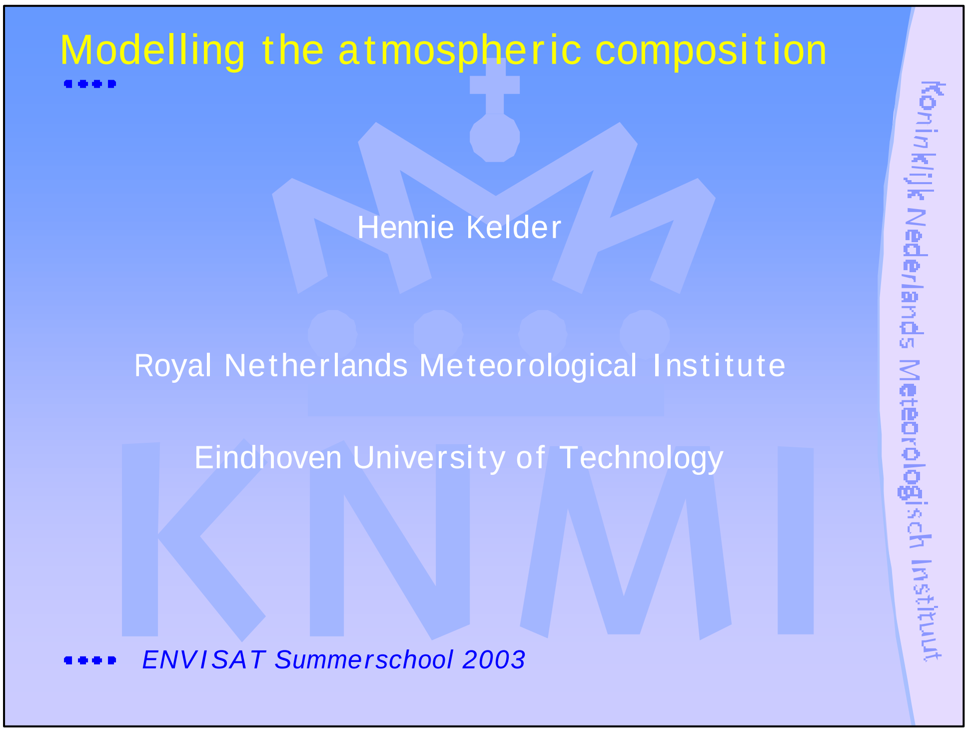

# Modelling the atmospheric composition

Hennie Kelder

Royal Netherlands Meteorological Institute

Eindhoven University of Technology

*ENVISAT Summerschool 2003*

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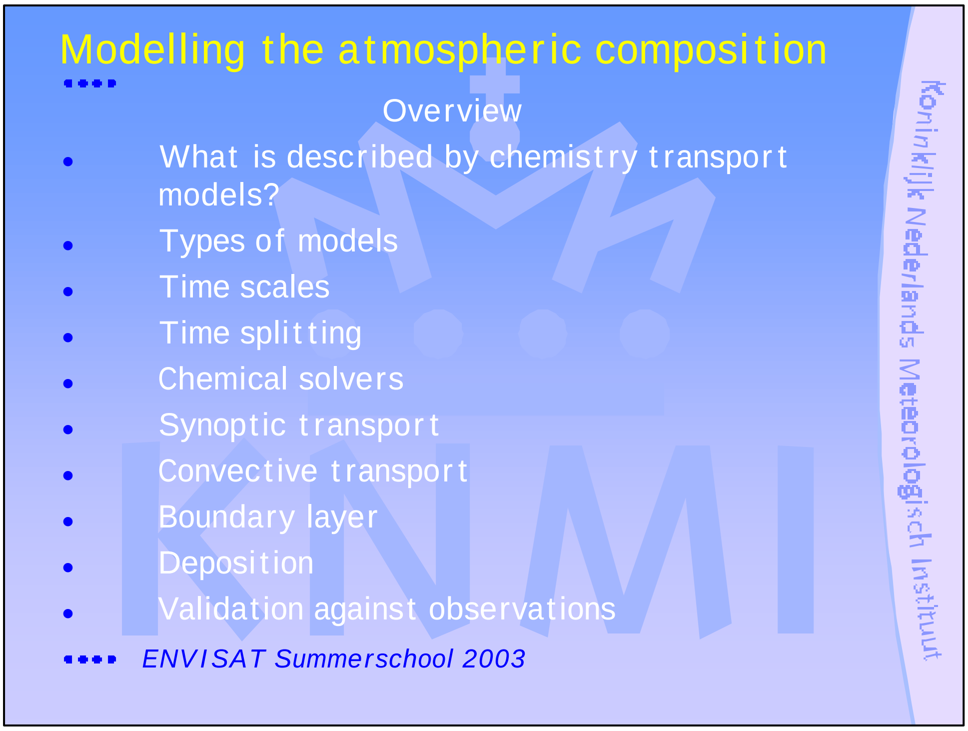

## Modelling the atmospheric composition

Overview

- What is described by chemistry transport models?
- Types of models
- Time scales
- Time splitting
- Chemical solvers
- Synoptic transport
- Convective transport
- Boundary layer
- Deposition
- Validation against observations

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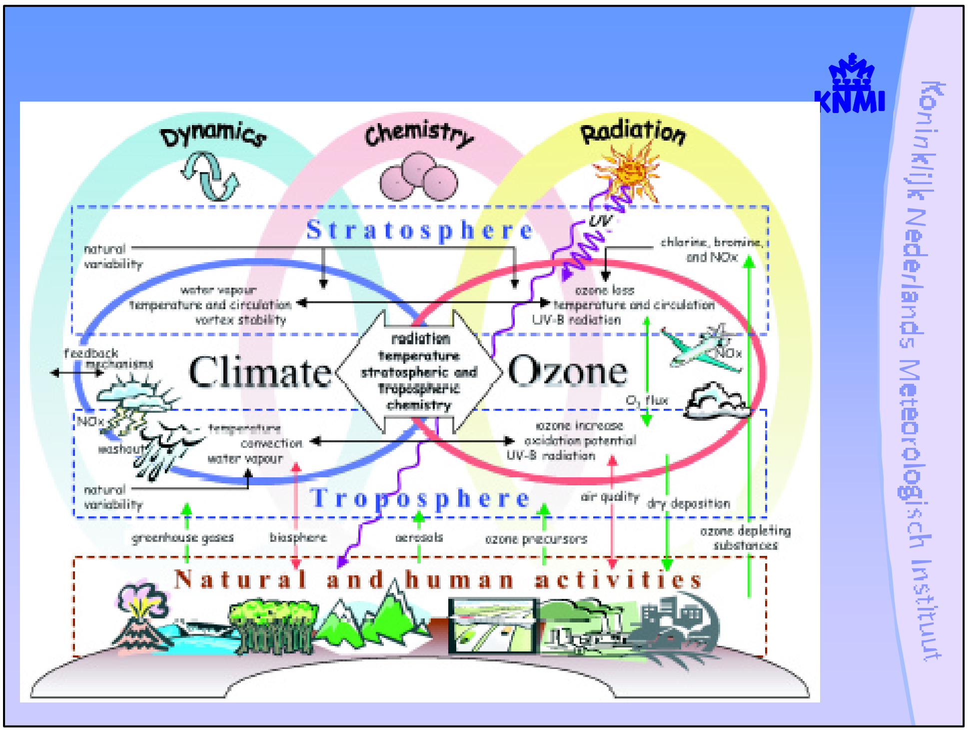
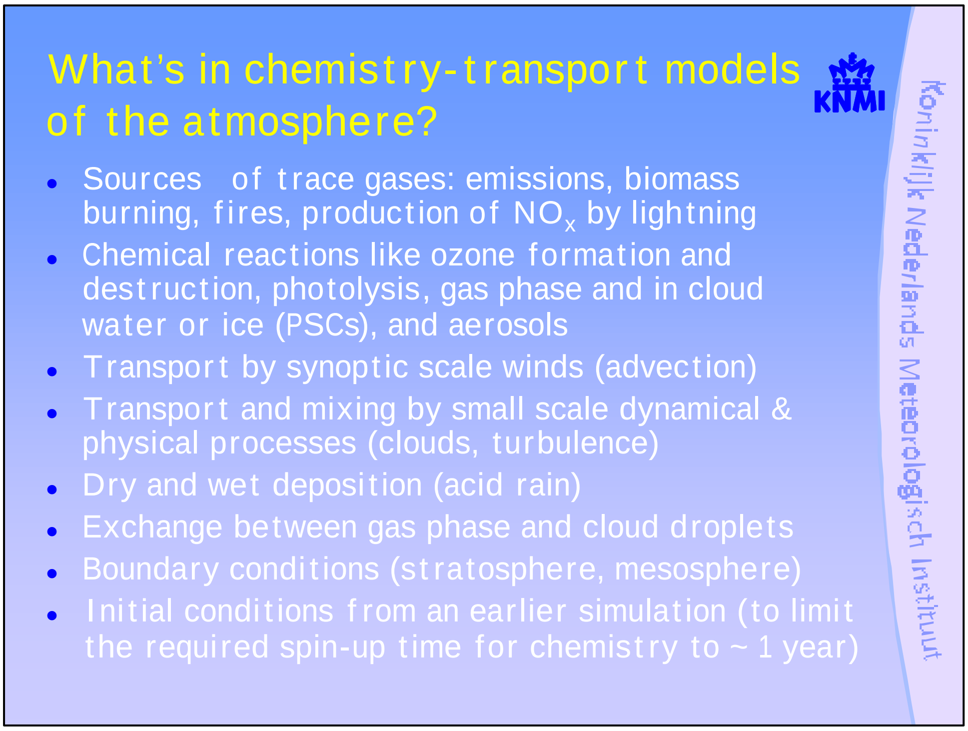
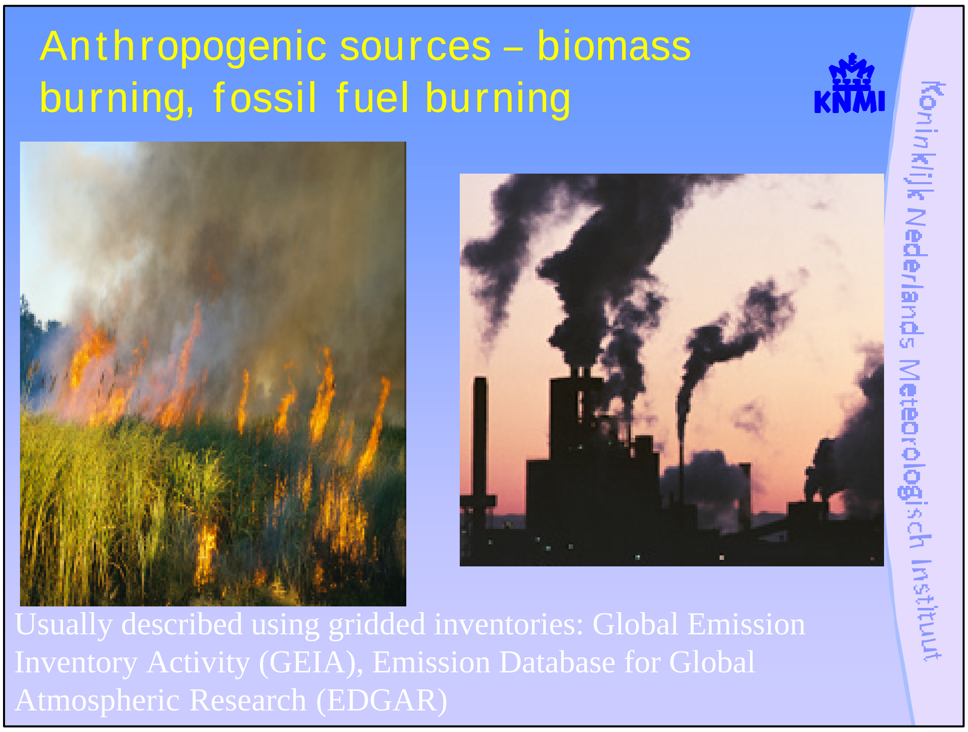




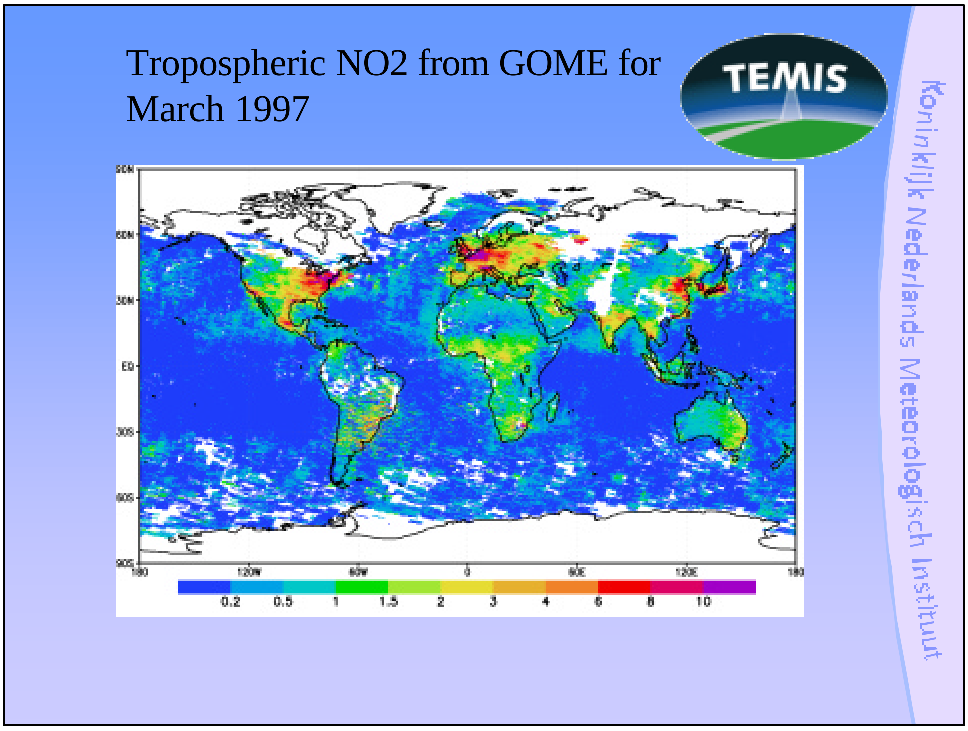
## What's in chemistry-transport models of the atmosphere?

- Sources of trace gases: emissions, biomass burning, fires, production of $NO_x$ by lightning
- Chemical reactions like ozone formation and destruction, photolysis, gas phase and in cloud water or ice (PSCs), and aerosols
- Transport by synoptic scale winds (advection)
- Transport and mixing by small scale dynamical & physical processes (clouds, turbulence)
- Dry and wet deposition (acid rain)
- Exchange between gas phase and cloud droplets
- Boundary conditions (stratosphere, mesosphere)
- Initial conditions from an earlier simulation (to limit the required spin-up time for chemistry to ~ 1 year)

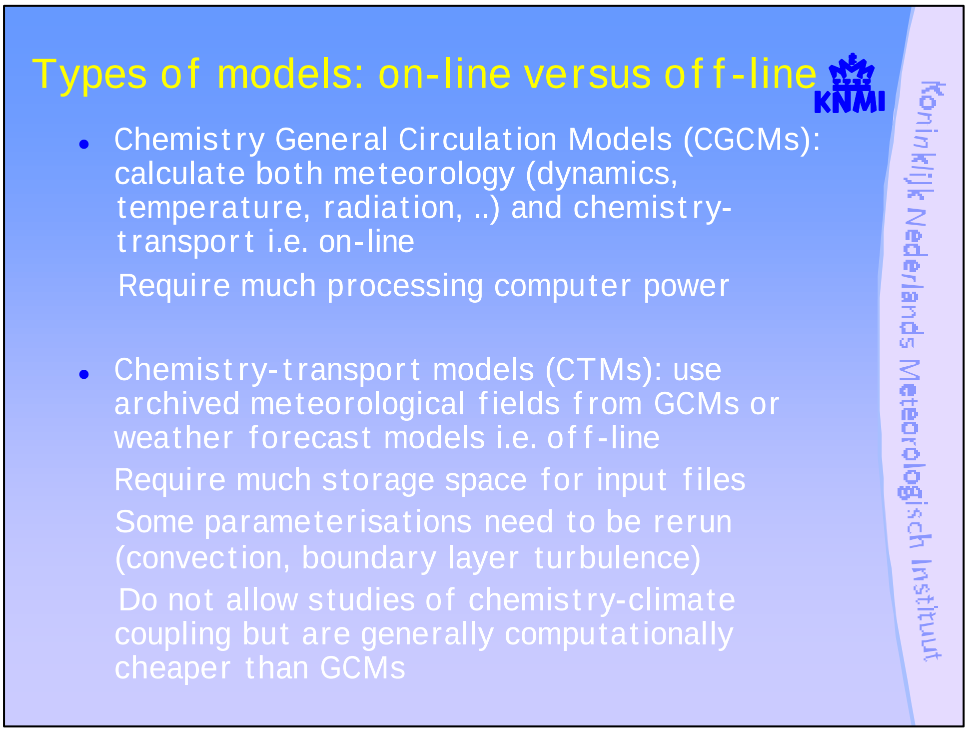


## Anthropogenic sources – biomass burning, fossil fuel burning

Usually described using gridded inventories: Global Emission Inventory Activity (GEIA), Emission Database for Global Atmospheric Research (EDGAR)



## Tropospheric NO2 from GOME for March 1997



## Types of models: on-line versus off-line

- Chemistry General Circulation Models (CGCMs): calculate both meteorology (dynamics, temperature, radiation, ..) and chemistry-transport i.e. on-line

  Require much processing computer power

- Chemistry-transport models (CTMs): use archived meteorological fields from GCMs or weather forecast models i.e. off-line

  Require much storage space for input files

  Some parameterisations need to be rerun (convection, boundary layer turbulence)

  Do not allow studies of chemistry-climate coupling but are generally computationally cheaper than GCMs

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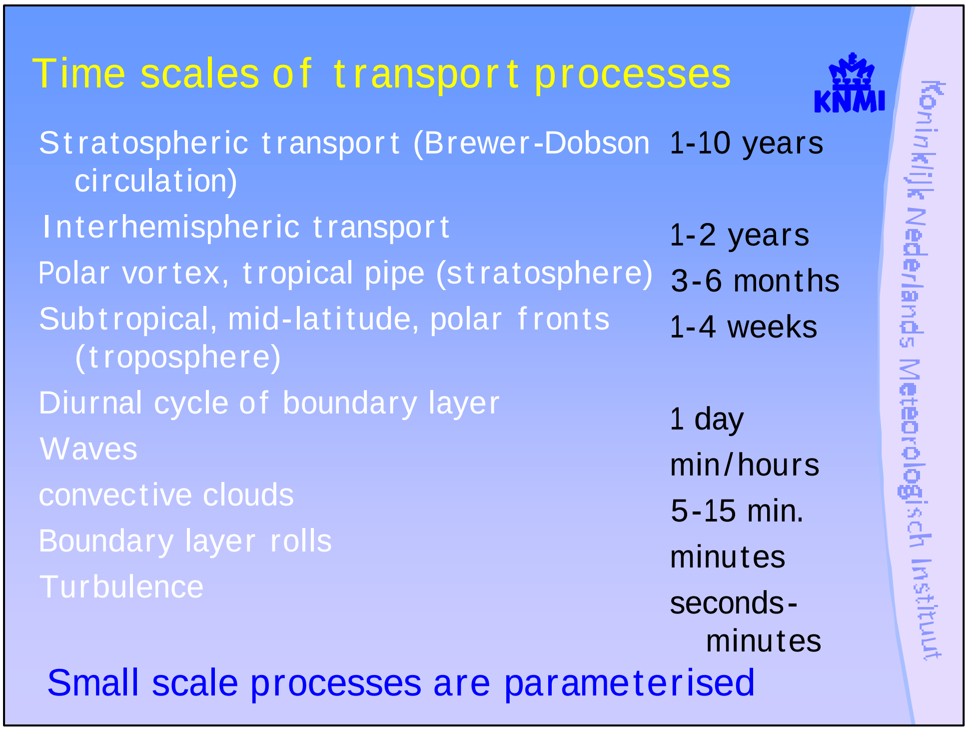

## Time scales of transport processes

| | |
|---|---|
| Stratospheric transport (Brewer-Dobson circulation) | 1-10 years |
| Interhemispheric transport | 1-2 years |
| Polar vortex, tropical pipe (stratosphere) | 3-6 months |
| Subtropical, mid-latitude, polar fronts (troposphere) | 1-4 weeks |
| Diurnal cycle of boundary layer | 1 day |
| Waves | min/hours |
| convective clouds | 5-15 min. |
| Boundary layer rolls | minutes |
| Turbulence | seconds-minutes |

Small scale processes are parameterised

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## Lifetimes of reactive chemical compounds

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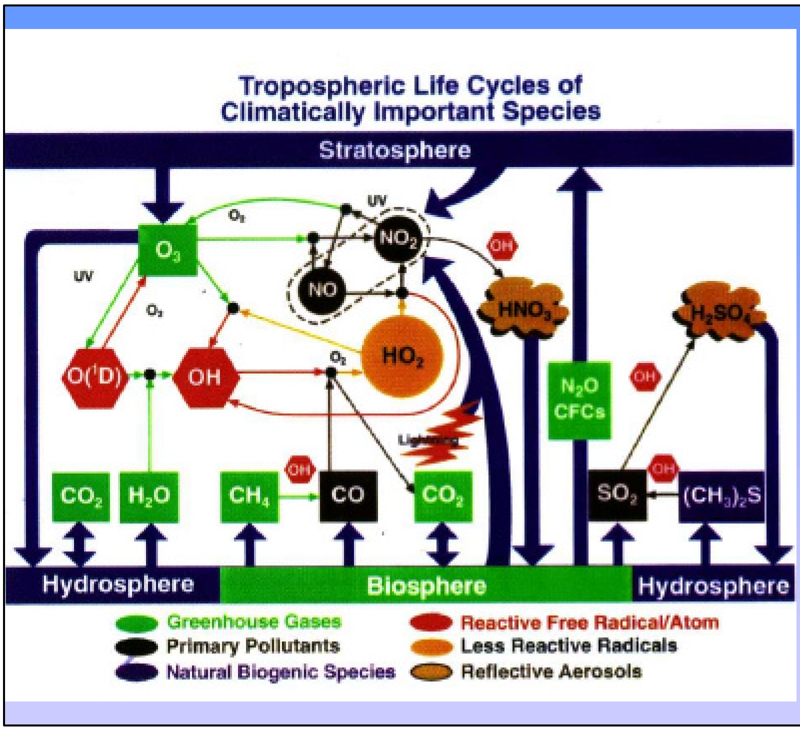
| | |
|---|---|
| $CH_4$ | 5-8 years |
| $O_3$ | weeks (troposphere)-months (stratosphere) |
| CO | 2-4 weeks |
| Stable hydrocarbons (e.g PAN) | days-weeks |
| Short-lived hydrocarbons | minutes-hours |
| $NO_x$ ($NO+NO_2$) | 2 (boundary layer)-20 days (lowermost stratosphere) |
| NO, $NO_2$ | 5-15 minutes |
| OH | milliseconds |

Short-lived compounds are assumed to be in quasi-steady state: family concept



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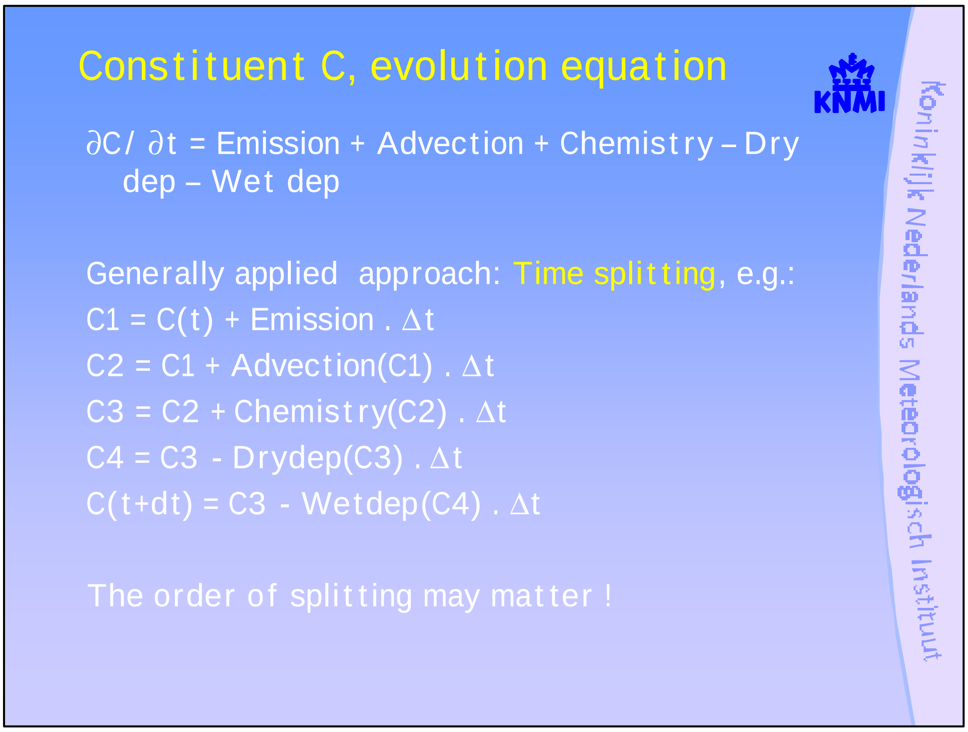

## Constituent C, evolution equation

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$\partial C/\partial t$ = Emission + Advection + Chemistry – Dry dep – Wet dep

Generally applied approach: Time splitting, e.g.:

$C1 = C(t) + \text{Emission} \,.\, \Delta t$

$C2 = C1 + \text{Advection}(C1) \,.\, \Delta t$

$C3 = C2 + \text{Chemistry}(C2) \,.\, \Delta t$

$C4 = C3 - \text{Drydep}(C3) \,.\, \Delta t$

$C(t+dt) = C3 - \text{Wetdep}(C4) \,.\, \Delta t$

The order of splitting may matter !

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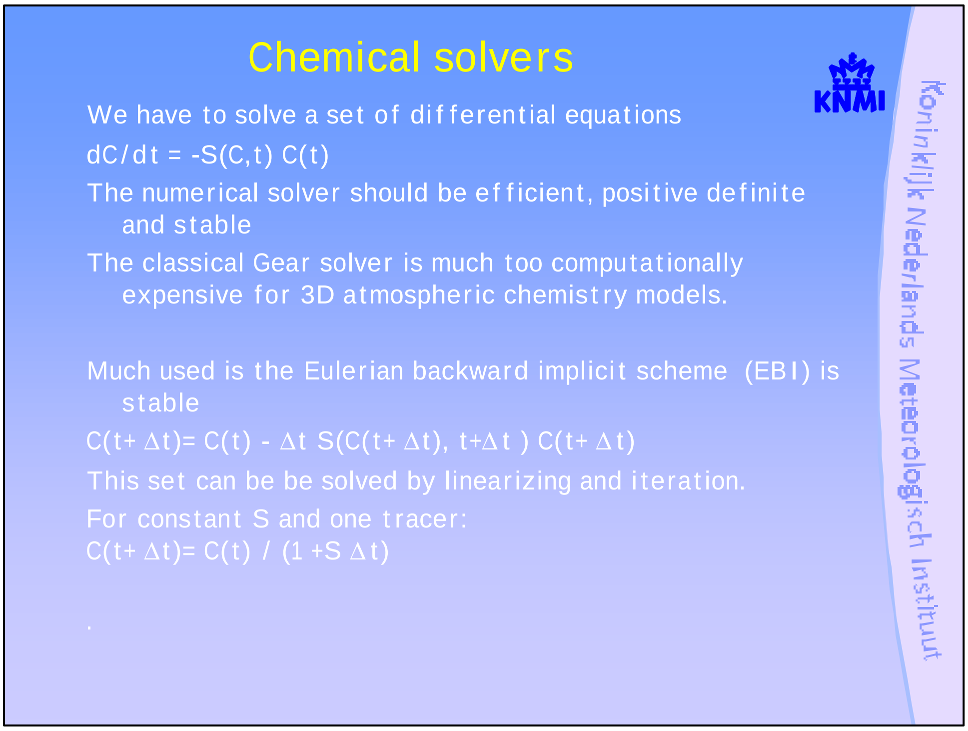

## Chemical solvers

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We have to solve a set of differential equations

$dC/dt = -S(C,t)\, C(t)$

The numerical solver should be efficient, positive definite and stable

The classical Gear solver is much too computationally expensive for 3D atmospheric chemistry models.

Much used is the Eulerian backward implicit scheme (EBI) is stable

$C(t+\Delta t) = C(t) - \Delta t\, S(C(t+\Delta t), t+\Delta t)\, C(t+\Delta t)$

This set can be be solved by linearizing and iteration.

For constant S and one tracer:

$C(t+\Delta t) = C(t) / (1 + S\,\Delta t)$

.

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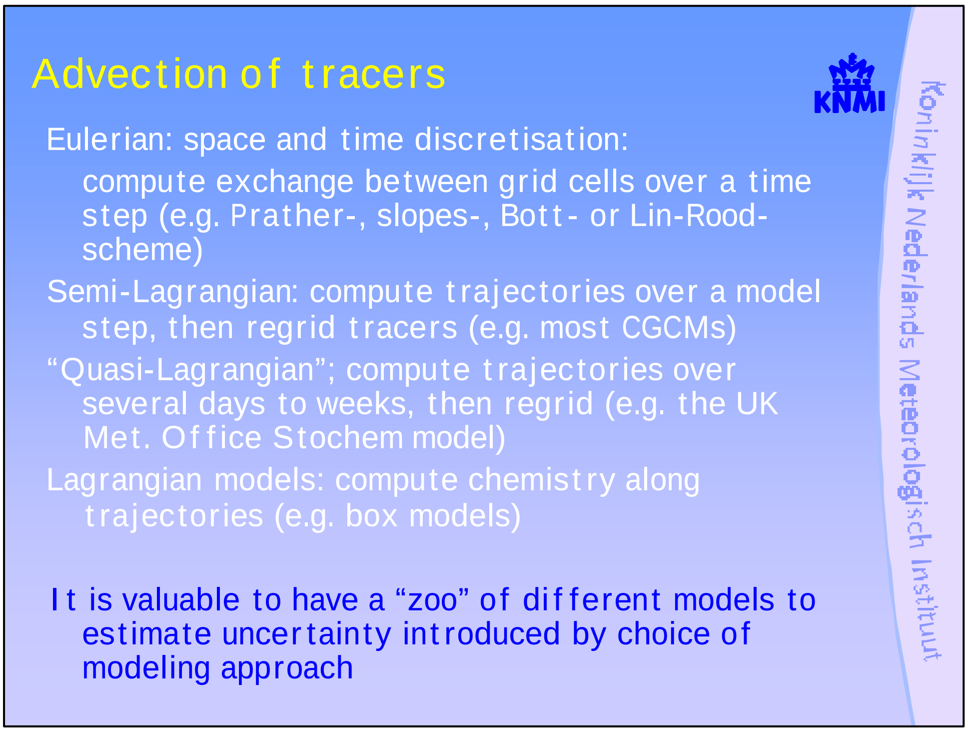


## Advection of tracers

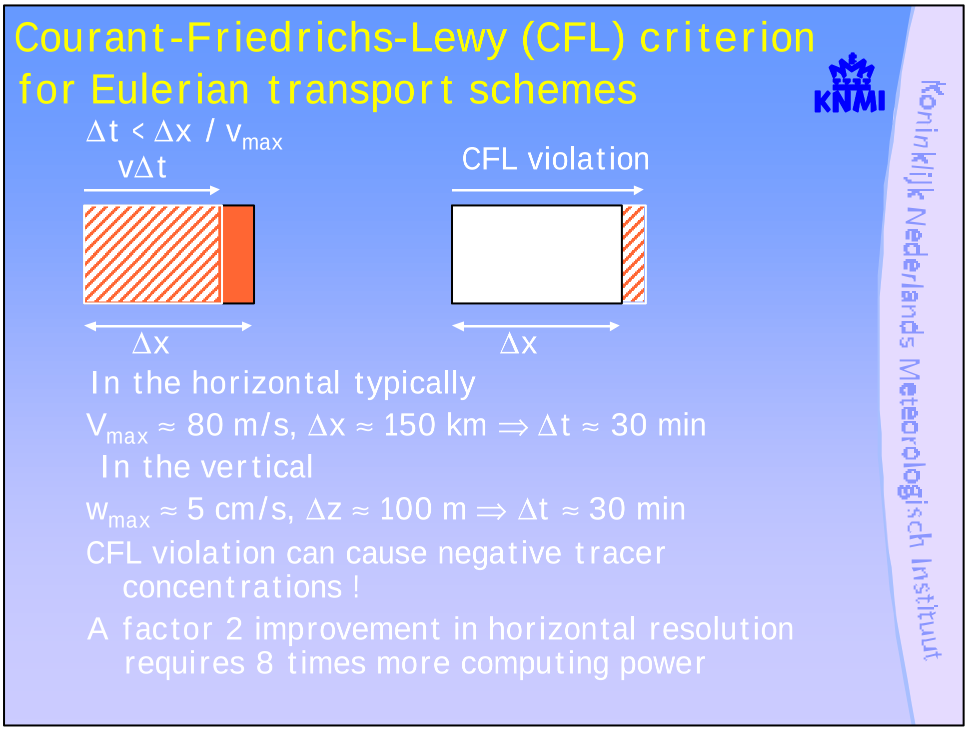
Eulerian: space and time discretisation:
- compute exchange between grid cells over a time step (e.g. Prather-, slopes-, Bott- or Lin-Rood-scheme)

Semi-Lagrangian: compute trajectories over a model step, then regrid tracers (e.g. most CGCMs)

“Quasi-Lagrangian”; compute trajectories over several days to weeks, then regrid (e.g. the UK Met. Office Stochem model)

Lagrangian models: compute chemistry along trajectories (e.g. box models)

It is valuable to have a “zoo” of different models to estimate uncertainty introduced by choice of modeling approach



## Courant-Friedrichs-Lewy (CFL) criterion for Eulerian transport schemes

$\Delta t < \Delta x / v_{max}$

In the horizontal typically

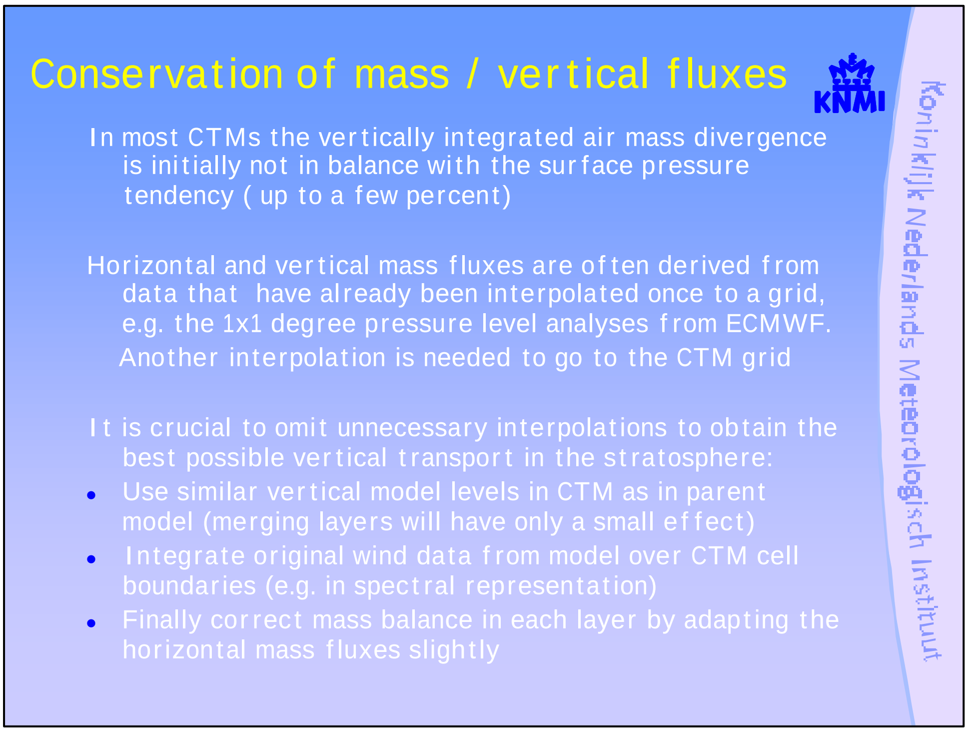
$V_{max} \approx 80$ m/s, $\Delta x \approx 150$ km $\Rightarrow \Delta t \approx 30$ min

In the vertical

$w_{max} \approx 5$ cm/s, $\Delta z \approx 100$ m $\Rightarrow \Delta t \approx 30$ min

CFL violation can cause negative tracer concentrations !

A factor 2 improvement in horizontal resolution requires 8 times more computing power



## Conservation of mass / vertical fluxes

In most CTMs the vertically integrated air mass divergence is initially not in balance with the surface pressure tendency ( up to a few percent)

Horizontal and vertical mass fluxes are often derived from data that have already been interpolated once to a grid, e.g. the 1x1 degree pressure level analyses from ECMWF. Another interpolation is needed to go to the CTM grid

It is crucial to omit unnecessary interpolations to obtain the best possible vertical transport in the stratosphere:

- Use similar vertical model levels in CTM as in parent model (merging layers will have only a small effect)
- Integrate original wind data from model over CTM cell boundaries (e.g. in spectral representation)
- Finally correct mass balance in each layer by adapting the horizontal mass fluxes slightly

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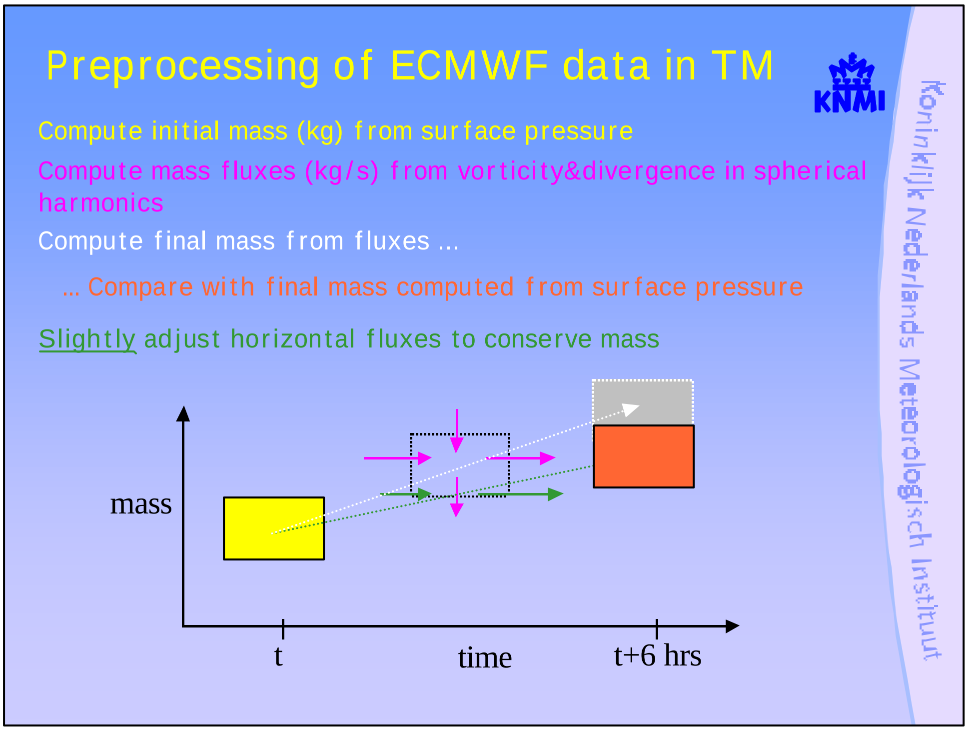

## Preprocessing of ECMWF data in TM

Compute initial mass (kg) from surface pressure

Compute mass fluxes (kg/s) from vorticity&divergence in spherical harmonics

Compute final mass from fluxes ...

... Compare with final mass computed from surface pressure

Slightly adjust horizontal fluxes to conserve mass

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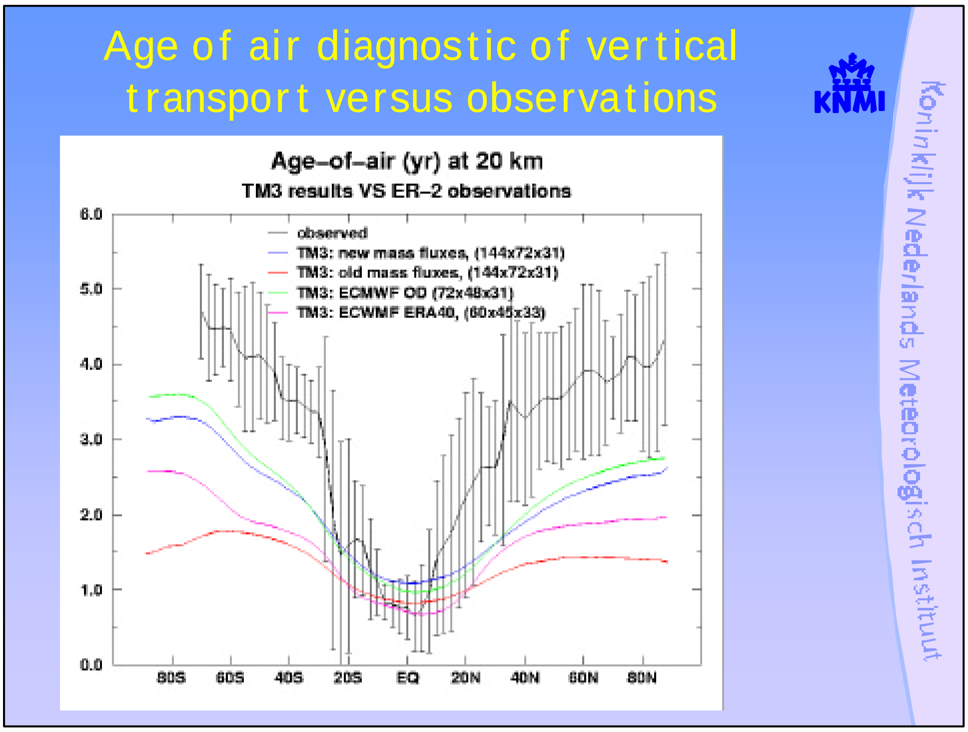
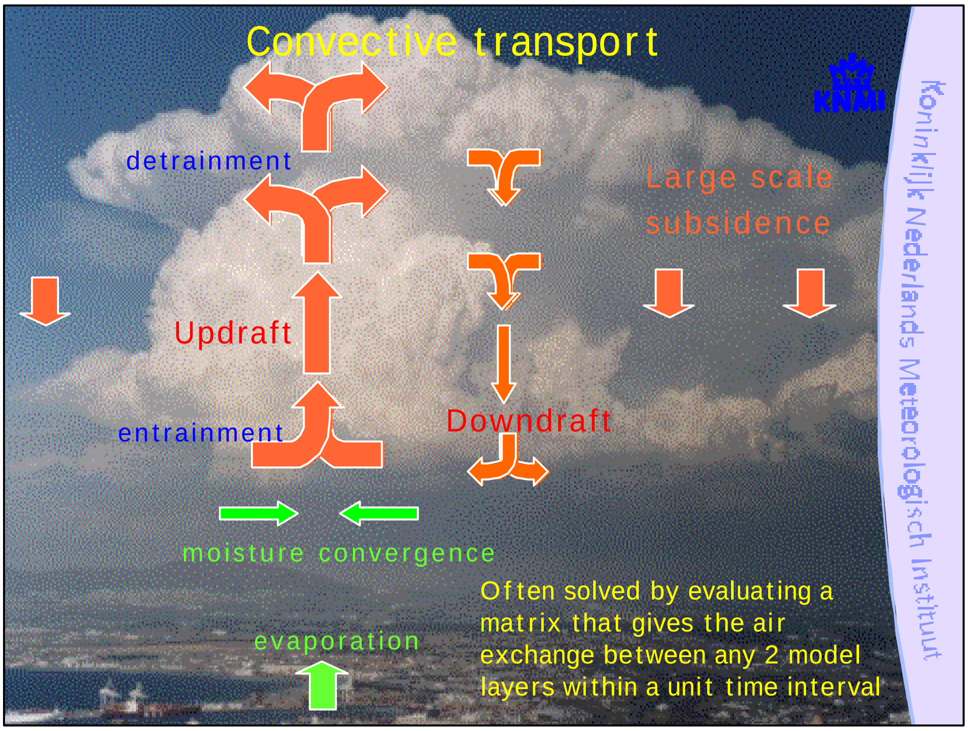
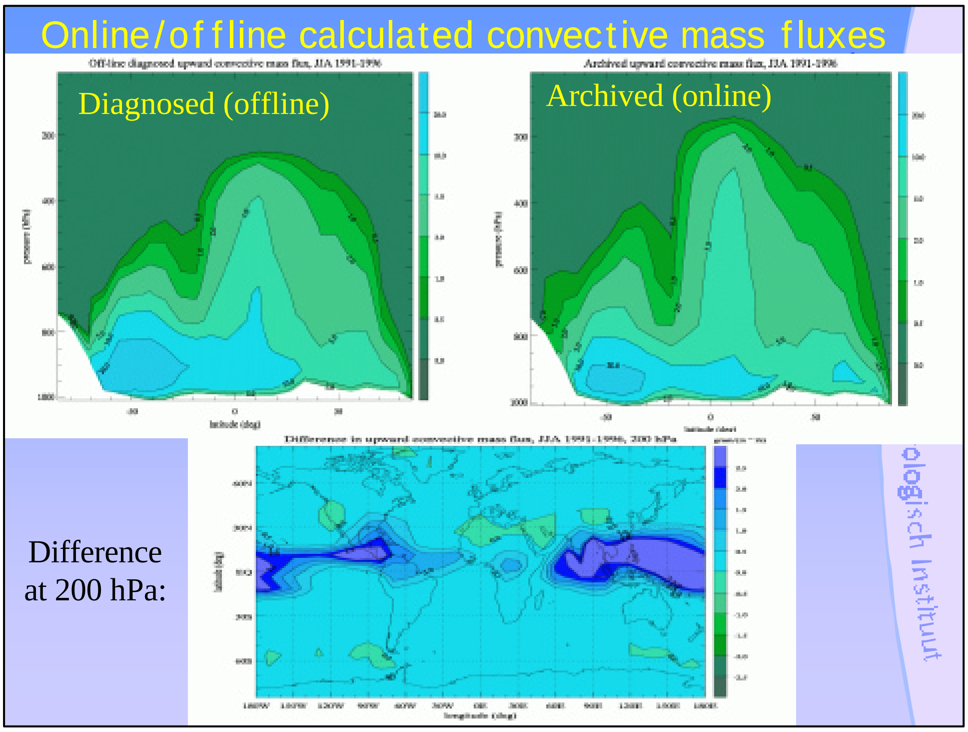


## Age of air diagnostic of vertical transport versus observations



## Convective transport

Often solved by evaluating a matrix that gives the air exchange between any 2 model layers within a unit time interval

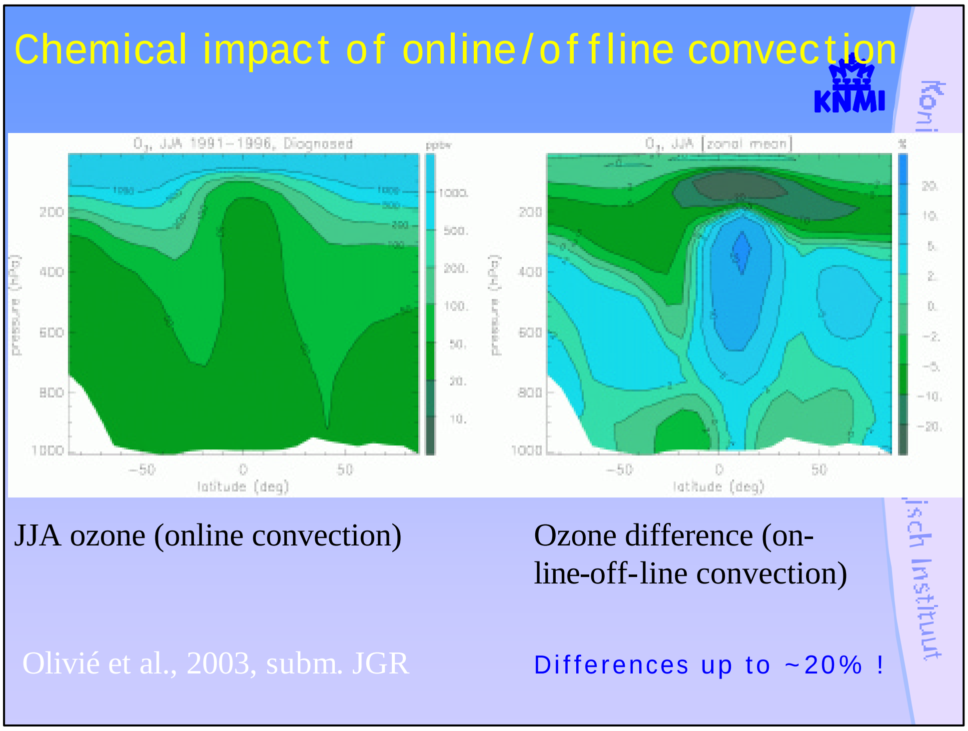


## Online/offline calculated convective mass fluxes

Diagnosed (offline)

Archived (online)

Difference at 200 hPa:



## Chemical impact of online/offline convection

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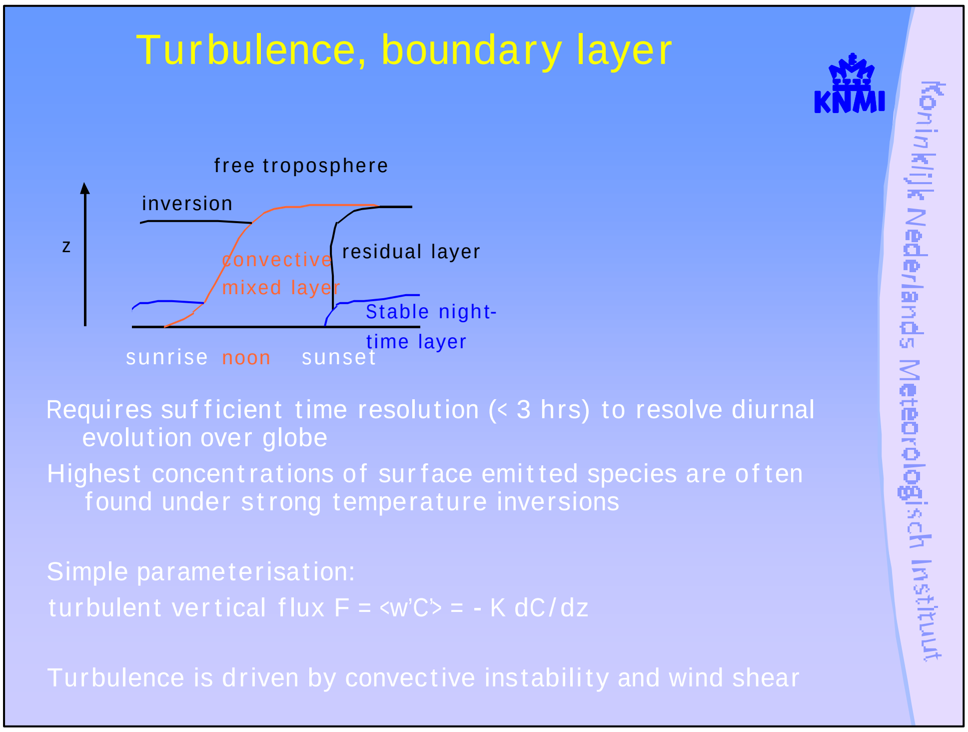
JJA ozone (online convection)

Ozone difference (on-line-off-line convection)

Olivié et al., 2003, subm. JGR

Differences up to ~20% !



## Turbulence, boundary layer

Requires sufficient time resolution (< 3 hrs) to resolve diurnal evolution over globe

Highest concentrations of surface emitted species are often found under strong temperature inversions

Simple parameterisation:

turbulent vertical flux F = <w'C'> = - K dC/dz

Turbulence is driven by convective instability and wind shear

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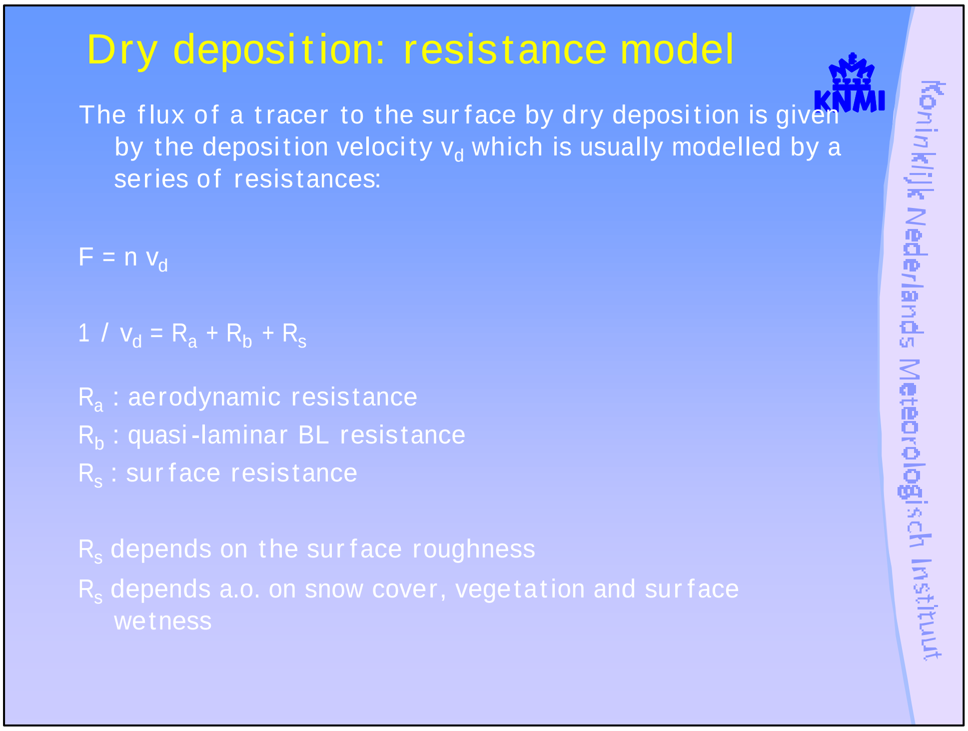

## Dry deposition: resistance model

The flux of a tracer to the surface by dry deposition is given by the deposition velocity $v_d$ which is usually modelled by a series of resistances:

$F = n\ v_d$

$1\ /\ v_d = R_a + R_b + R_s$

$R_a$ : aerodynamic resistance

$R_b$ : quasi-laminar BL resistance

$R_s$ : surface resistance

$R_s$ depends on the surface roughness

$R_s$ depends a.o. on snow cover, vegetation and surface wetness

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## Atmospheric chemistry is still observation limited

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Techniques for validation with observations:

- Nudging = relaxation towards meteorological analyses from the major weather forecast centres
- Nesting grids of different spatial resolution: zooming into the region where observations are made
- Chemical data assimilation: objective determination of model+observation errors
- Inverse modelling of observations and emissions
- Chemical re-analysis: Use meteorological re-analyses to check if historical trends are reproduced

## Inverse modelling example

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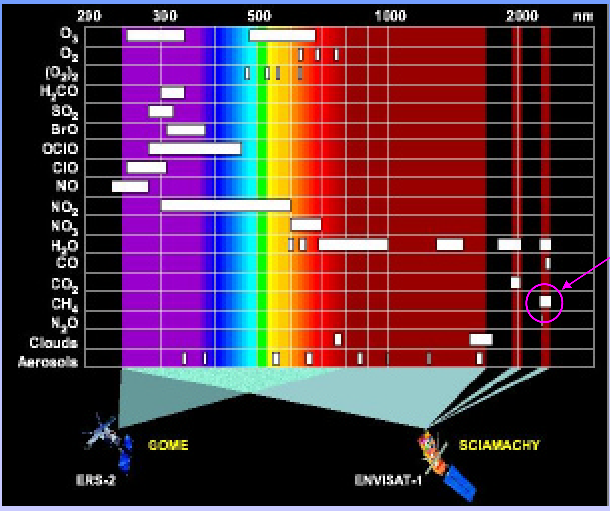
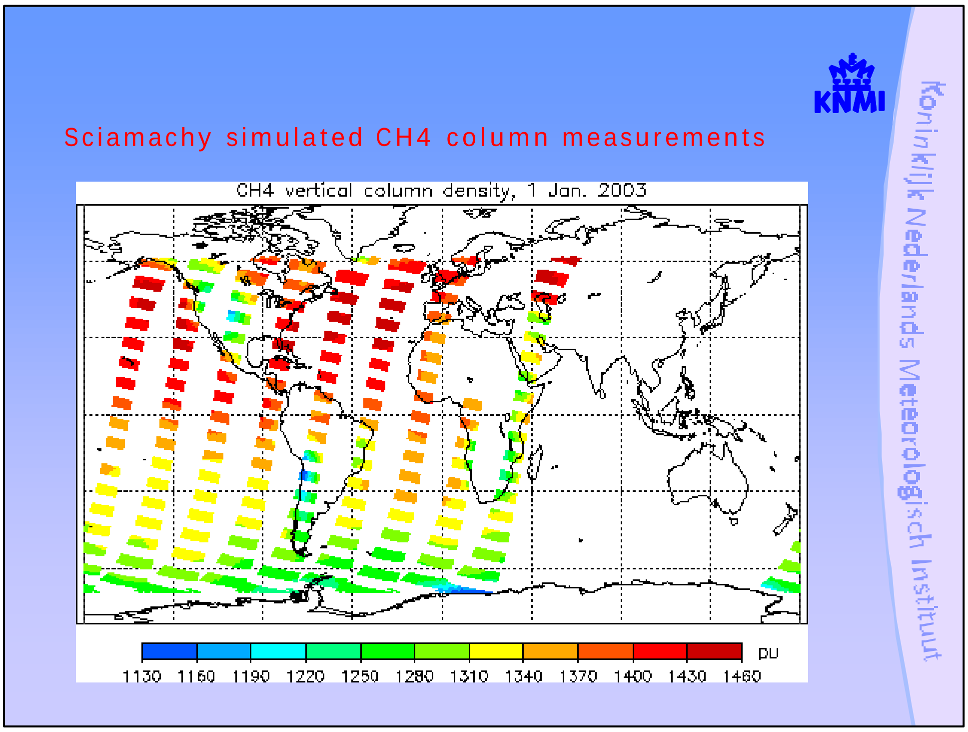
Sciamachy
methane



$CH_4$



## Sciamachy simulated CH4 column measurements

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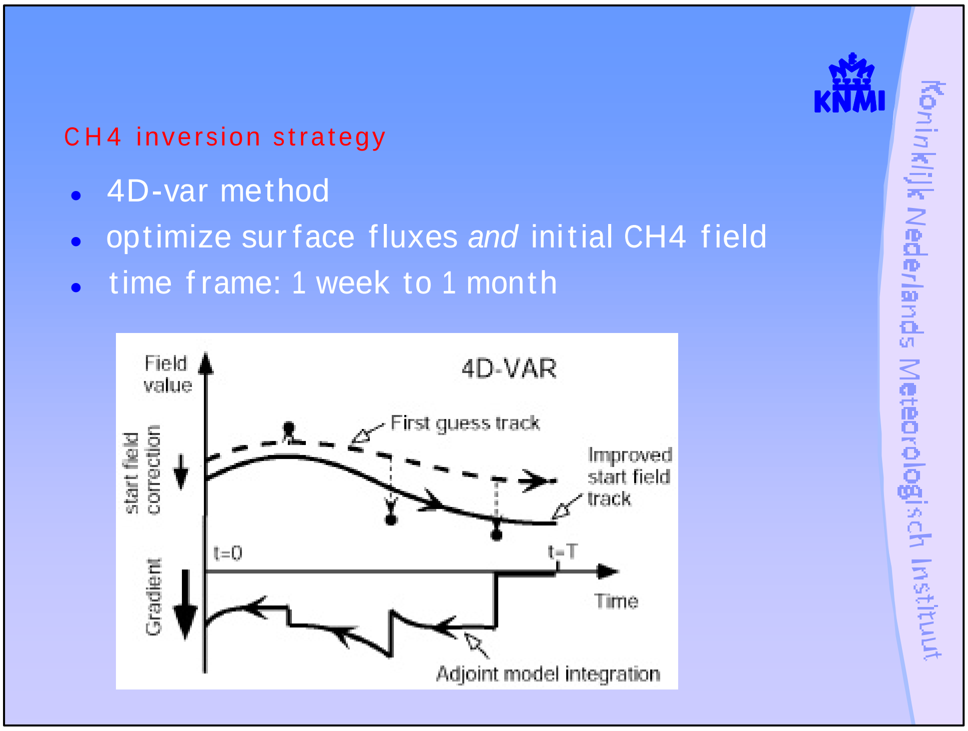

## CH4 inversion strategy

- 4D-var method
- optimize surface fluxes *and* initial CH4 field
- time frame: 1 week to 1 month

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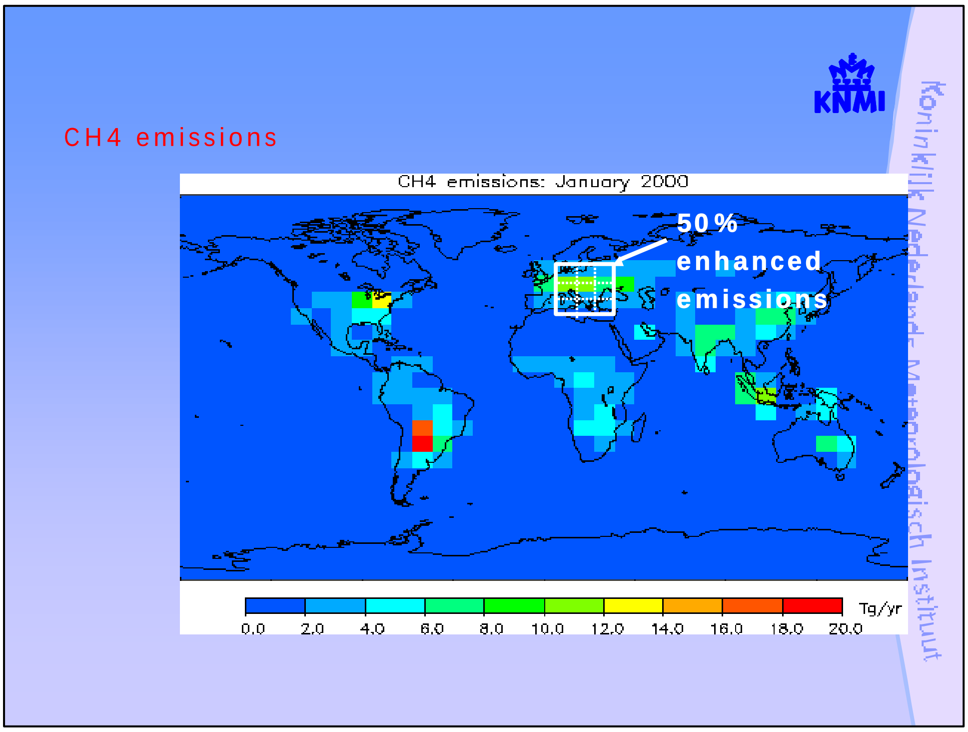

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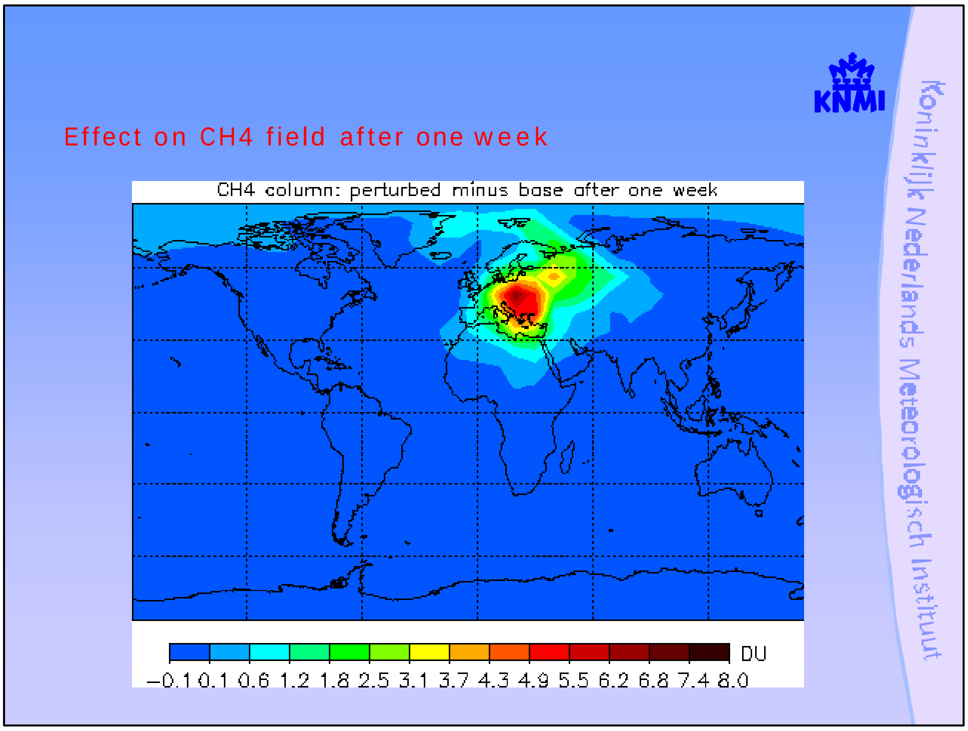
CH4 emissions



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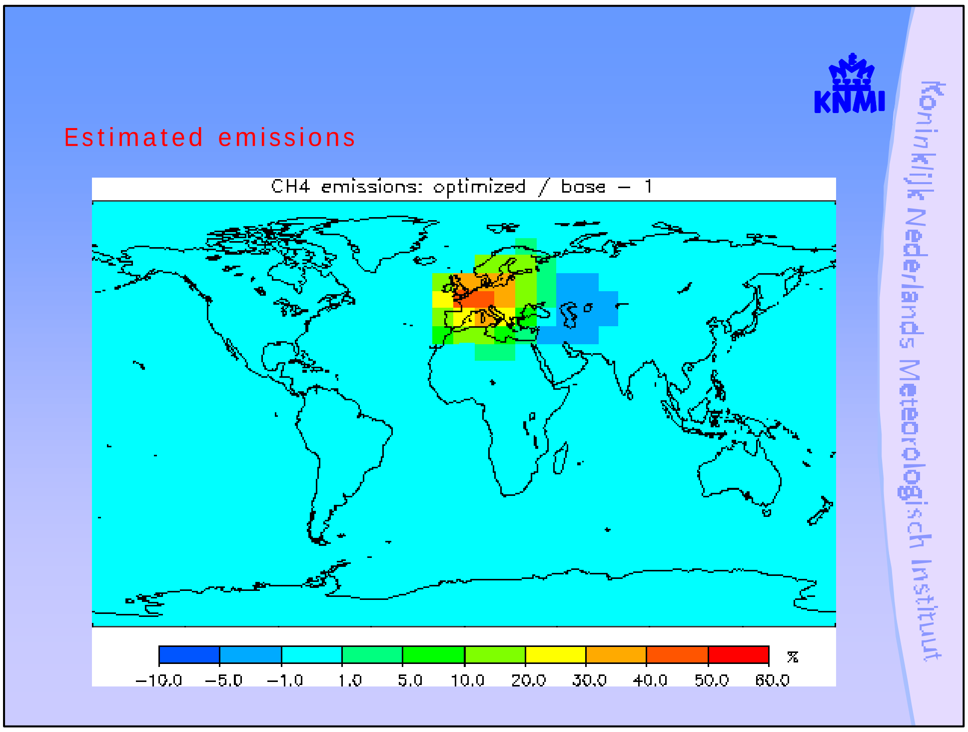
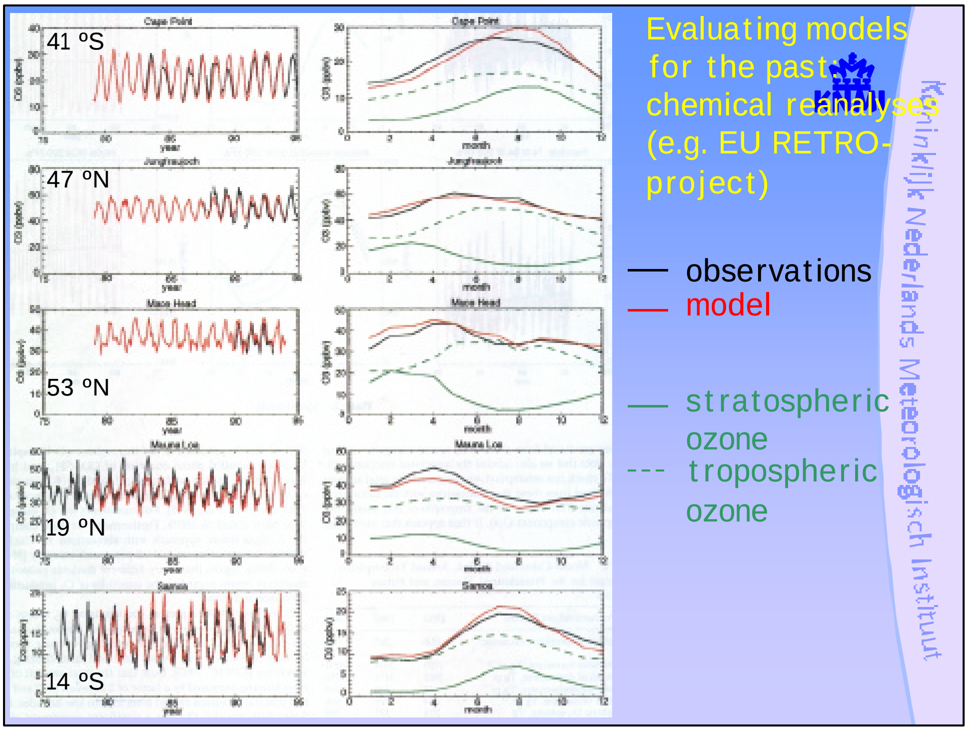
Effect on CH4 field after one week



Estimated emissions



Evaluating models for the past: chemical reanalyses (e.g. EU RETRO-project)

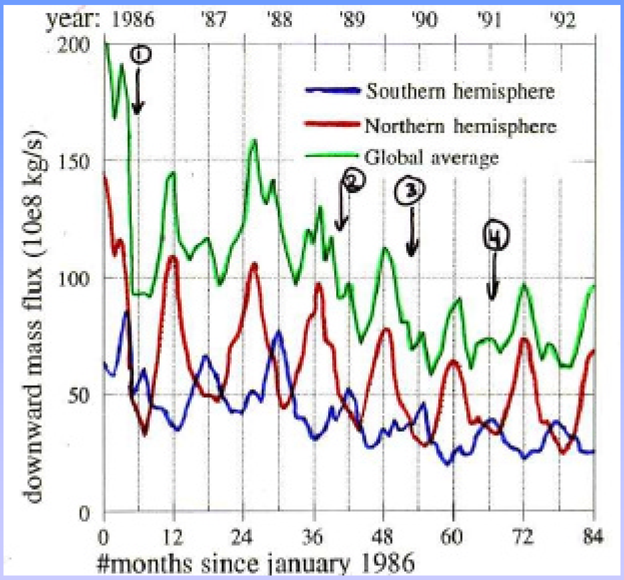
— observations

— model

— stratospheric ozone

--- tropospheric ozone

## Why use meteorological re-analyses?



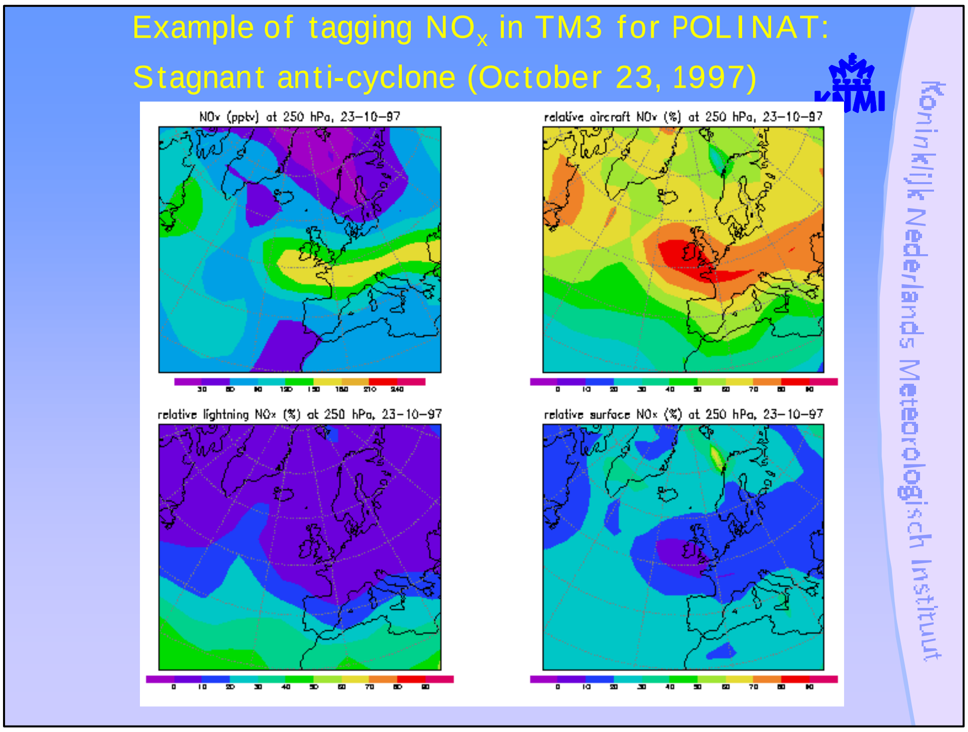
1,2,3,4
model changes

*Van Velthoven & Kelder, JGR (1996)*

## Tagging of constituent changes

Administrate changes in constituents due to a certain emission e.g. from $NO_x$ from aviation:

Attribute constituent changes to emissions from a certain sector or geographical region



Example of tagging $NO_x$ in TM3 for POLINAT: Stagnant anti-cyclone (October 23, 1997)

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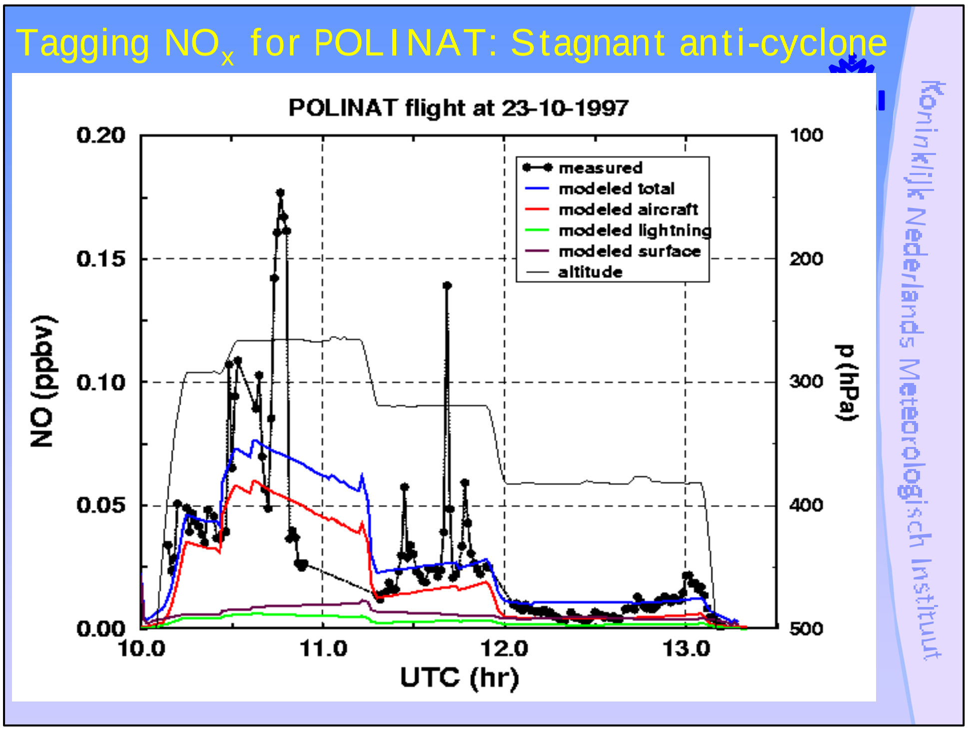

Tagging $NO_x$ for POLINAT: Stagnant anti-cyclone

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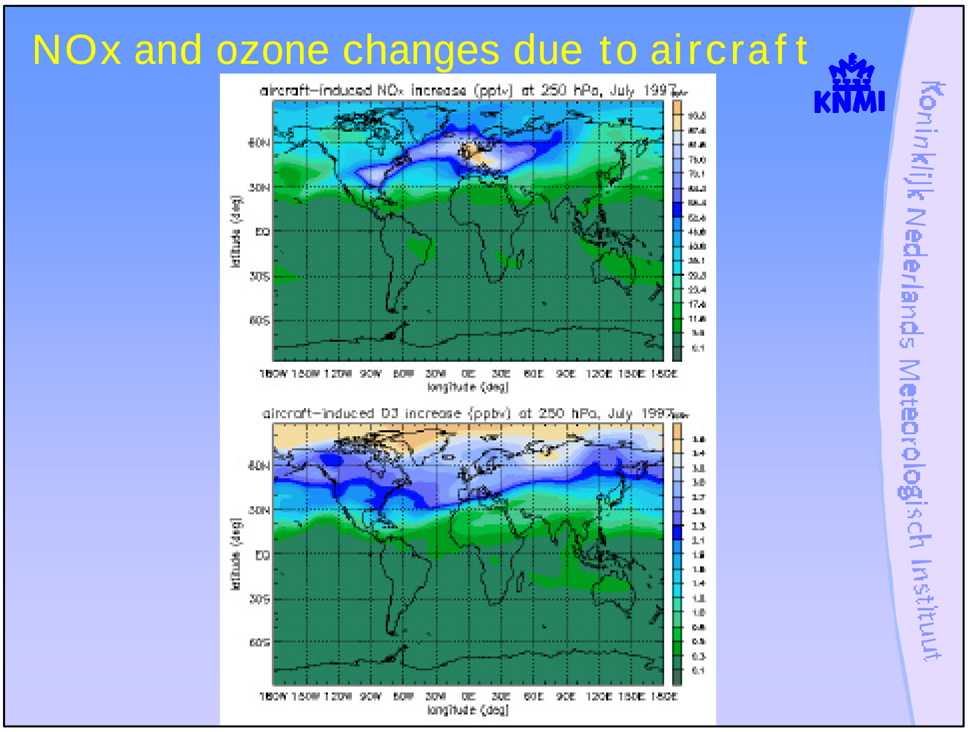

## NOx and ozone changes due to aircraft

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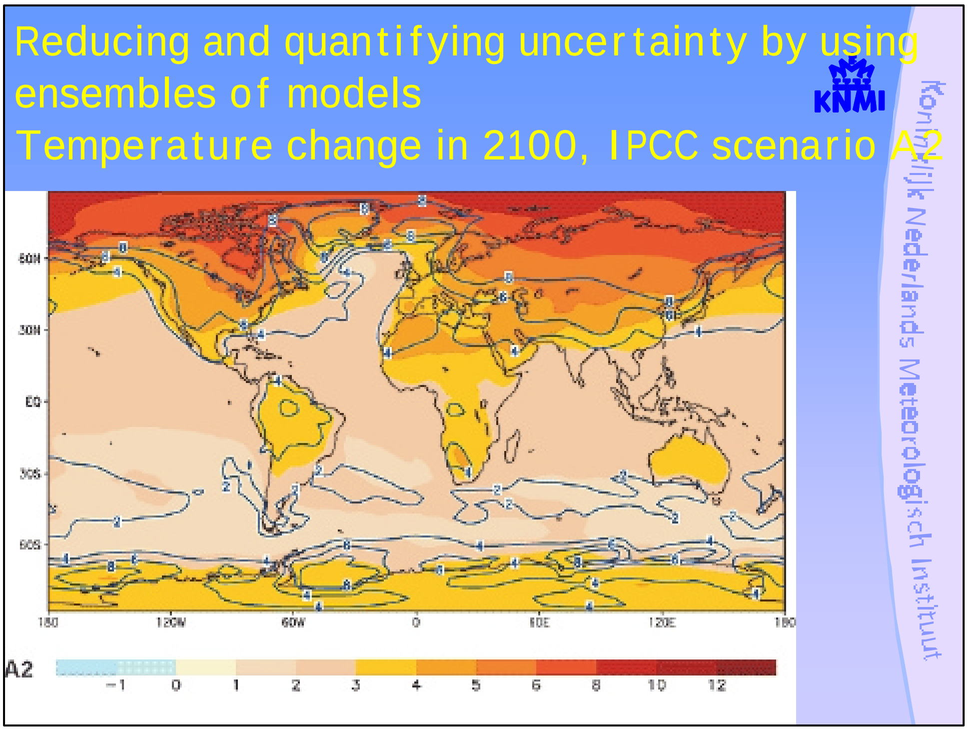

## Reducing and quantifying uncertainty by using ensembles of models
## Temperature change in 2100, IPCC scenario A2

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## Future climate change: Multiple models en scenarios

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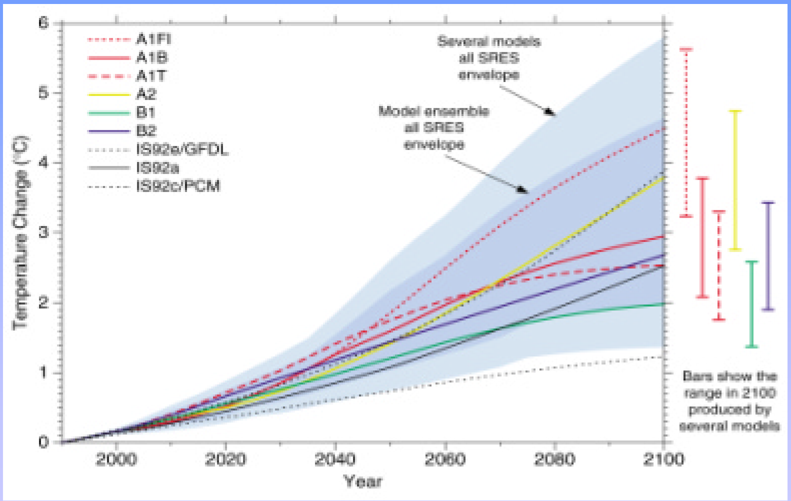

## Outlook

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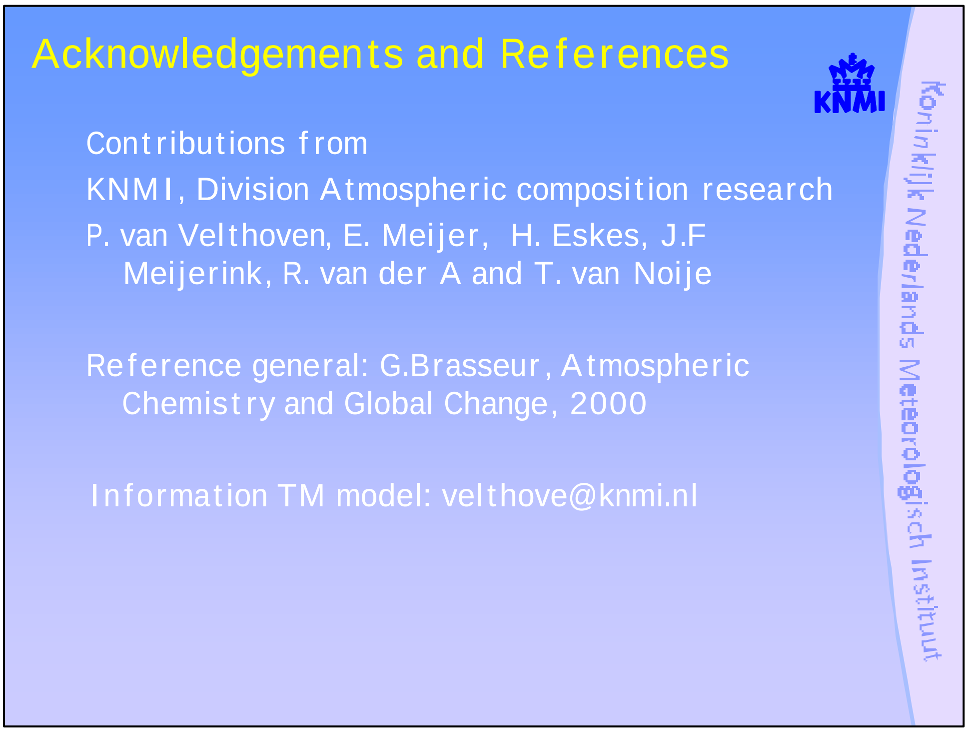
- Chemistry transport models useful for a comprehensive description of influence of chemistry and transport on atmospheric composition

Developments:

- Grid nesting to zoom into regions of interest
- Higher vertical and horizontal resolutions
- Models of troposphere and stratosphere
- Inclusion of sophisticated aerosol cycles
- Chemical data assimilation and forecasting
- Model evalution by comparison with observations, global satellite data sets are important



## Acknowledgements and References

Contributions from

KNMI, Division Atmospheric composition research

P. van Velthoven, E. Meijer, H. Eskes, J.F Meijerink, R. van der A and T. van Noije

Reference general: G.Brasseur, Atmospheric Chemistry and Global Change, 2000

Information TM model: velthove@knmi.nl