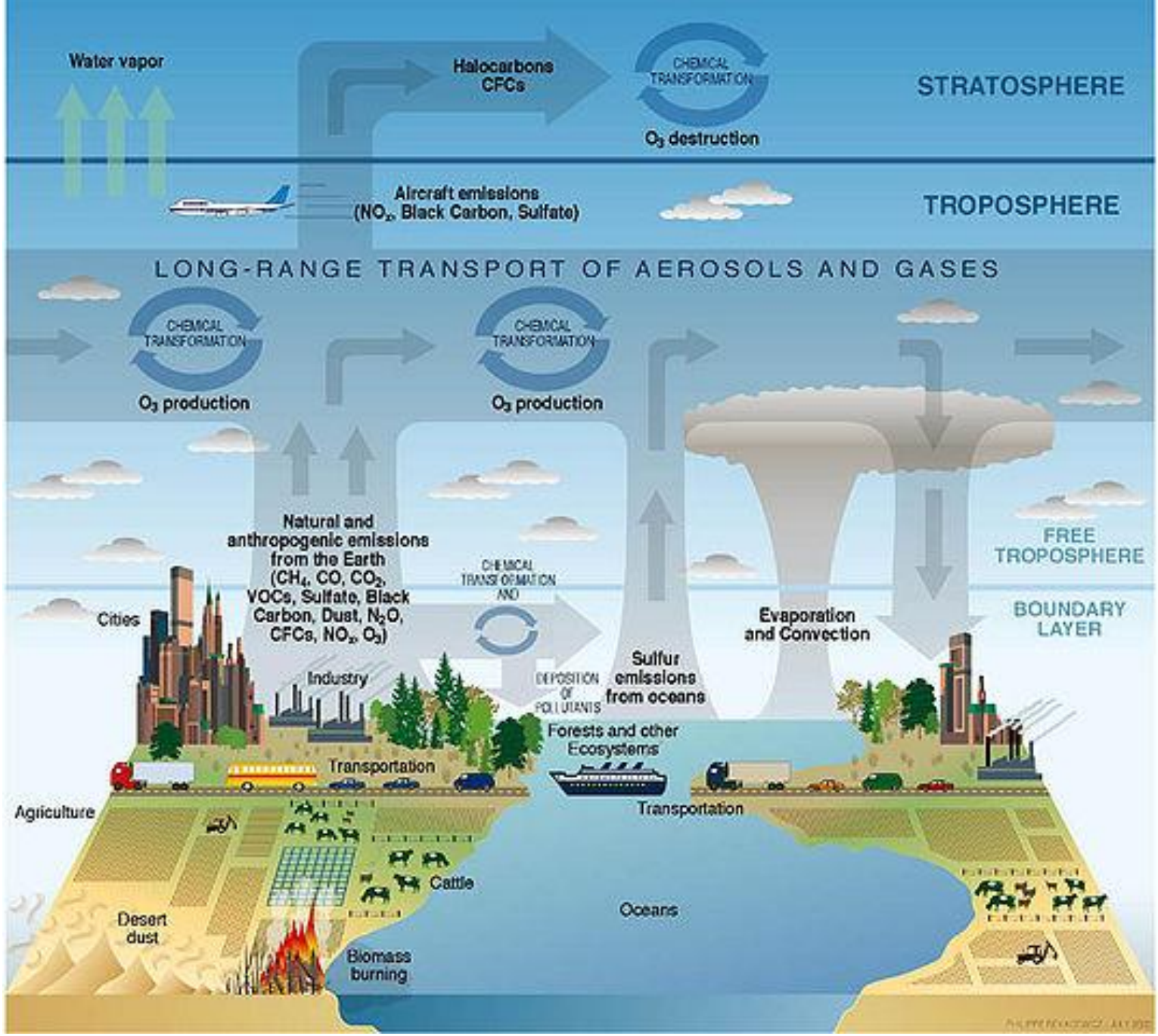
Why does resolution matter for tracers?





DLR, CO2Image

Back to atmospheric composition…



Strategic Plan for the U.S. Climate Change Science Program,

Conservation of mass for an atmospheric tracer (gas or aerosol): continuity equation

$$\frac{\partial [X]}{\partial t} = E_X - \nabla \cdot (U[X]) + P_X - L_X - D_X$$

Local change in concentration over time

Emissions

Transport (advection and convection), the flux divergence, where U is the wind vector

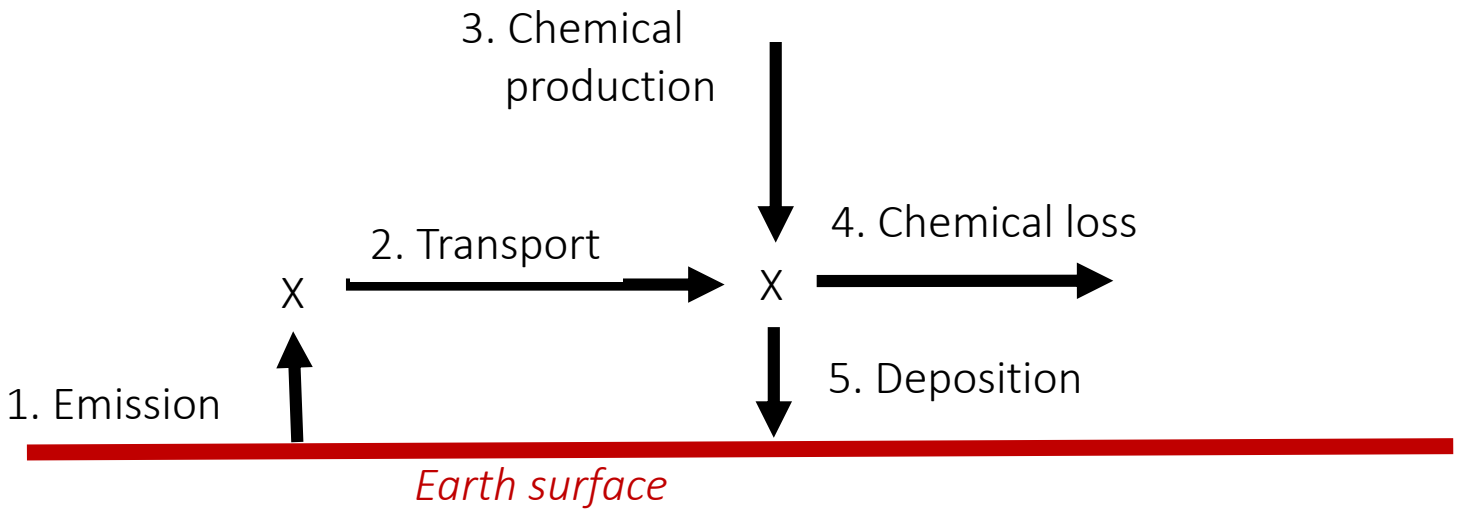
Chemical production

Chemical loss

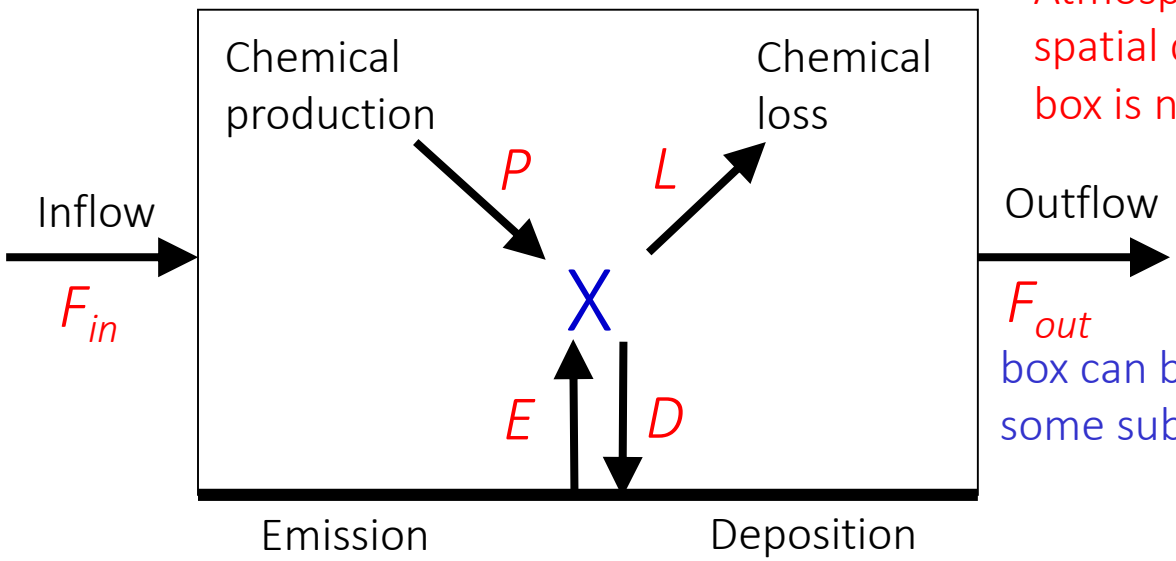
Deposition

Building a simple atmospheric chemistry model

Objective: predict the concentration of species X



The one-box model



Atmospheric "box";
spatial distribution of X within box is not resolved

F_{in}

F_{out}

box can be global atmosphere or some subdomain

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

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

The one-box model

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

Loss rate : $k = \frac{1}{\tau} = \frac{F_{out} + L + D}{m}$

Lifetimes add in parallel: $\frac{1}{\tau} = \frac{F_{out}}{m} + \frac{L}{m} + \frac{D}{m} = \frac{1}{\tau_{\text{out}}} + \frac{1}{\tau_{\text{chem}}} + \frac{1}{\tau_{\text{dep}}}$

Loss rate constants add in series: $k = \frac{1}{\tau} = k_{\text{out}} + k_{\text{chem}} + k_{\text{dep}}$

Fraction f removed by outflow:

Is k a constant?

In most models, it's a bit more complex!

- Example: RACM2 chemistry scheme (Goliff et al., 2013) has 363 chemical reactions affecting 17 stable inorganic species, 4 inorganic intermediates, 55 stable organic species (3 primarily of biogenic origin) and 43 organic intermediates
- Still a simplification of reality, with over 30 000 known VOCs emitted from plants alone
- Size distribution of aerosols often simplified into a few log-normal modes to reduce computational demands

Example

Consider a pollutant emitted in an urban area of 100 km dimension. The pollutant can be removed from the airshed by oxidation, precipitation scavenging, or export. The lifetime against oxidation is 1 day. It rains once a week. The wind is 20 km/h. Which is the dominant pathway for removal?

$$\tau_{chem} = ? \qquad \tau_{dep} = ? \qquad \tau_{out} = ?$$

Example

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$$\tau_{chem} = 1\ \mathrm{d} \qquad \tau_{dep} = 7\ \mathrm{d} \qquad \tau_{out} = 5\ h$$

So the dominant pathway is outflow. What fraction of total removal does it account for?

.

$k_{out} = 0.2\ h^{-1} = 4.8\ d^{-1}$ $k_{chem} = 1\ d^{-1}$ $k_{dep} = 0.14\ d^{-1}$

Total loss rate constant $k = k_{out} + k_{chem} + k_{dep} = 5.9\ d^{-1}$

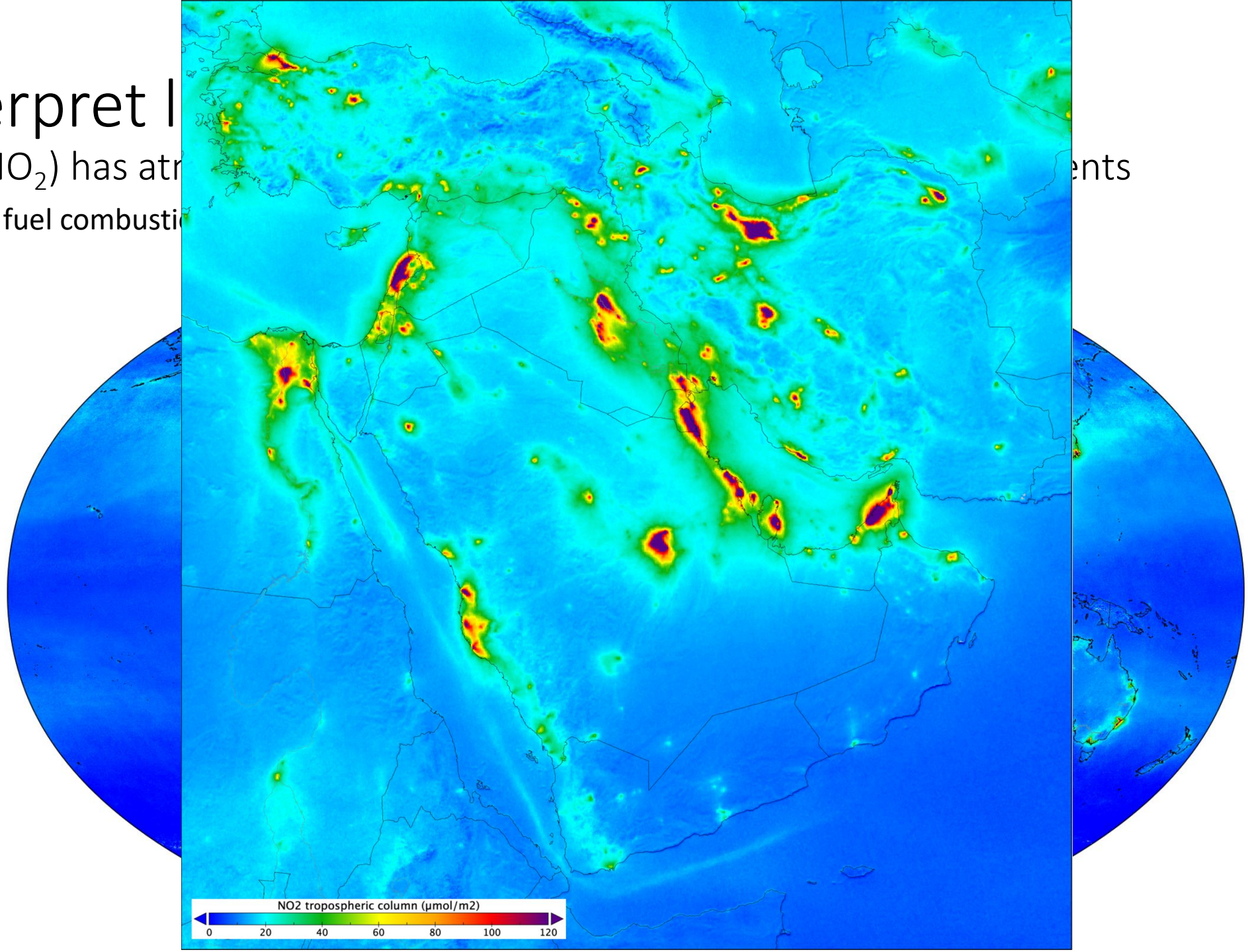
So the fraction removed by outflow is $k_{out}/k = 4.8/5.9 = 0.81$ or 81%.

How to interpret l

Nitrogen dioxide (NO_2) has atr ents

Source: fossil fuel combusti

[TROPOMI NO_2](#) between April and September 2018 (ESA)

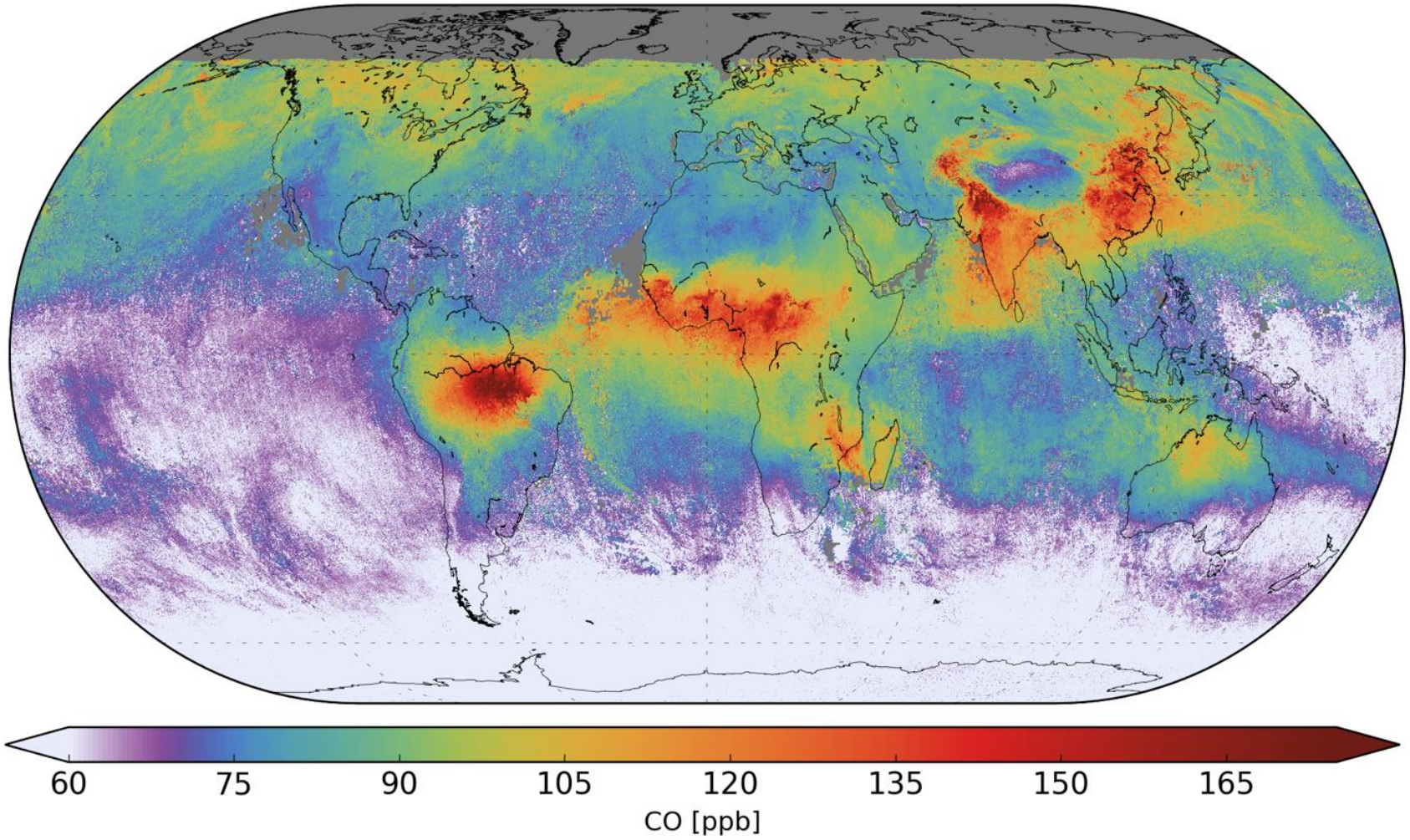


[regional view](#)

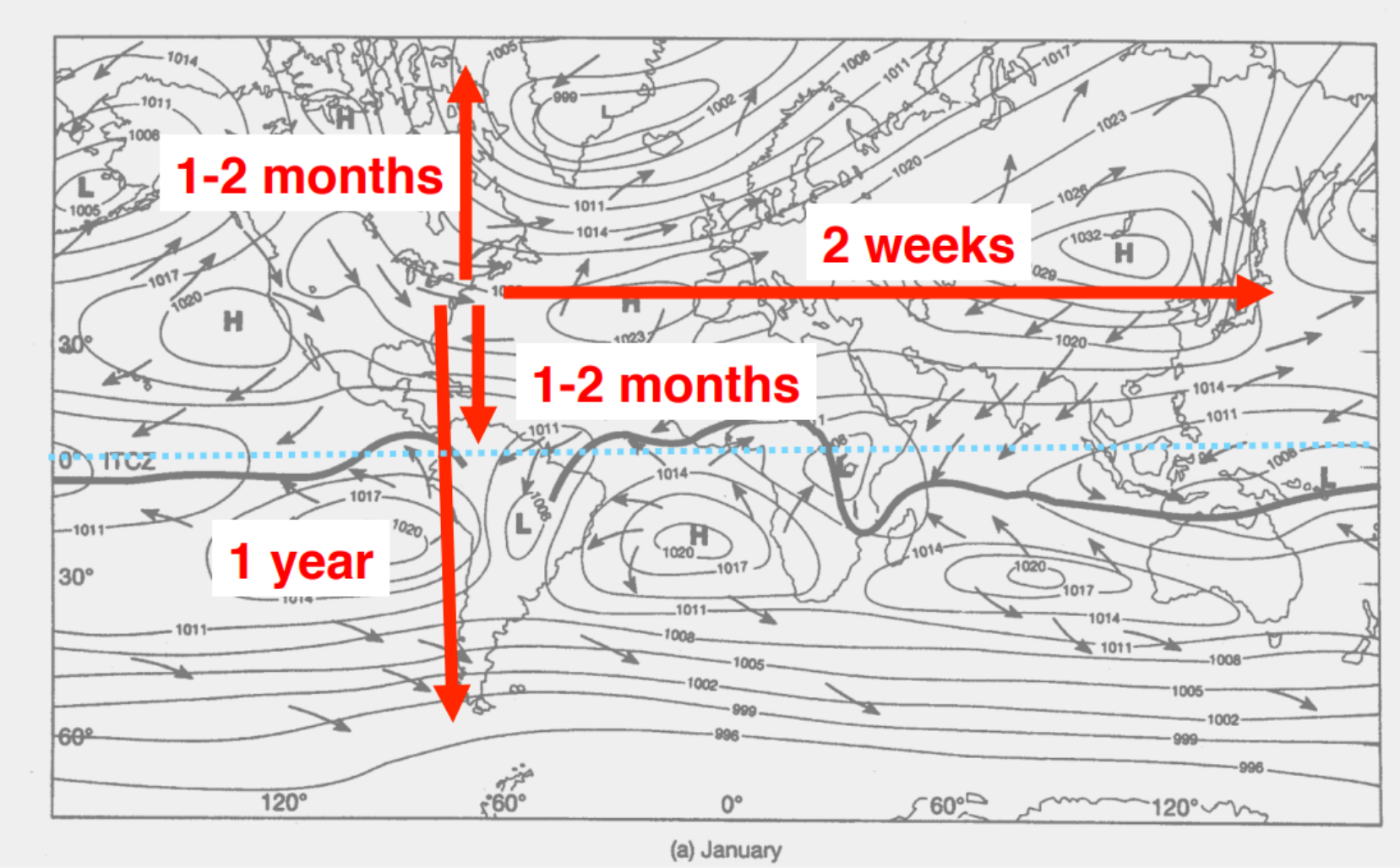
Carbon monoxide (CO) has an atmospheric lifetime of ~ 2 months: mixing around latitude bands

Source: combustion Sink: oxidation

TROPOMI CO



Typical timescales for mixing within the atmosphere



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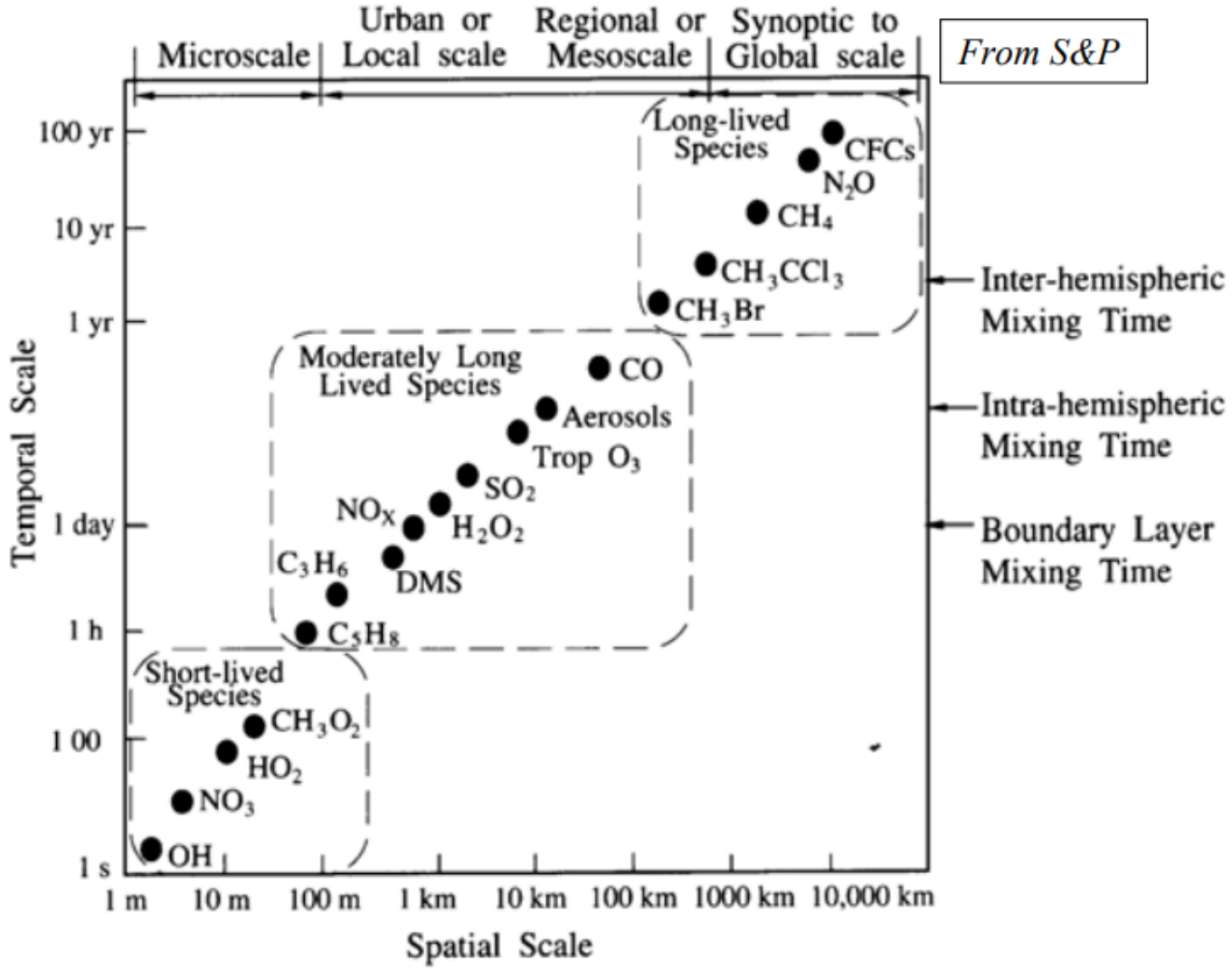
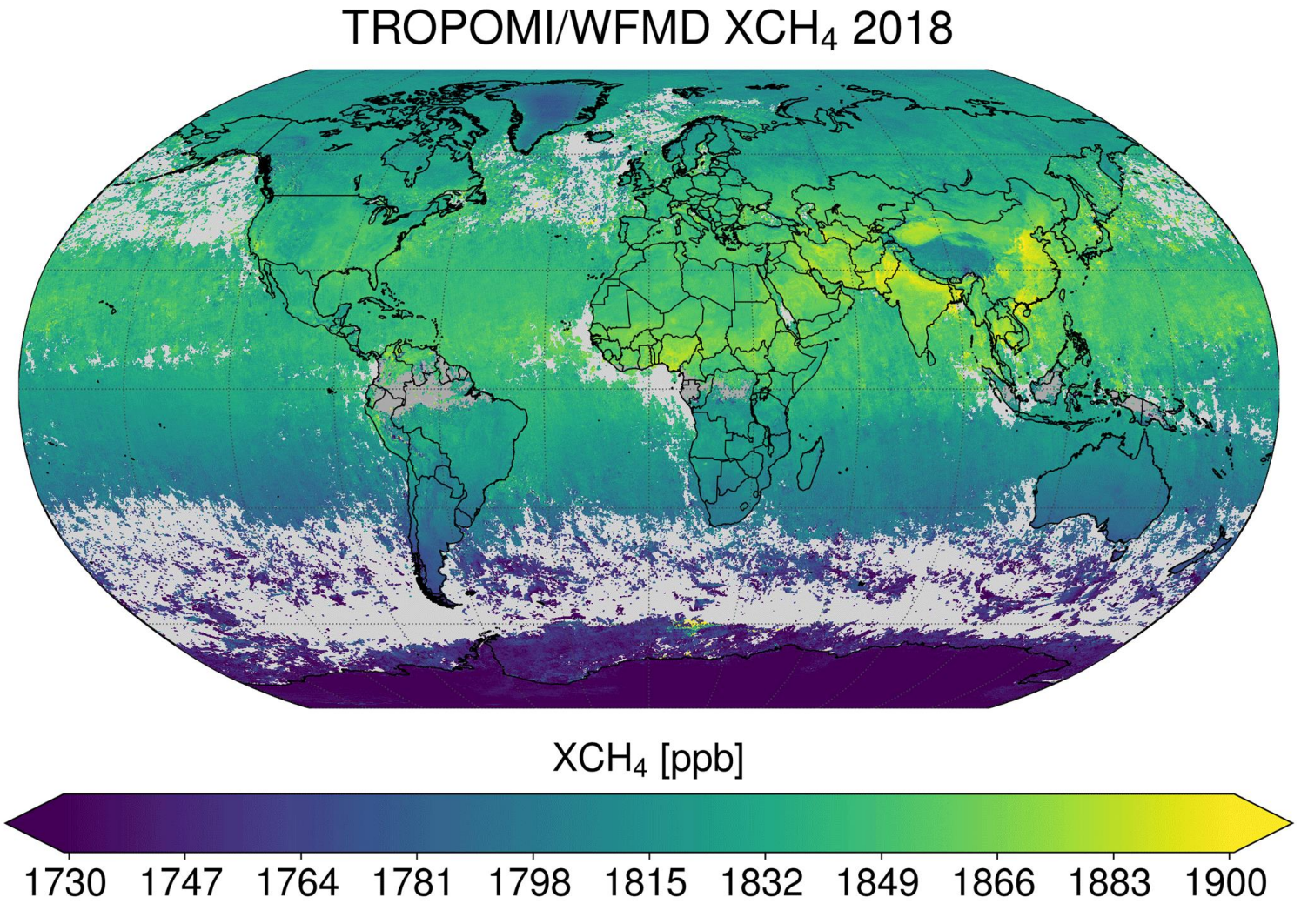


Seinfeld and Pandis, Fig. 1.17

Methane (CH_4) has atmospheric lifetime of ~10 years: global mixing

Sources: wetlands, livestock, oil/gas/coal production, landfills, wastewater treatment
Sink: oxidation

TROPOMI CH4
[Schneising et al., 2019]

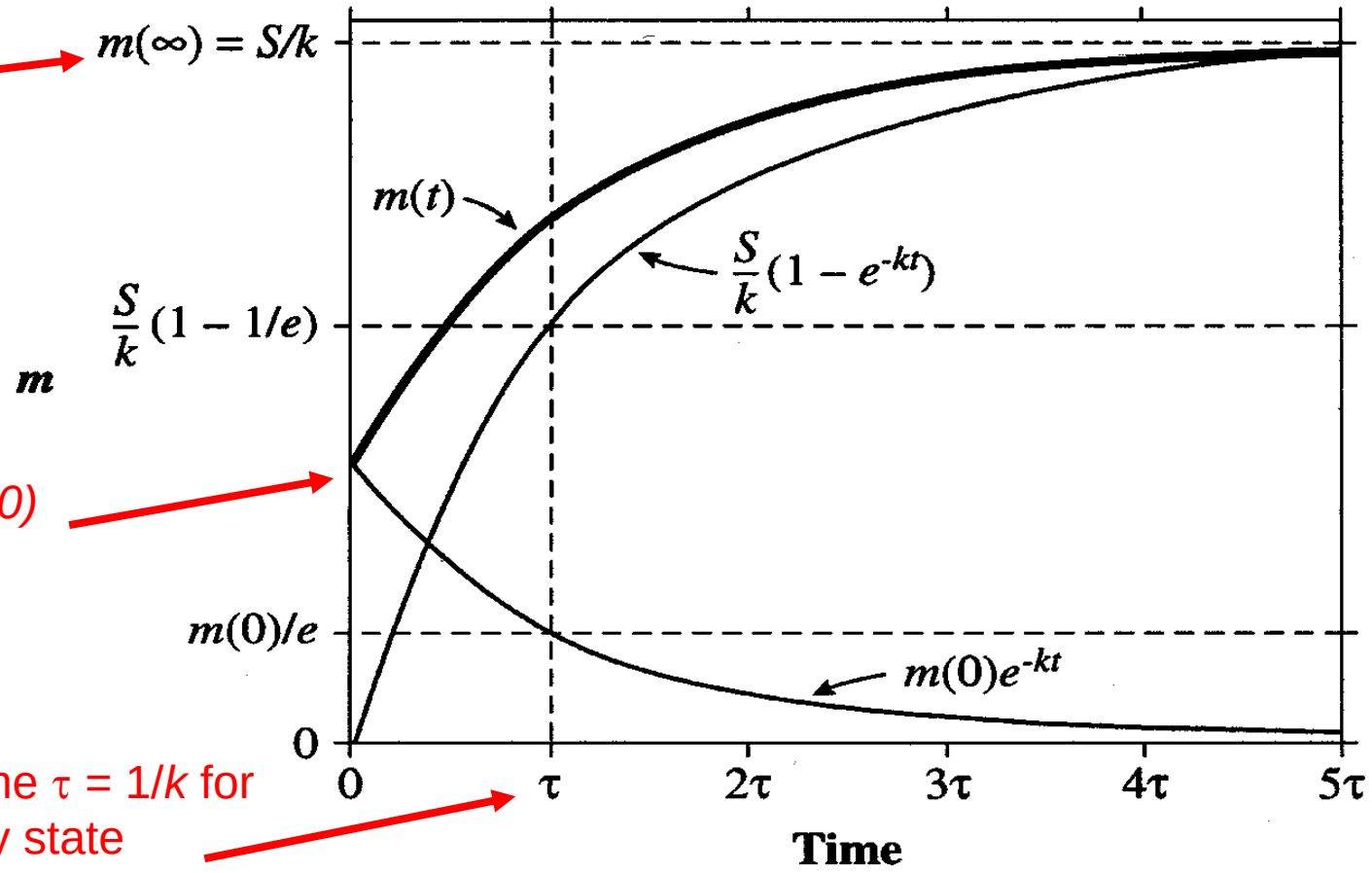


Simple models can still be valid and insightful! Consider methane:

Special case: constant source, first-order sink

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

Steady state solution (*dm/dt = 0*)

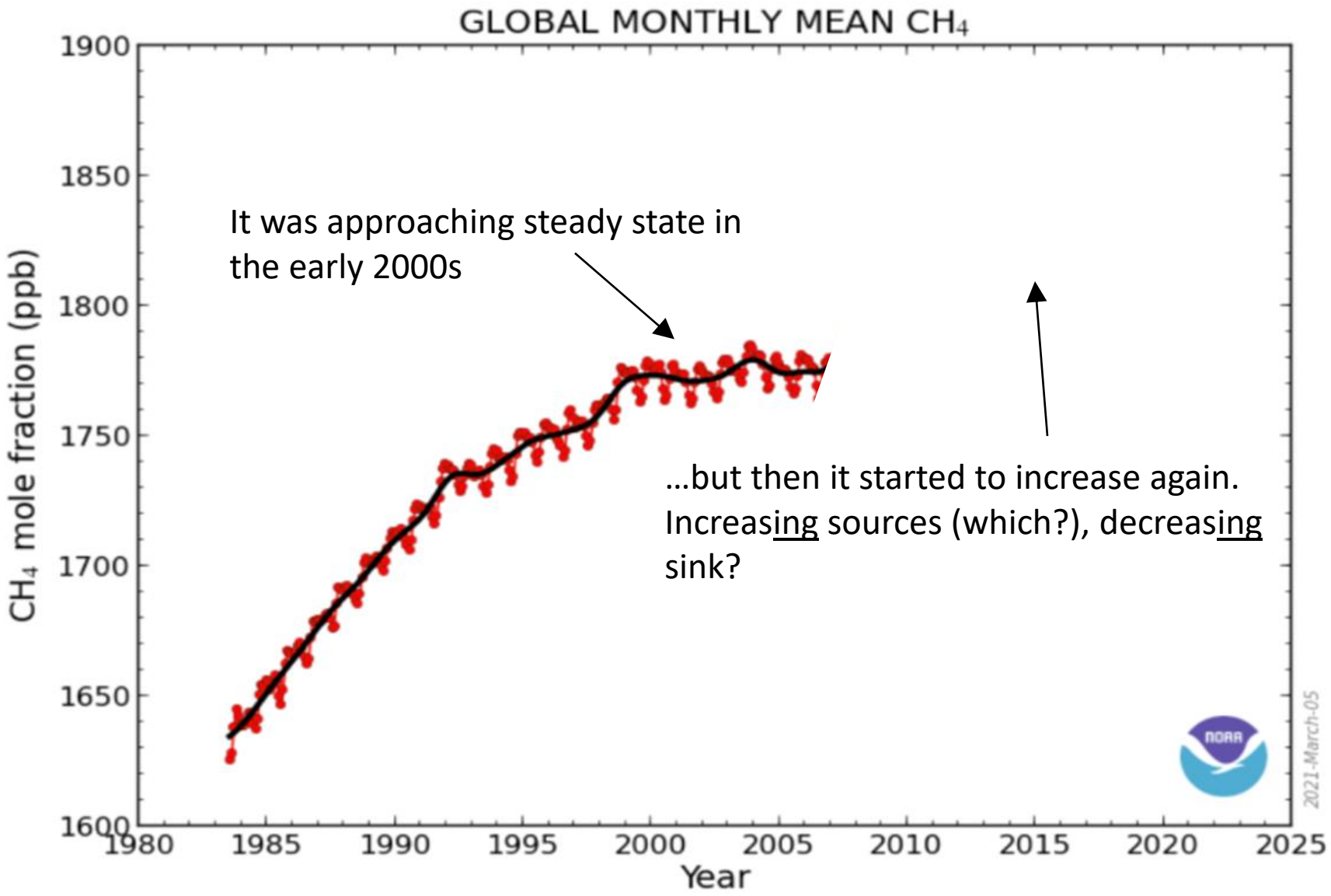


Initial condition *m(0)*

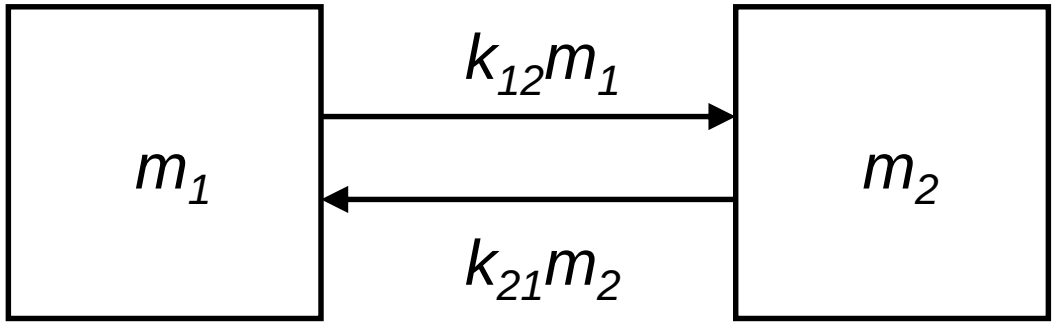
Characteristic time $\tau = 1/k$ for
- reaching steady state
- decay of initial condition

If *S*, *k* are constant over $t >> \tau$, then $dm/dt \rightarrow 0$ and $m \rightarrow S/k$: (steady state)

The enigma of atmospheric methane



TWO-BOX MODEL
defines spatial variation between two domains



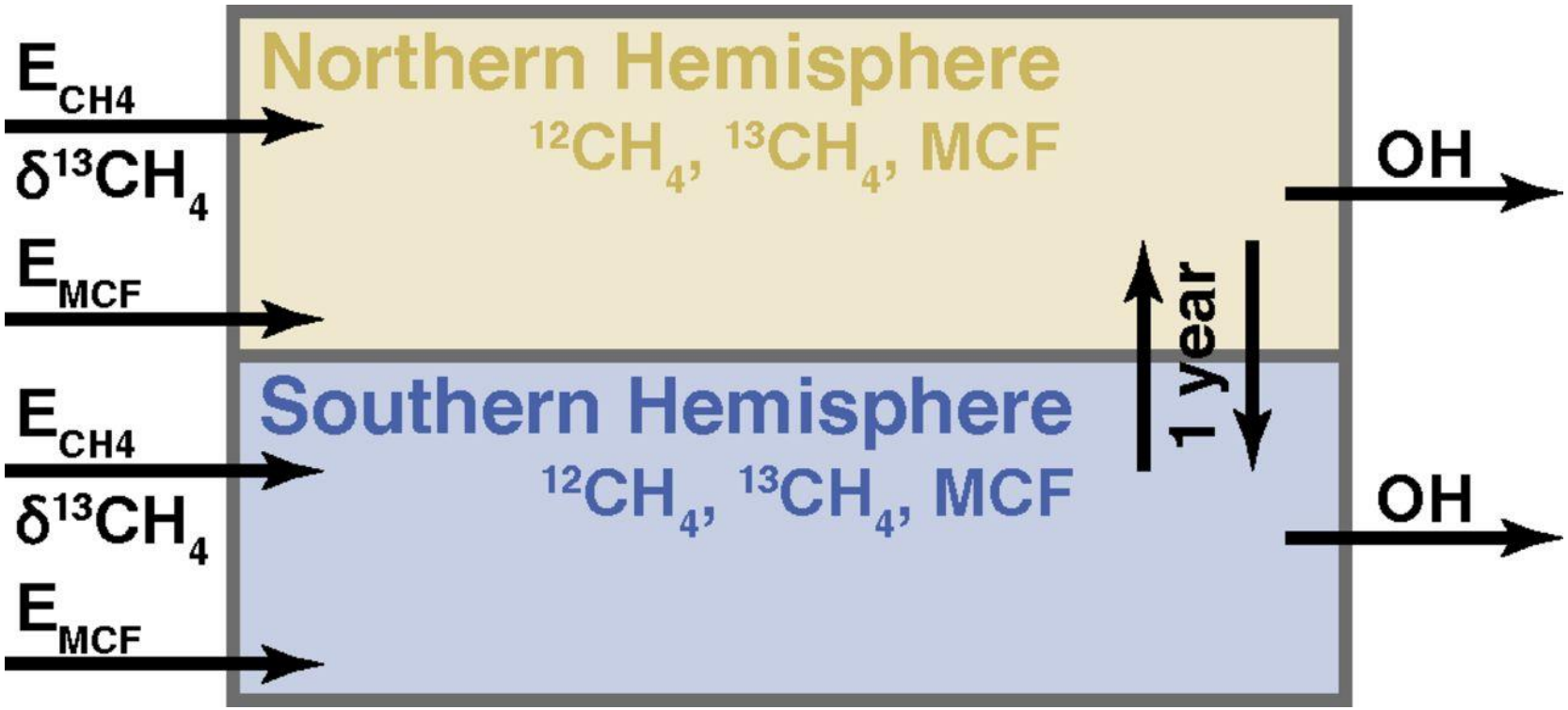
Mass balance equations:

$$\frac{dm_1}{dt} = E_1 + P_1 - L_1 - D_1 - k_{12}m_1 + k_{21}m_2$$

$$\frac{dm_2}{dt} = E_2 + P_2 - L_2 - D_2 + k_{12}m_1 - k_{21}m_2$$

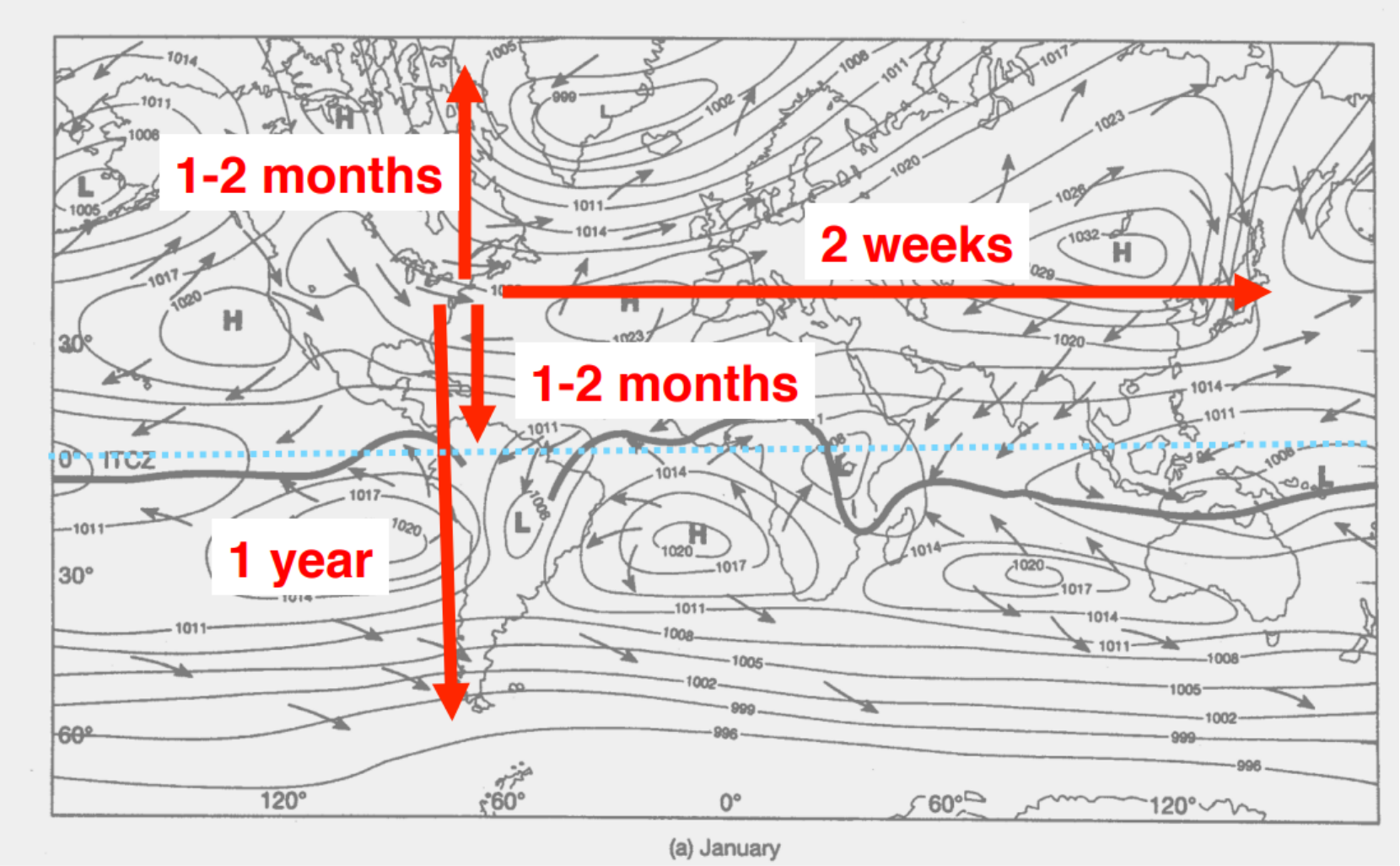
⇨ system of two coupled ordinary differential equations
(or algebraic equations if system is assumed to be at steady state)

Was used to argue that the increase was caused by changes in the *OH sink*



Turner et al., PNAS, 2017

Recall: Typical timescales for mixing within the atmosphere



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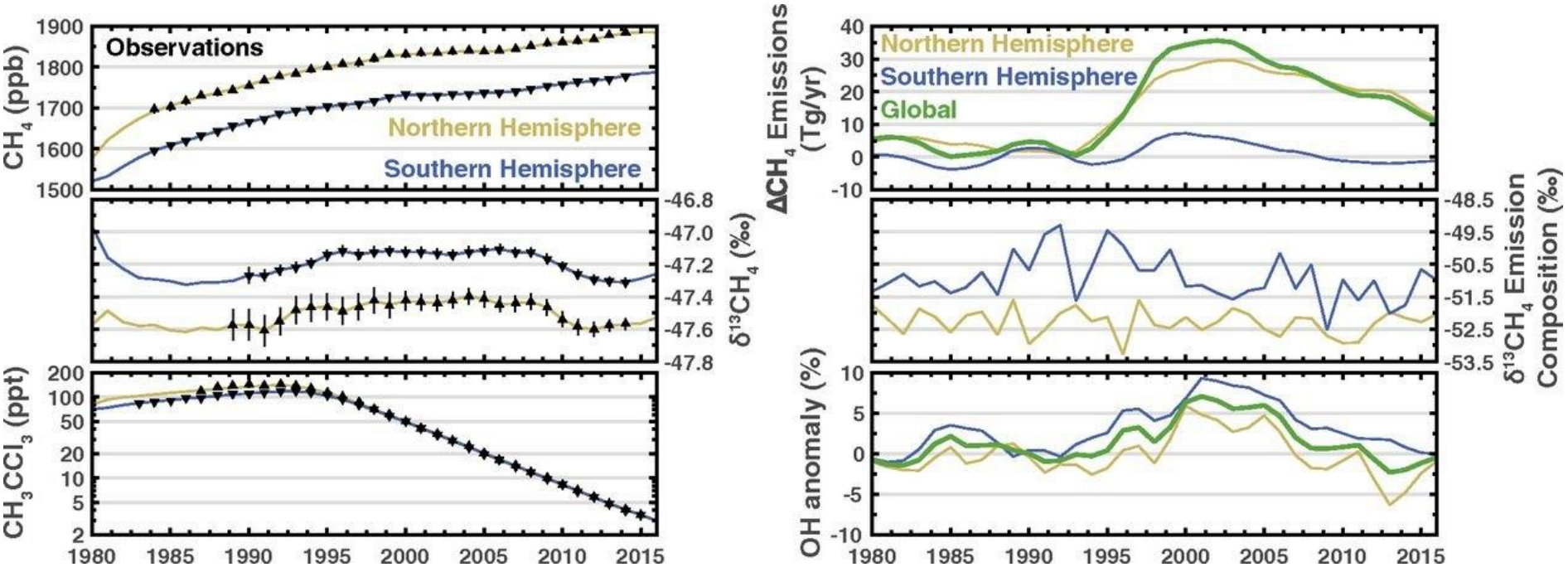
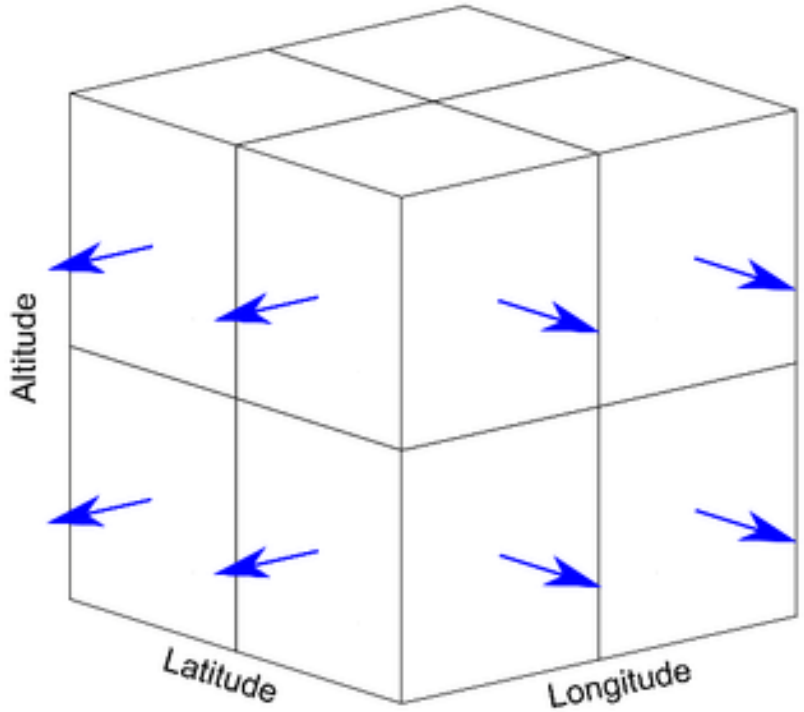
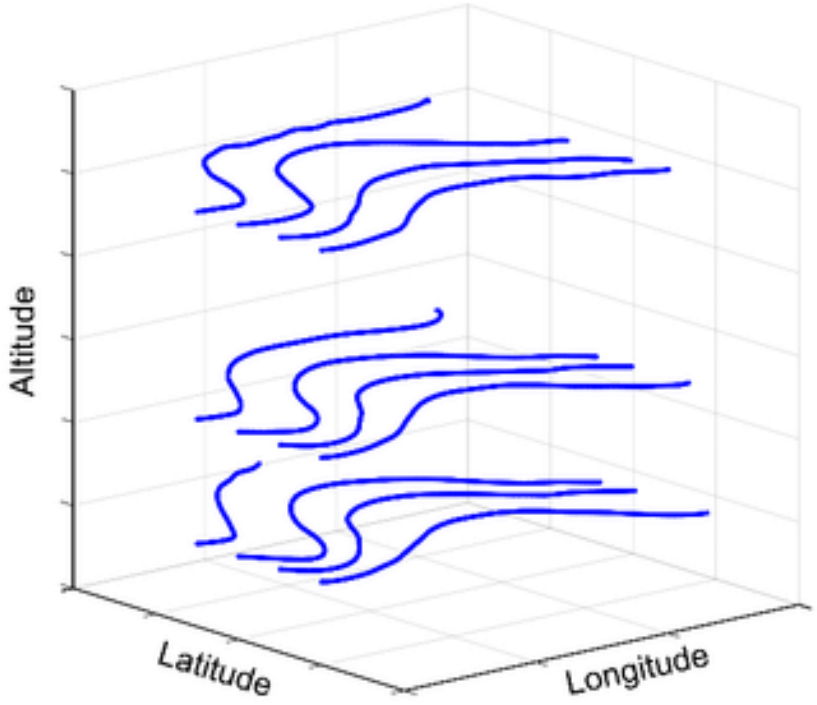


"Here we use a multispecies inversion to determine the cause of these decadal trends. The most likely explanation for the renewed growth in atmospheric methane involves a decrease in hydroxyl (OH), the main sink for atmospheric methane, that is partially offset by a decrease in methane emissions."

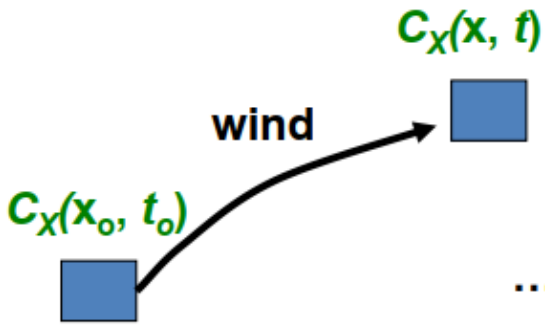
Turner et al., PNAS, 2017

Eulerian vs. Lagrangian models





Other model forms: Lagrangian models

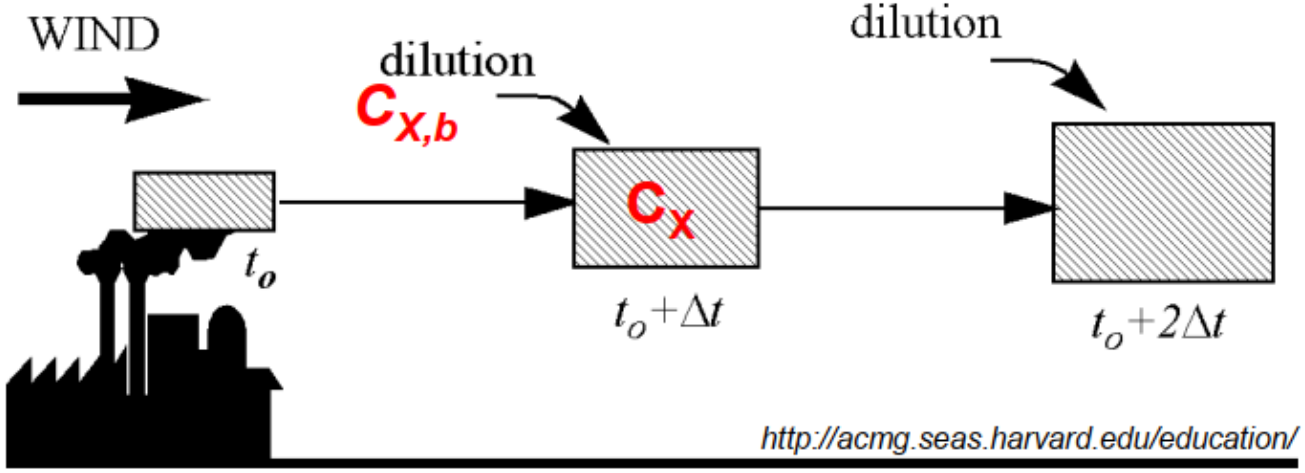


In the moving box (*C* is the concentration),

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

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

Application to the chemical evolution of an isolated pollution plume:



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

Used both for plume modelling (in the forward direction) and for inverse modelling (with time inverted). Can be very efficient!

An iterative process, to improve our understanding of the atmosphere