Atmospheric models

Chem 5151 - Christoph Knote - NCAR
Spring 2013

based on:
Introduction to Atmospheric Chemistry, D. Jacob, Princeton Press, 1999
Prof. Colette Heald's course http://www.atmos.colostate.edu/~heald/teaching.html

NCAR

total change in
X over time

Continuity equation

$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

Nothing is ever lost.

The change of a quantity X over time
is the net result of *sources minus sinks*.

Source and sink terms depend on the application.

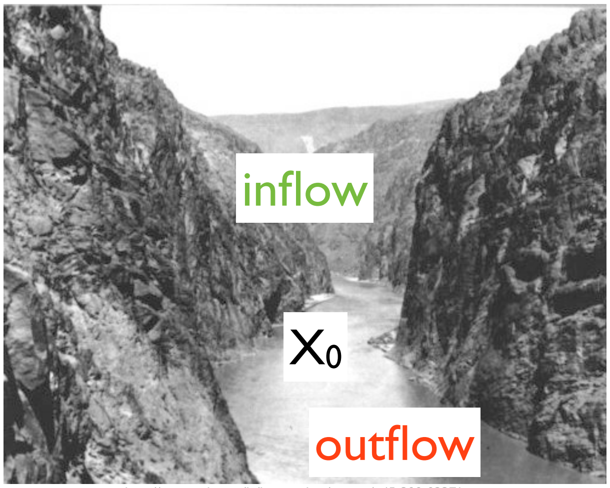
total change in
X over time

Transport

$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

transport

Example (X == water)



http://www.usbr.gov/lc/hooverdam/images/p45-300-02371.jpg

F_{in} (inflow) - F_{out} (outflow)

in this example $\approx$*0.0*

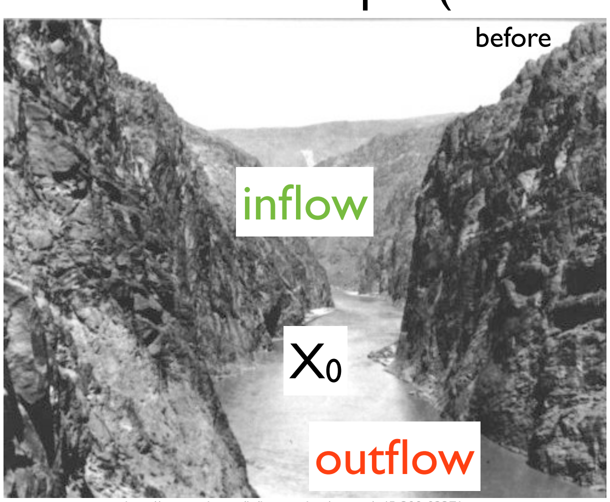
total change in
X over time

Transport

$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

transport

Example (X == water) + Hoover dam



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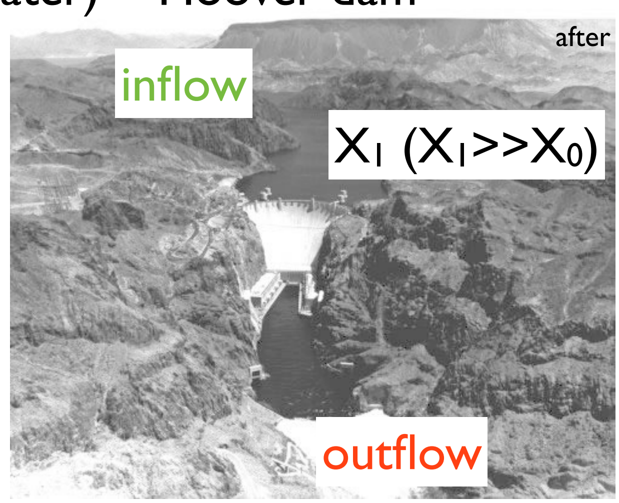


http://www.usbr.gov/lc/hooverdam/images/p45-300-01501.jpg

Clicker question

Did the transport term F_X (on average) change after construction of the Hoover dam?

A. yes, it is now > 0.0

B. yes, it is now < 0.0

C. no

D. yes, it is now == 0.0

E. I don't know

Clicker question

Did the transport term F_X (on average) change after construction of the Hoover dam?

A. yes, it is now > 0.0

B. yes, it is now < 0.0

C. no

D. yes, it is now == 0.0

E. I don't know

C no (on average), because the reservoir would overflow if the term is still positive once the reservoir is full.

transport is always:
F_{in} - F_{out}

Emissions

total change in X over time

$$\frac{dX}{dt} = F_X + \underbrace{E_X}_{\textbf{emissions}} + P_X - L_X - D_X$$

based on **emission factors** and **activity rates:**

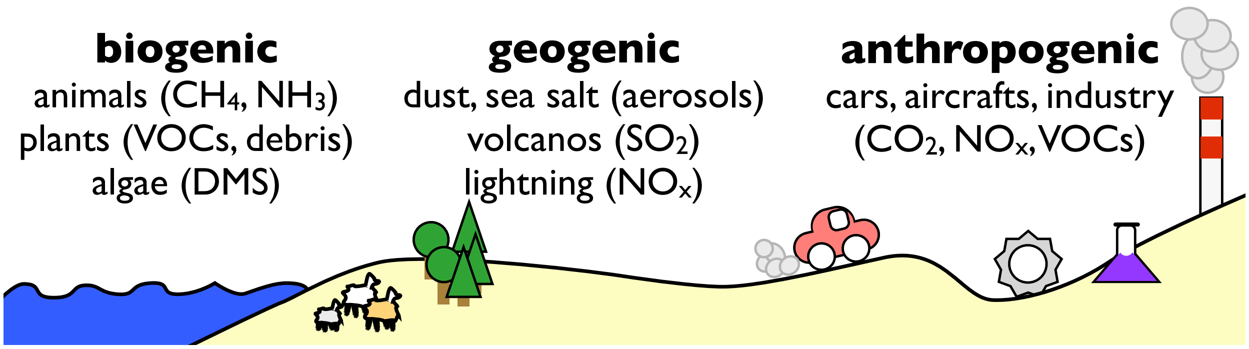
$$E_X = EF_X \cdot A_X$$ = 368 kg CO_2 emitted

Example: 368 g CO_2 / km   1.000 km driven

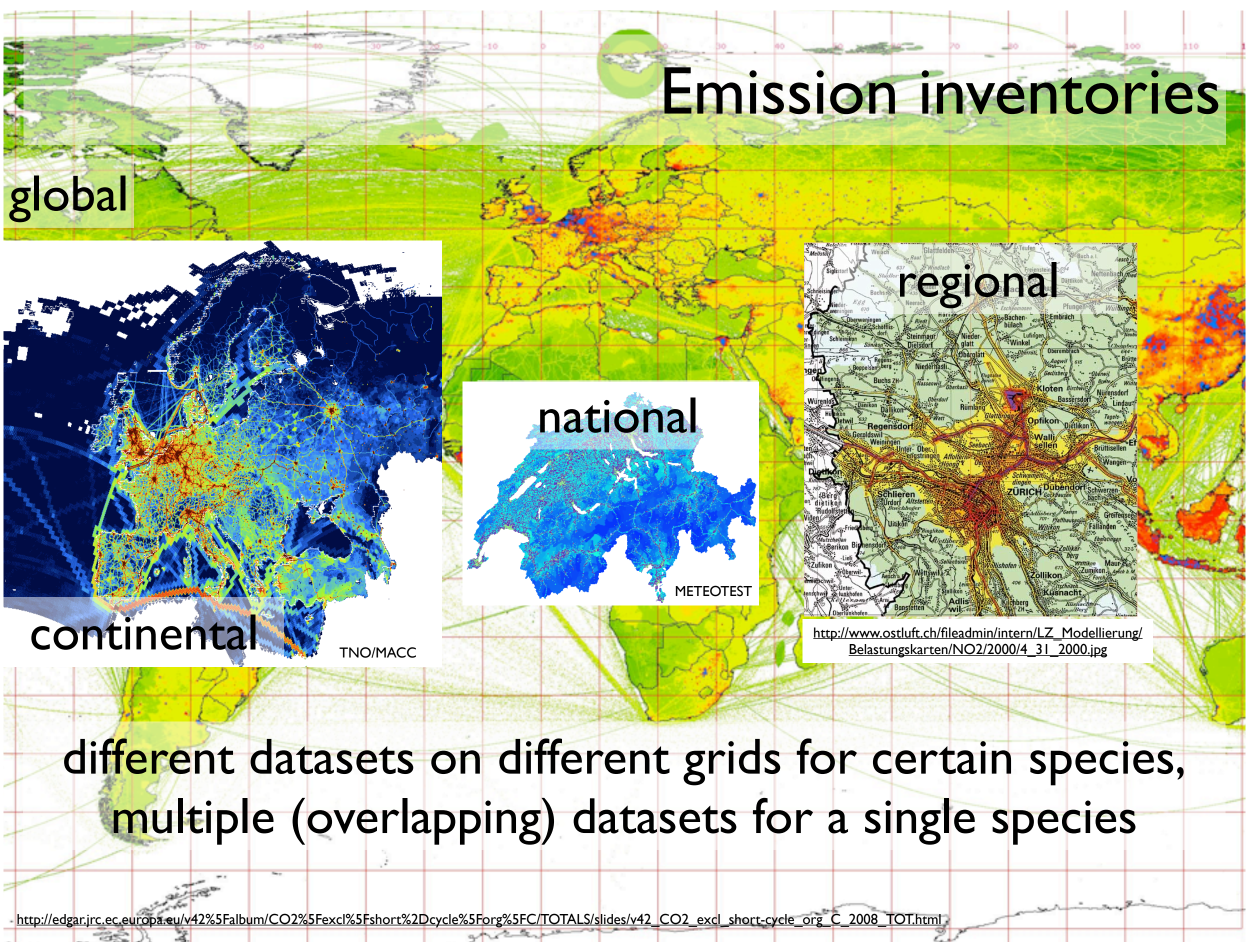
biogenic
animals (CH_4, NH_3)
plants (VOCs, debris)
algae (DMS)

geogenic
dust, sea salt (aerosols)
volcanos (SO_2)
lightning (NO_x)

anthropogenic
cars, aircrafts, industry
(CO_2, NO_x, VOCs)



Emission inventories



different datasets on different grids for certain species, multiple (overlapping) datasets for a single species total change in X over time

Chemical reactions

$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

chemical Production / Loss

e.g. tropospheric ozone (photostationary state)

production

$$NO_2 + h\nu \rightarrow NO + O(^3P)$$

$$O(^3P) + O_2 + M \rightarrow O_3 + M$$

loss

$$NO + O_3 \xrightarrow{k} NO_2 + O_2$$

in our model e.g.:

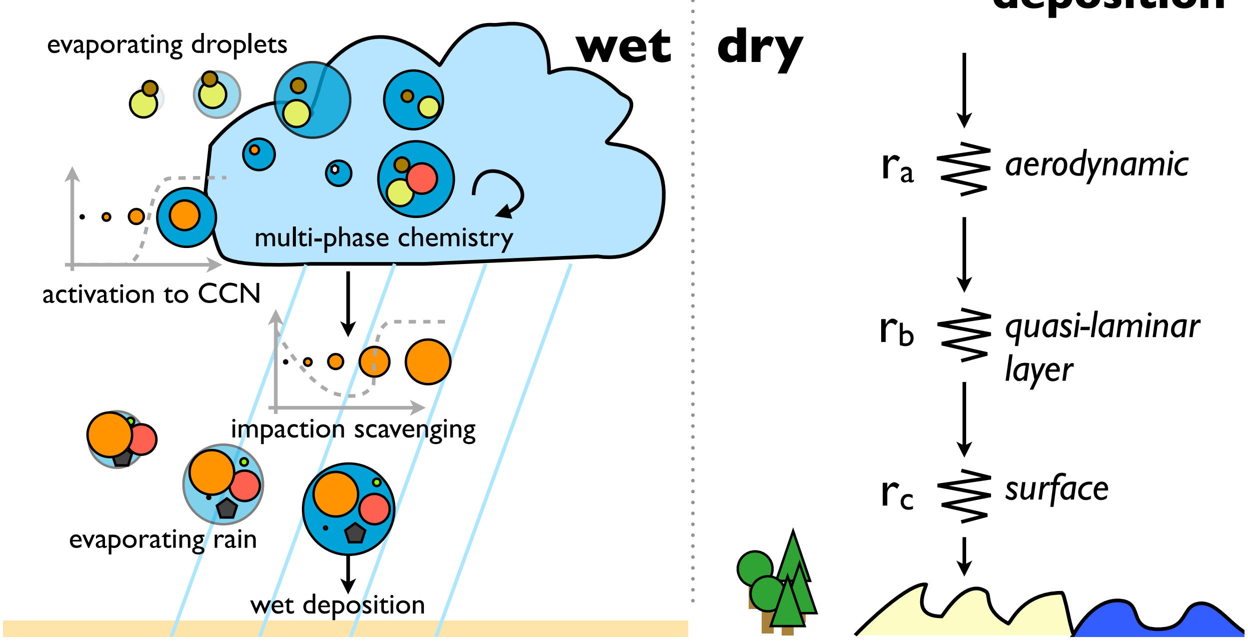
$$= \boxed{J_{NO_2}[NO_2] + f([O(^3P)], [O_2], [M])} \boxed{- k_{NO,O_3}[NO][O_3]}$$

total change in X over time

Deposition

$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

deposition



Resistance approach

Calculation of dry dep. flux $F_X = v_{dep}[X]$

deposition velocity — concentration of X

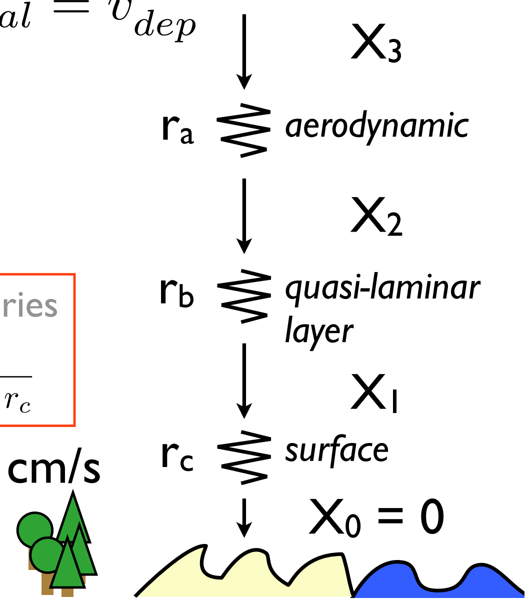
based on resistance analogy $r_{total} = v_{dep}^{-1}$

$$F_X = \frac{X_3 - X_2}{r_a} = \frac{X_2 - X_1}{r_b} = \frac{X_1 - \cancel{X_0}}{r_c} = \frac{X_3 - \cancel{X_0}}{r_{tot}}$$

$$= \frac{X_3 - (F_X r_b + X_1)}{r_a}$$

$$= \frac{X_3 - (F_X r_b + F_X r_c)}{r_a}$$

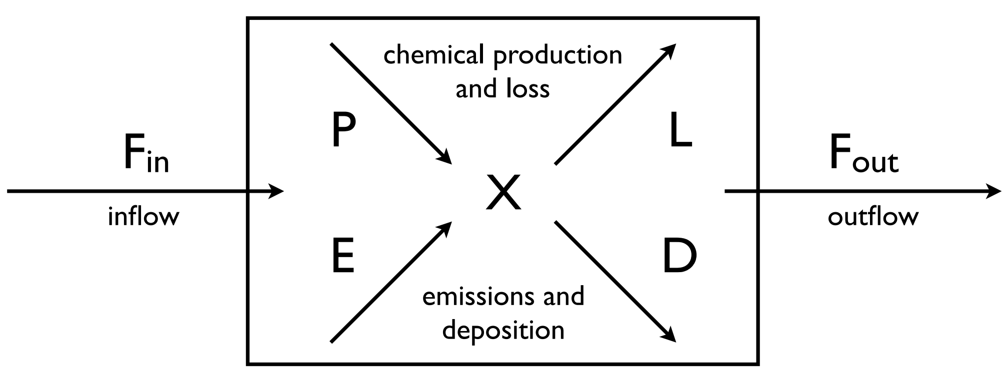
$$F_X = \frac{X}{r_a + r_b + r_c} \rightarrow \boxed{\text{resistances in series} \quad v_{dep} = \frac{1}{r_a + r_b + r_c}}$$



typical values of v_{dep} for gases: 0.5 cm/s

see also: Wesely and Hicks, Atm. Env., 34, 2000

Box models

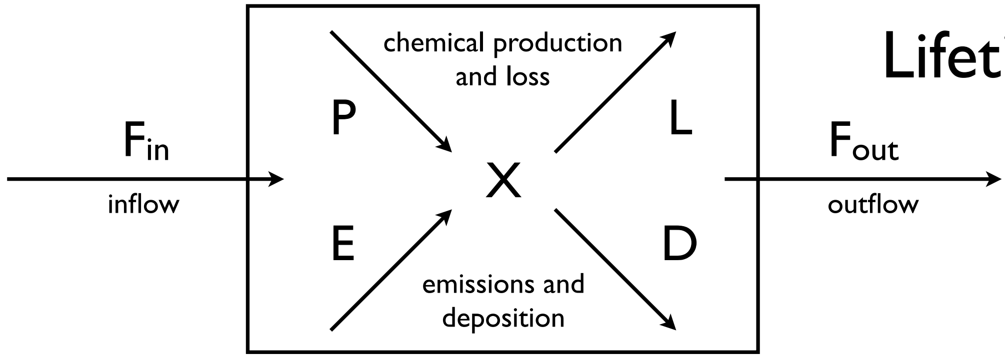


adapted from Introduction to Atmospheric Chemistry, D. Jacob

All variables (e.g. X) and environmental conditions (temperature, pressure, ...) are homogeneous within the box:

„well-mixed“ assumption

Lifetime



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mass balance:

$$\frac{dX}{dt} = \sum sources - \sum sinks = F_{in} - F_{out} + E_X + P_X - L_X - D_X$$

$$\boxed{\text{atmospheric lifetime: } \tau = \frac{X}{F_{out} + L_X + D_X} \quad \text{(s)}}$$

lifetimes add in parallel: $\frac{1}{\tau} = \frac{1}{\tau_{outflow}} + \frac{1}{\tau_{chemical\ loss}} + \frac{1}{\tau_{deposition}}$

loss rates relate to lifetime: $k = \frac{1}{\tau}$ (s^{-1})

Clicker question

Box of 1 x 1 x 1 m. No transport.
20 ppbv of compound X in the box at steady state.
Chemical production of X: **0.1 ppbv/s**. Chemical loss (first order k): **0.005 1/s**. Emissions of **0.5 ppbv/s**.
Deposition: **0.025 ppbv/s**.

Lifetime of X against chemical loss?

A. 4000 s

B. 200 s

C. 160 s

D. 12000 s

E. I don't know

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Lifetime of X against chemical loss?

$$\tau = \frac{X}{F_{out} + L_X + D_X}$$

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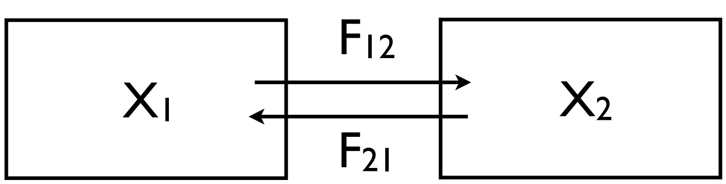
$$\frac{1}{\tau} = \frac{1}{\tau_{outflow}} + \boxed{\frac{1}{\tau_{chemical\ loss}}} + \frac{1}{\tau_{deposition}}$$

$$\tau_{chemical\ loss} = \tau_{L_x} = \frac{X}{L_X}$$

B

Two-box models



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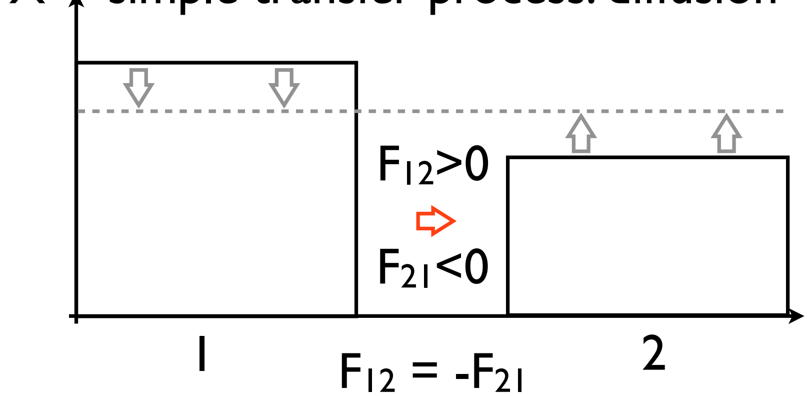
X simple transfer process: diffusion



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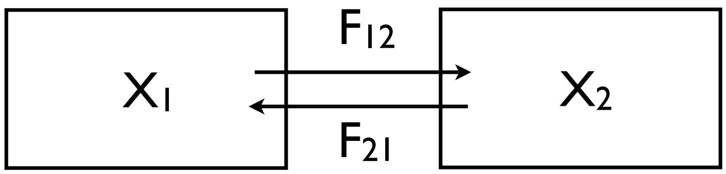


adapted from Introduction to Atmospheric Chemistry, D. Jacob

extended continuity eq. for X_1

$$\frac{dX_1}{dt} = E_1 + P_1 - L_1 - D_1 + F_{21} - F_{12}$$

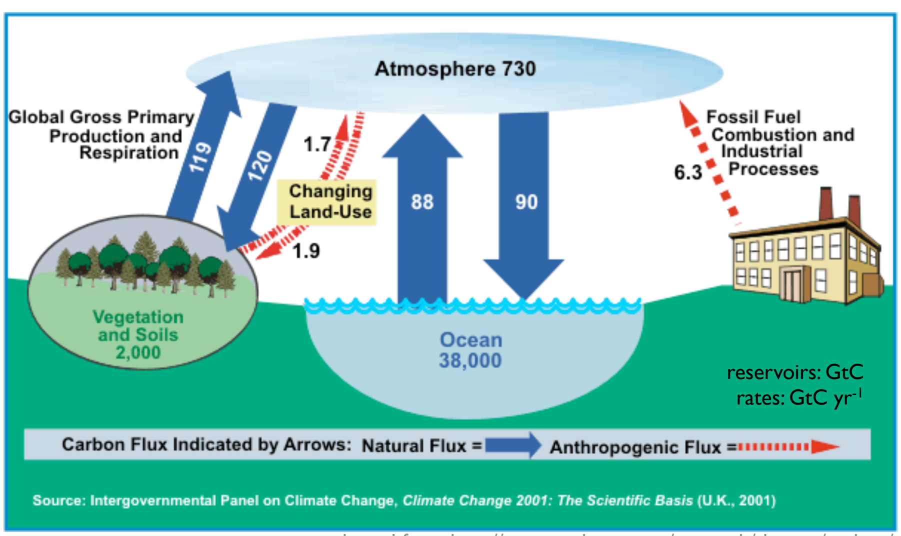
assume flux is mass times transport coefficient (k)

$$\frac{dX_1}{dt} = E_1 + P_1 - L_1 - D_1 + k_{21}X_2 - k_{12}X_1$$

system of coupled ODEs

(analytically solvable if in steady state)

Examples of box models



adapted from http://www.esrl.noaa.gov/research/themes/carbon/

- hemispheric exchange studies, emission estimates
- lifetime and lifecycle assessments for longer lived species (e.g. CO_2, HFCs, CH_4)

Clicker question

What is the lifetime of C in the atmosphere?

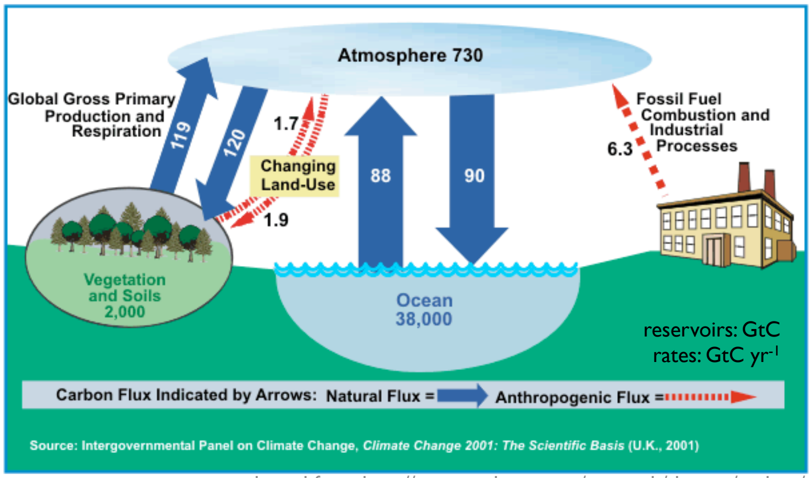
A. 1.6 yrs

B. 3.4 yrs

C. 2.8 yrs

D. 4.9 yrs

E. I don't know



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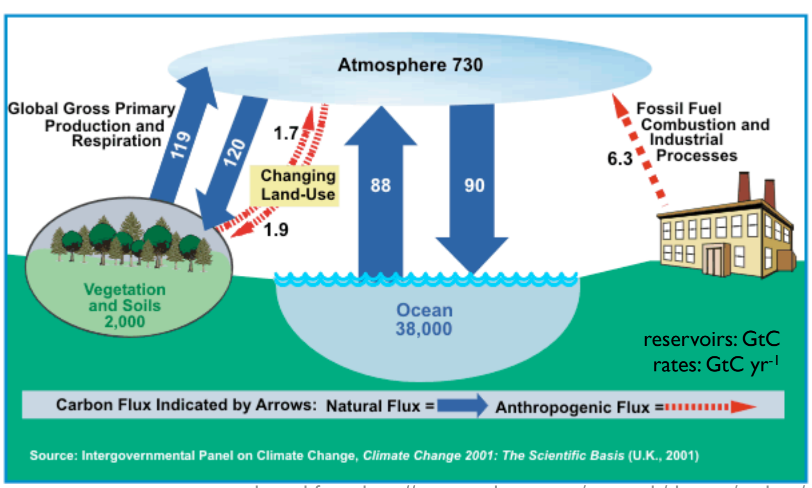

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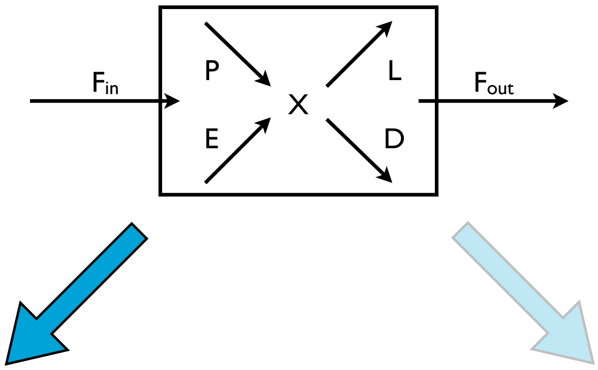
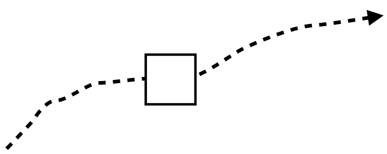
B. $= \frac{730}{90+120+1.9} = 3.45\ yrs$

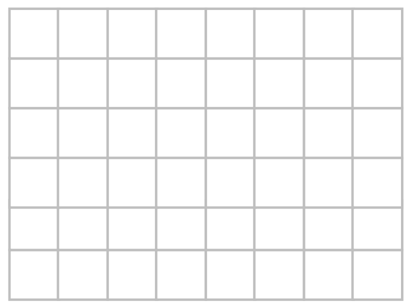
box models



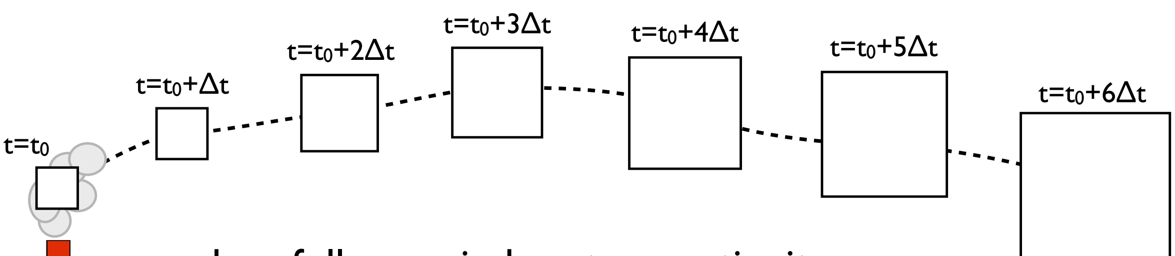
Lagrangian models

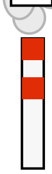
Eulerian models





Puff models





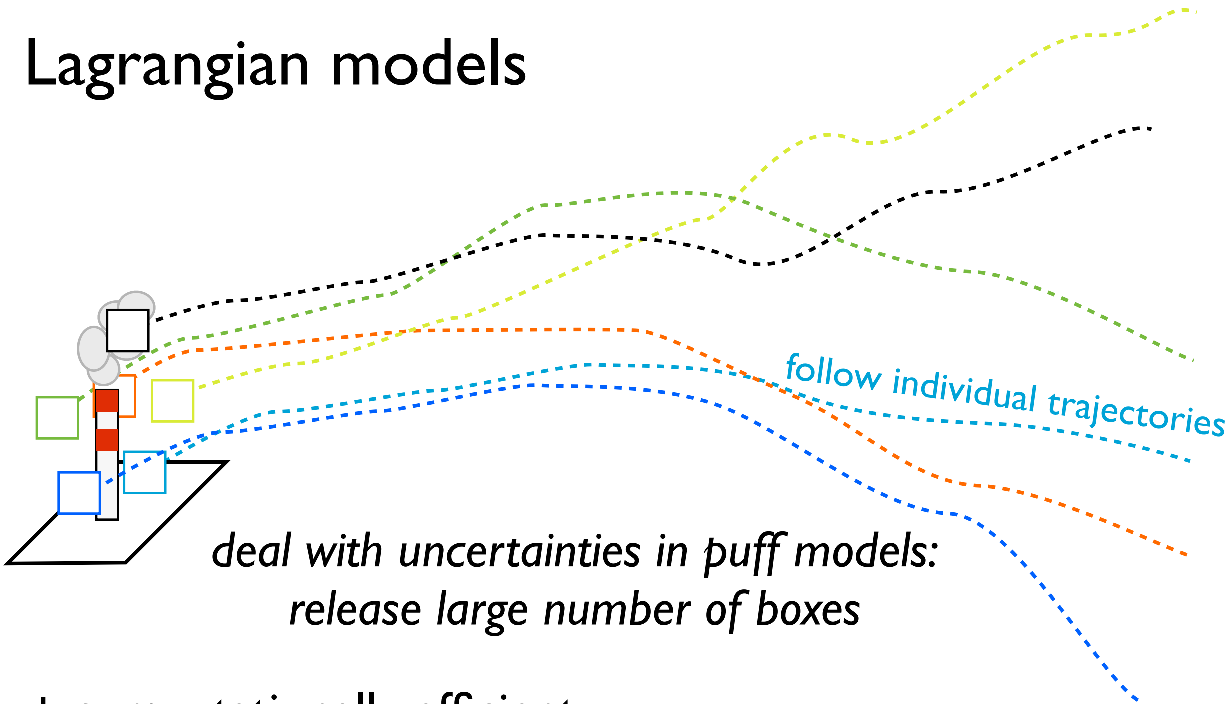
box follows wind vector, continuity eq.:

$$\frac{dX}{dt} = E + P - L - D \boxed{- k_{dil}(X - X_{env})}$$

dilution term - air in box mixes with surroundings

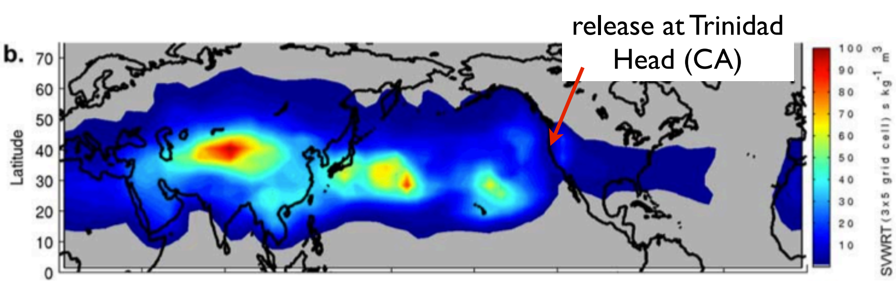
Large uncertainties in transport and dilution possible!
(additionally to uncert. in chemistry, emissions, removal)

Lagrangian models



deal with uncertainties in puff models:
release large number of boxes

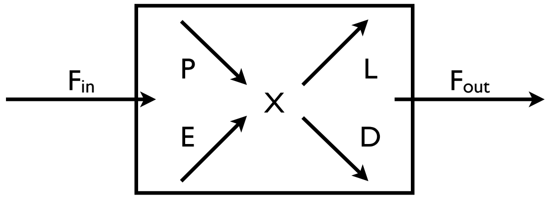
+ computationally efficient
- no mixing between individual boxes (chemistry!)
- statistical undersampling away from source



Example

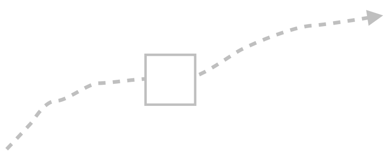
residence time

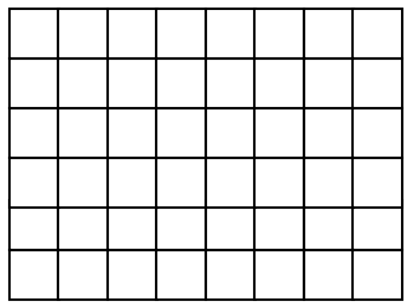
box models

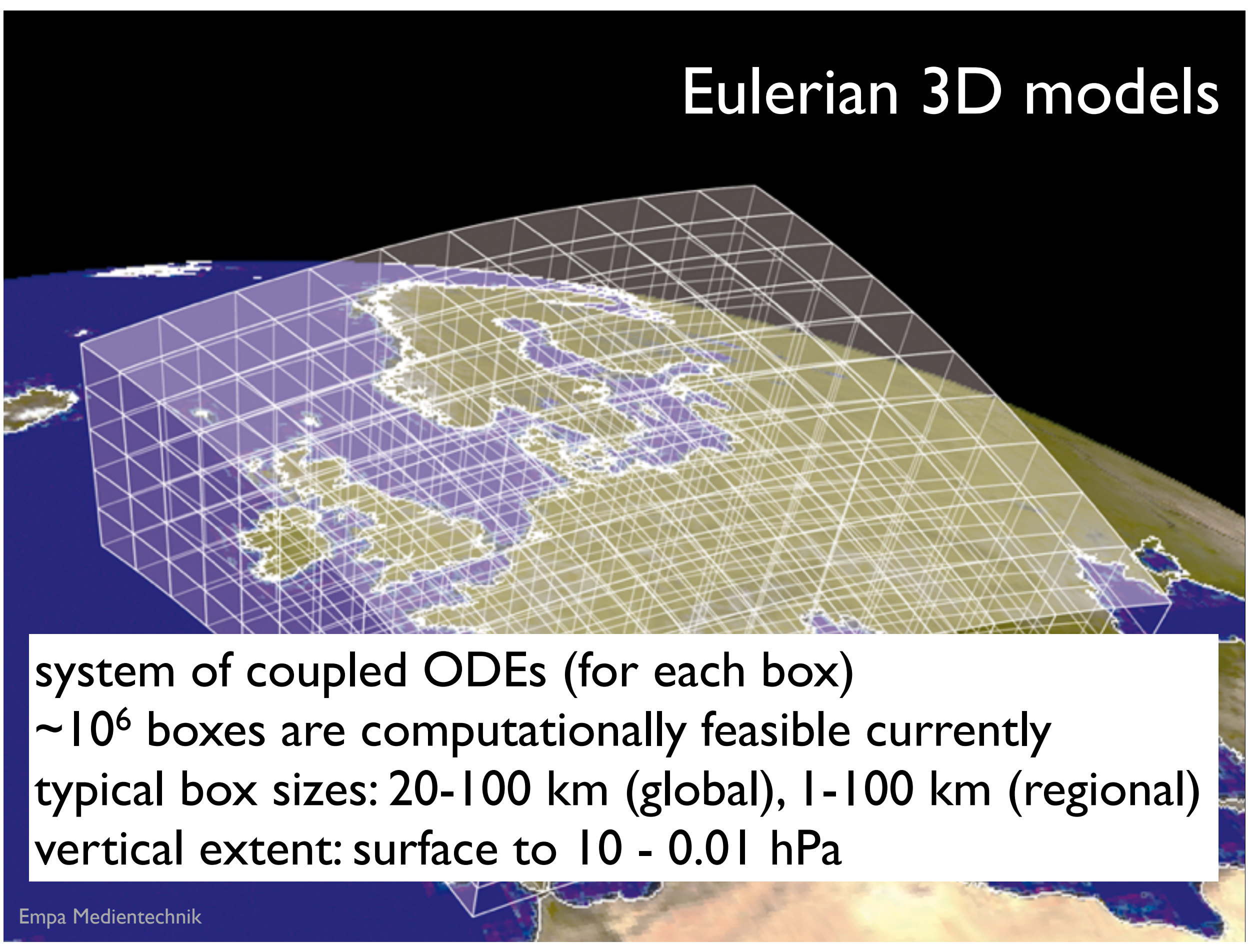


Lagrangian models

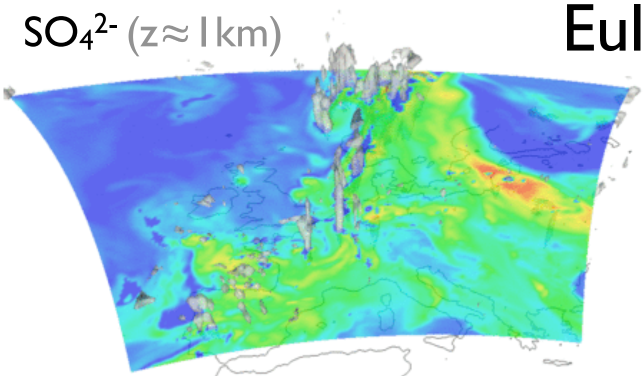
Eulerian models







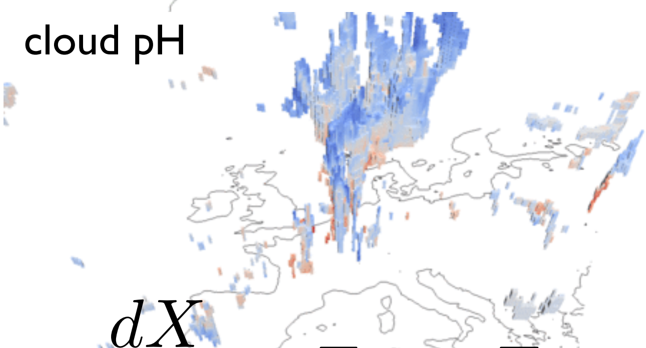
SO$_4^{2-}$ (z≈1km)



Eulerian model example

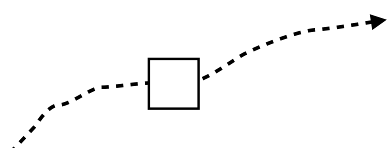
processes seen here:
transport, convection (F_X)
wet deposition (D_X)
aq.-phase chem. (P_X)

cloud pH



$$\frac{dX}{dt} = F_X + E_X + P_X - L_X - D_X$$

Lagrangian models

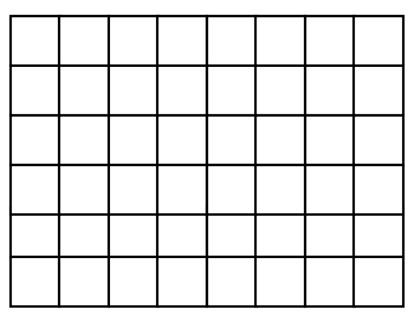


! output of Eulerian model („weather forecast“) necessary for wind vector !

boxes follow wind vector, transport term == 0

+ computationally efficient
+ no numerical diffusion
- no mixing (chemistry)
- statistical undersampling

Eulerian models

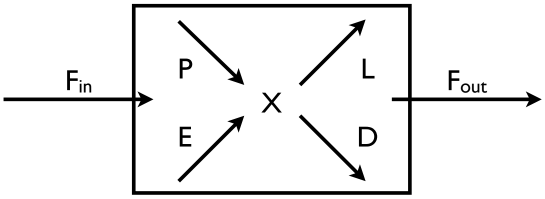


large # of boxes at fixed positions

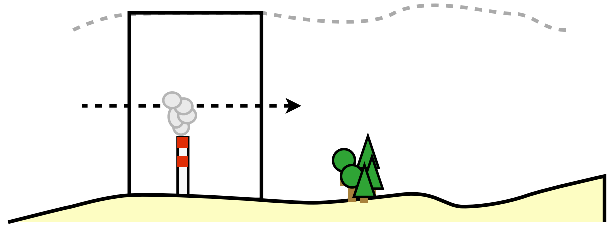
+ complex chemistry, interactions possible
- expensive computation
- numerical diffusion

Final overview

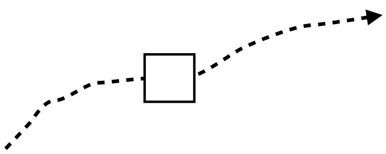
Box models



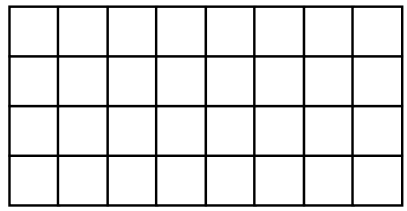
Column models



Lagrangian models



Eulerian models



various types of models, you decide depending on question you want to answer