Description of the chemical mechanism Chem-NWP in Enviro-HIRLAM. The importance of urban-aerosol-meteorology feedbacks (second indirect effect).

Allan Gross, Ulrik Korsholm, Alexander Baklanov

Danish Meteorological Institute, DMI

Research and Development Department

Lyngbyvej 100, 2100 Ø

Denmark

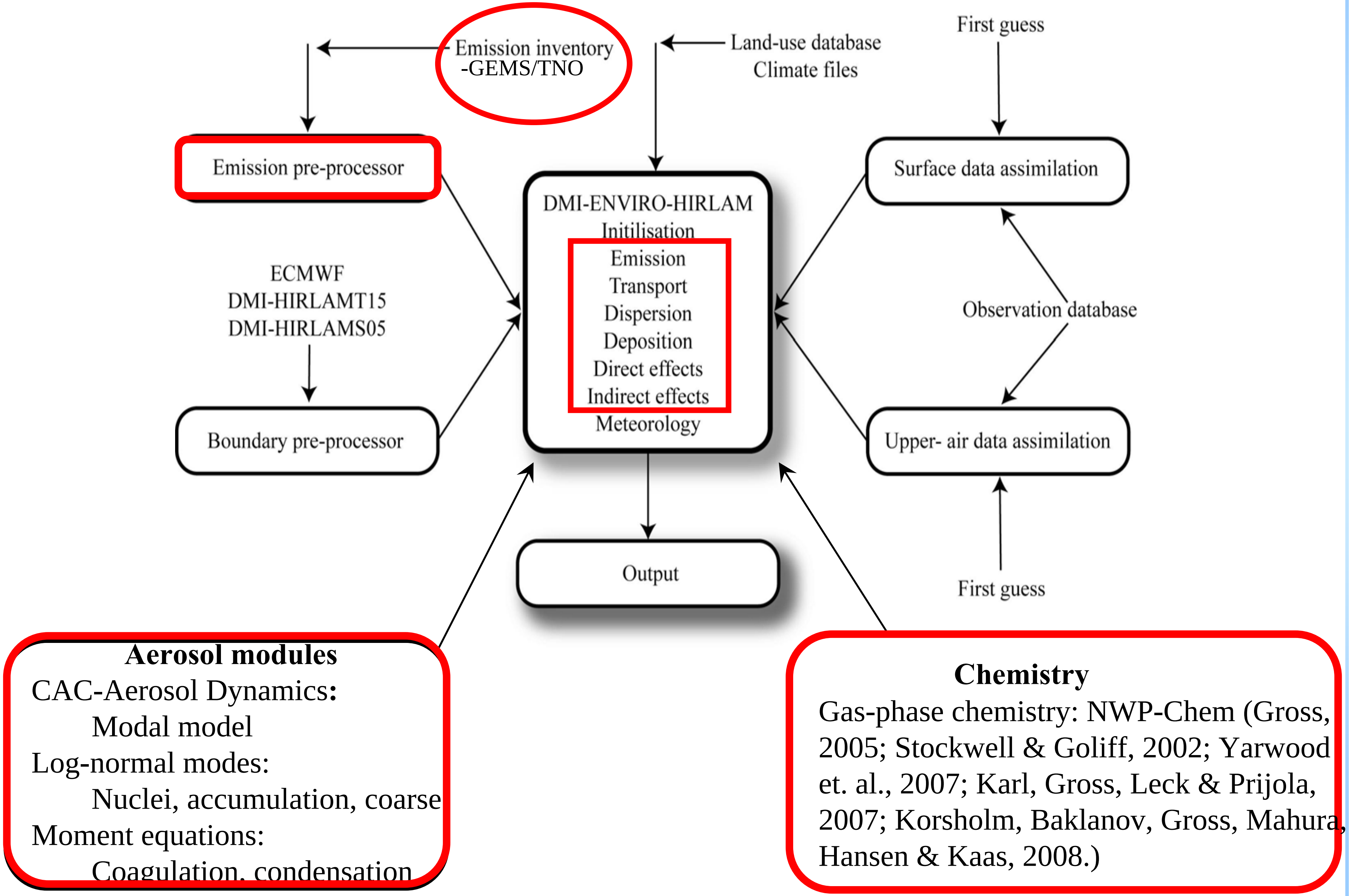
Strongest motivation for DMI to build an on-line model:

- Improve NWP forecasts.
- Improve air quality modelling and forecasts.
- Have one system for both.

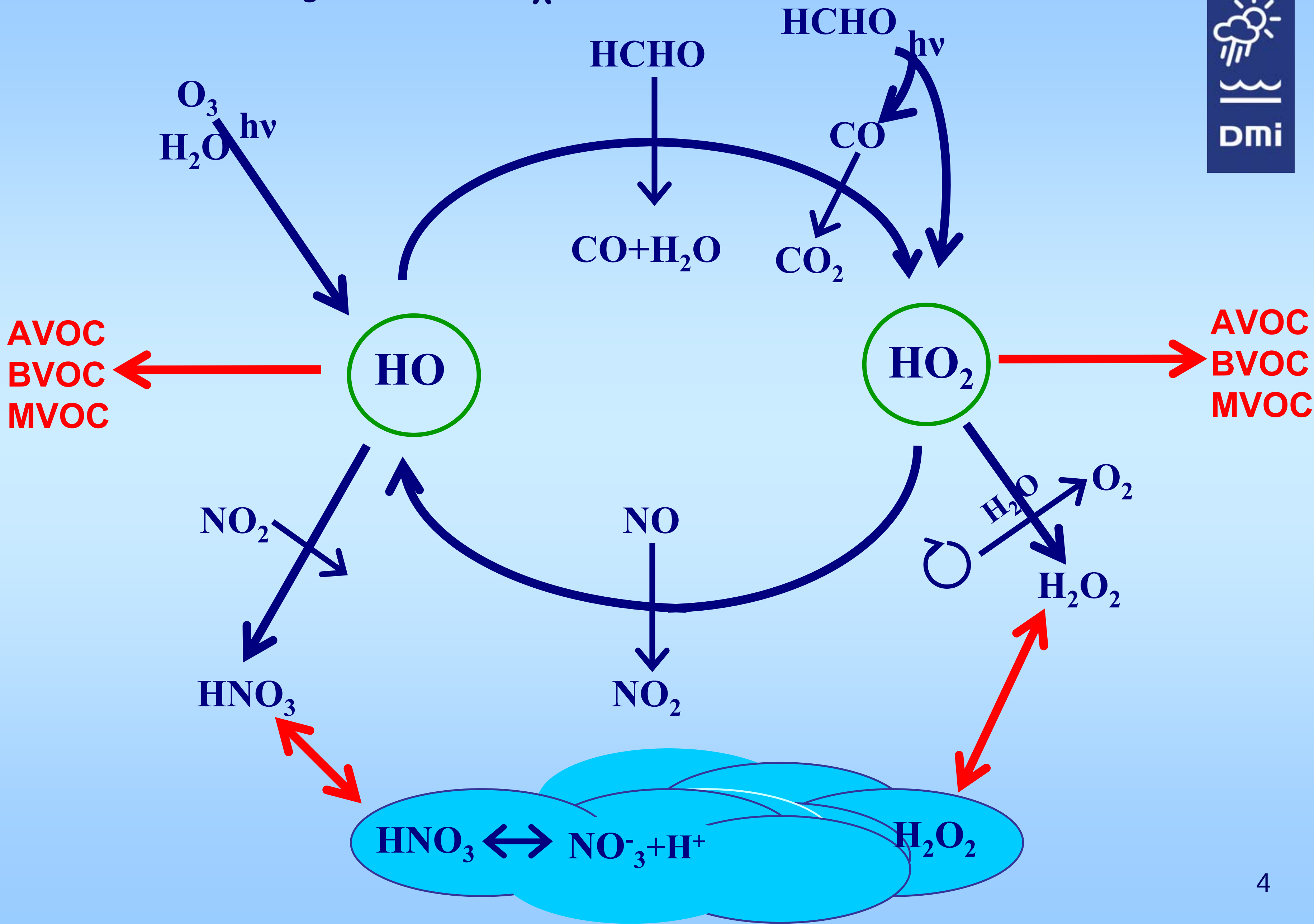
Contents

- Description of NWP-Chem in Enviro-HIRLAM.
- Aerosol dynamics in Enviro-HIRLAM.
- The second indirect effect.
- Model examples.
- Conclusion + next steps.
- The effect of air pollution on pollen.

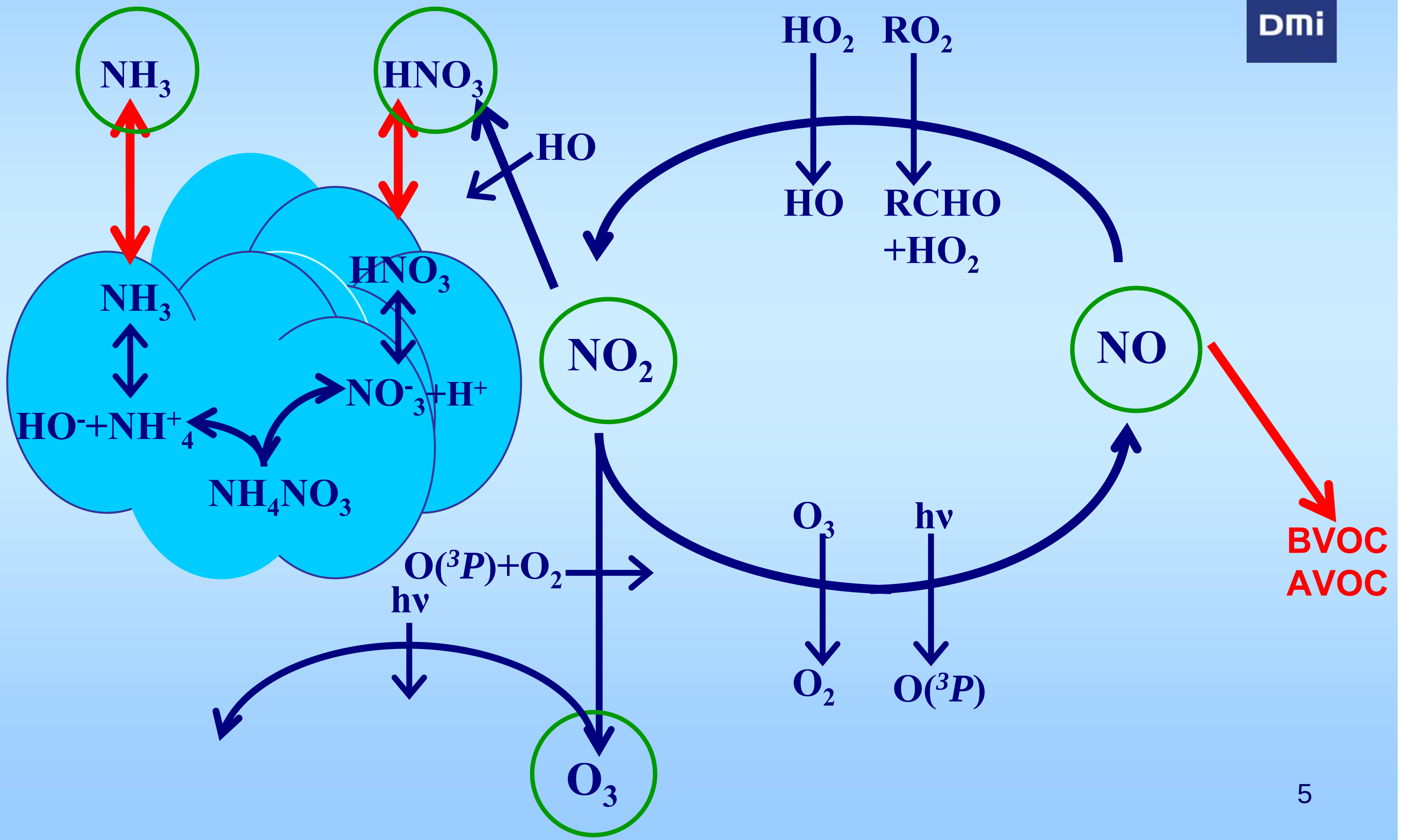
Version of Enviro-HIRLAM used in this study



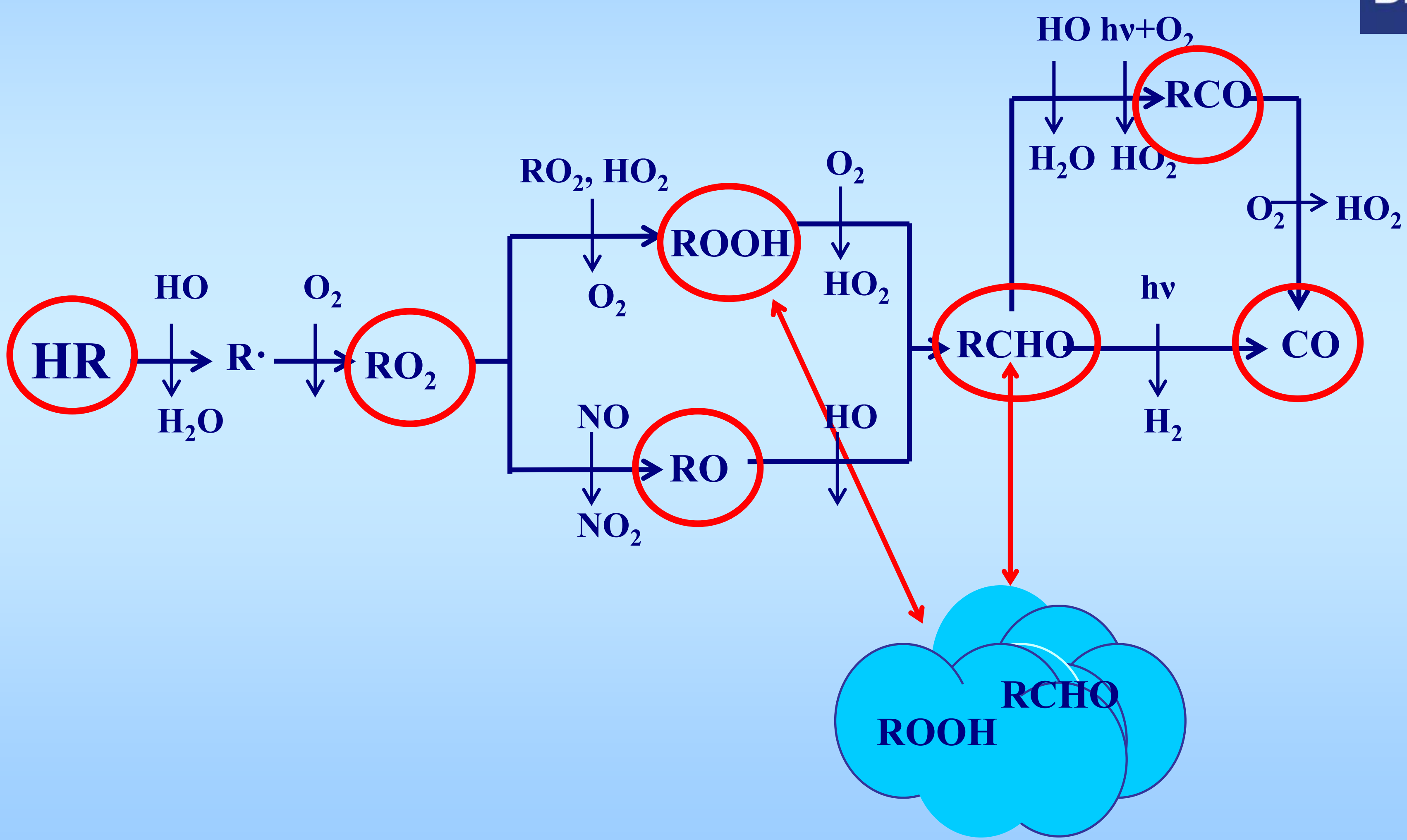
Reaction Cycle of HO_X



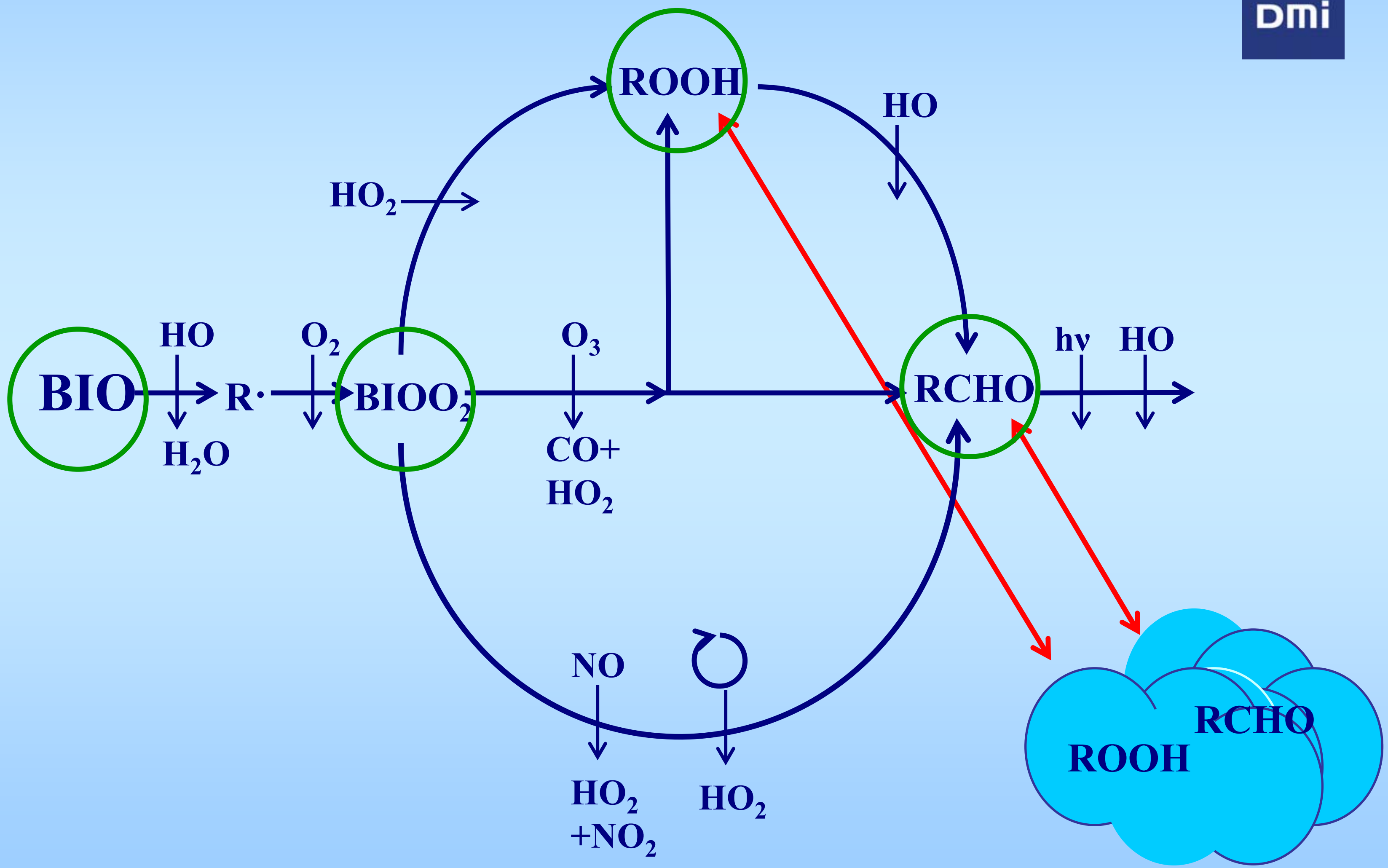
Reaction Cycle of NO_x



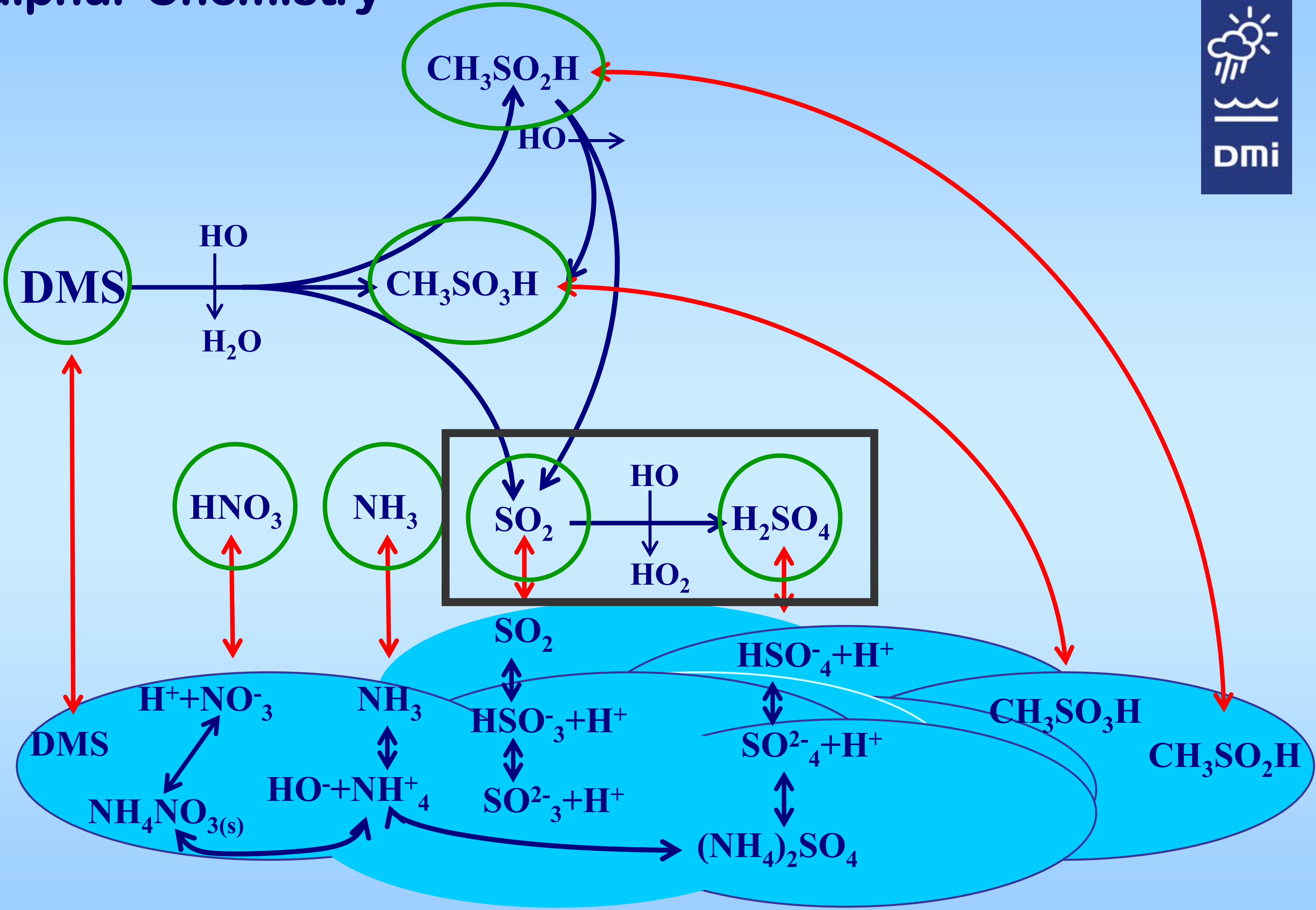
Anthropogenic VOC oxidation



Biogenic Chemistry

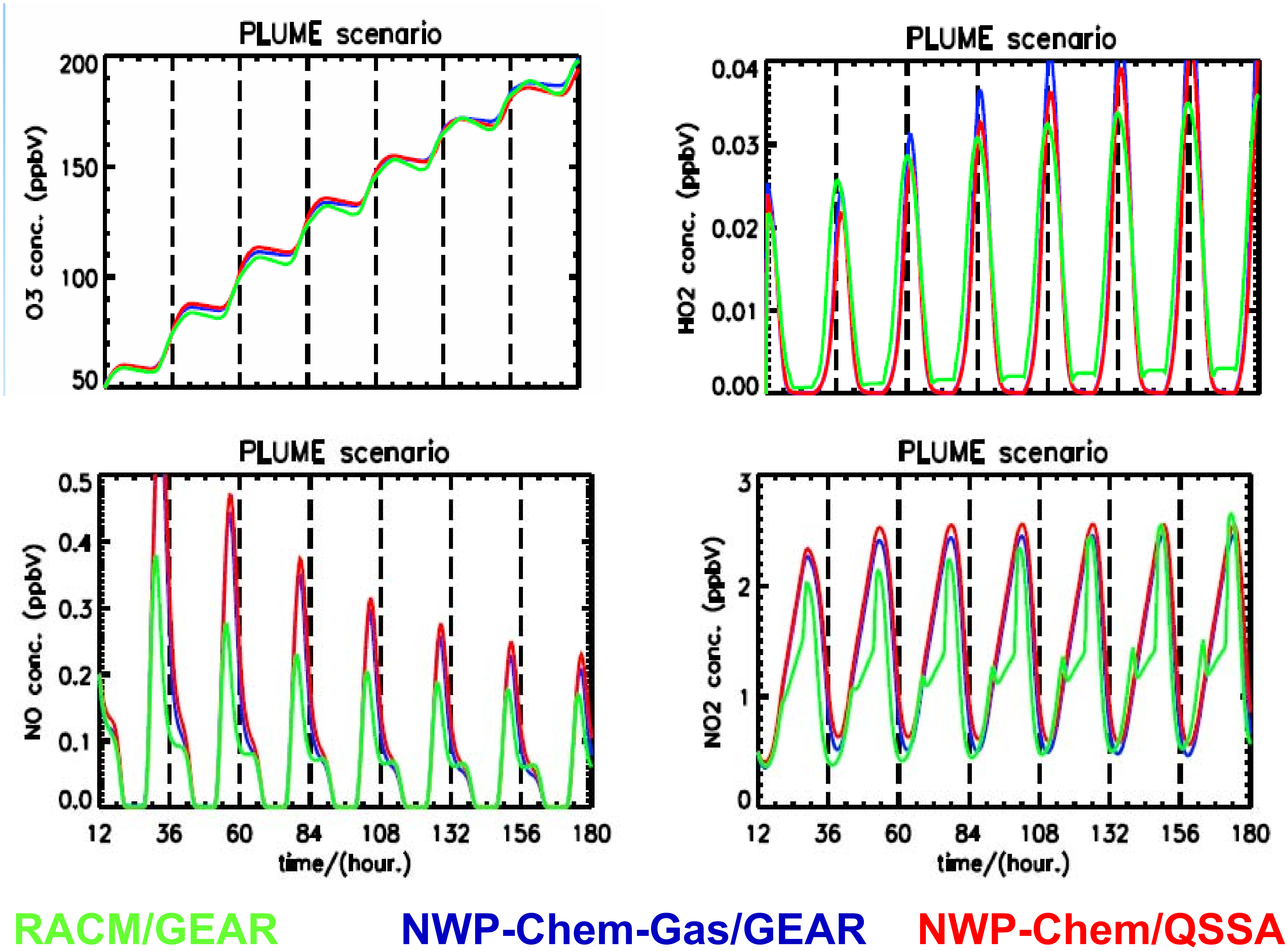


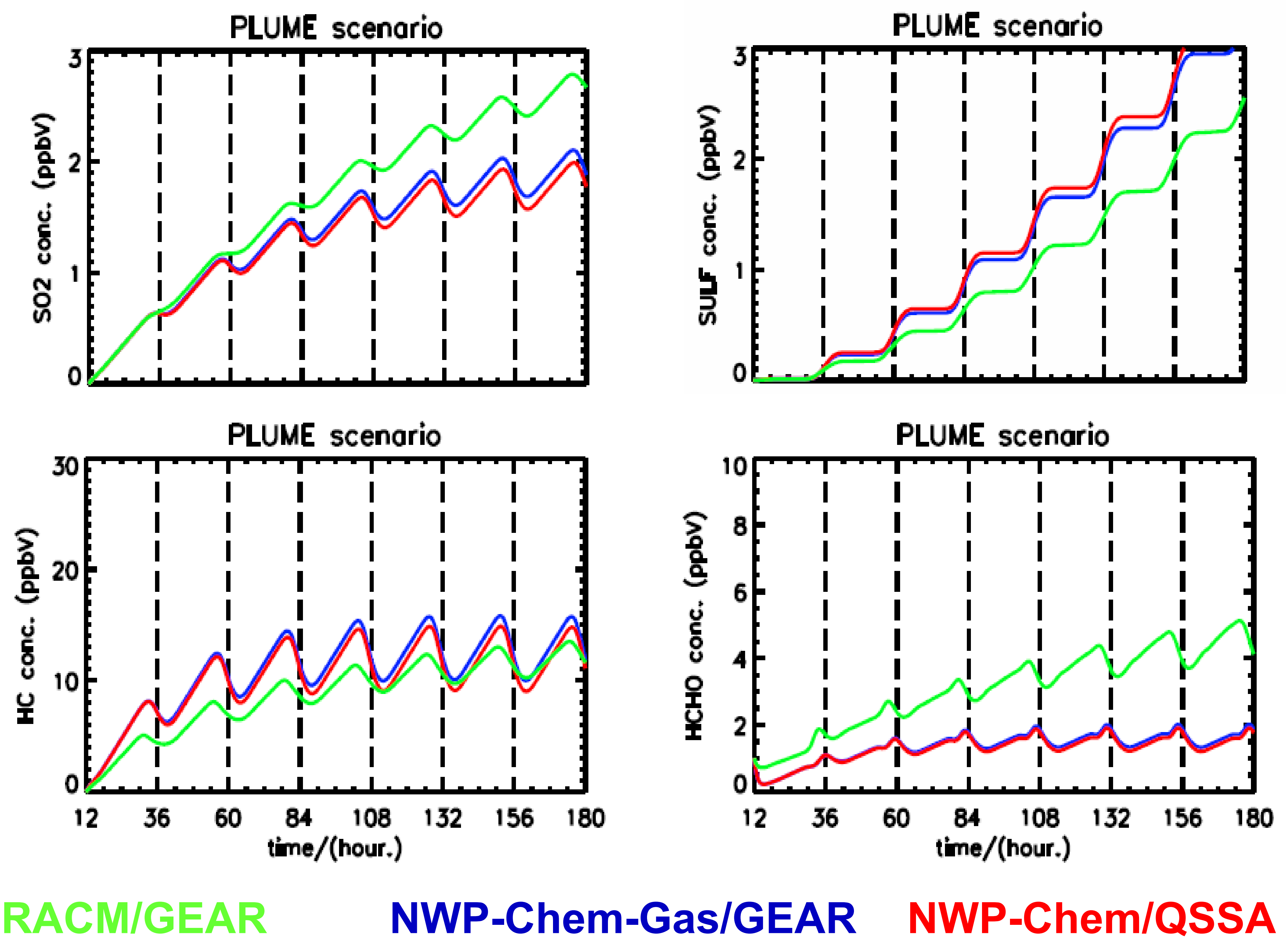
Sulphur Chemistry



Numerical solution of the chemistry

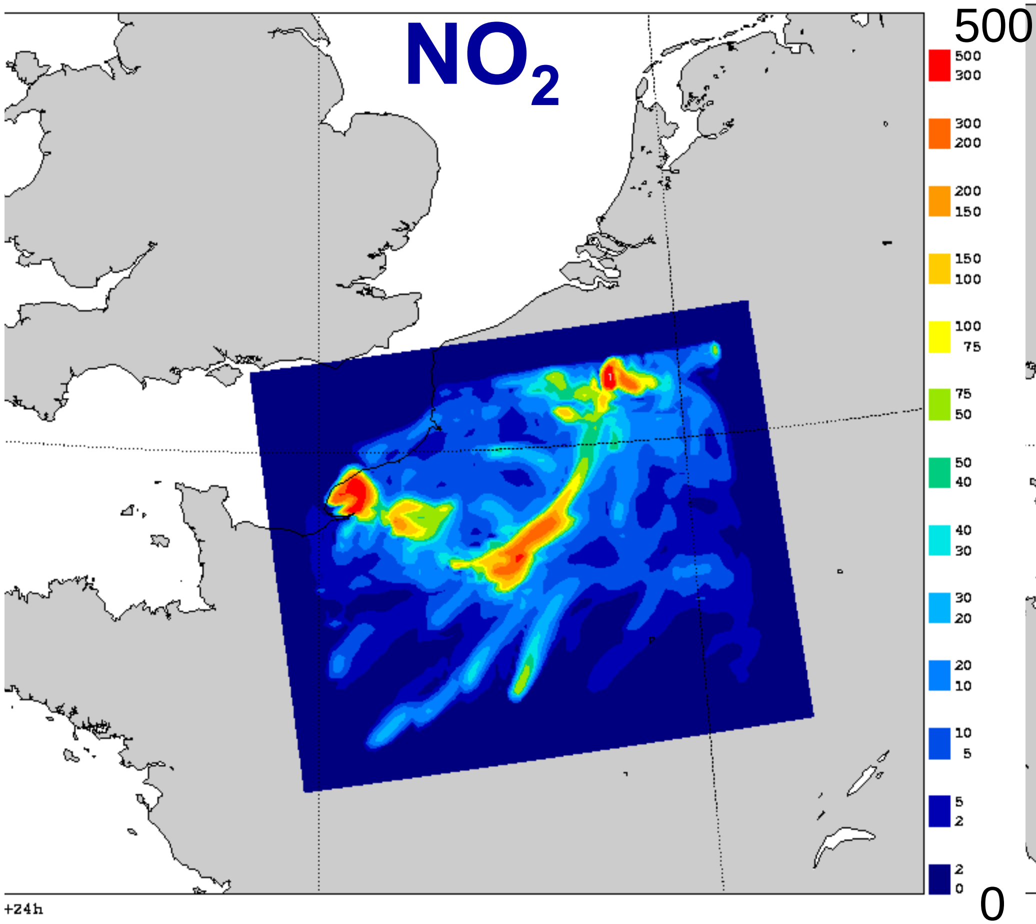
- Rates and coefficients in NWP-Chem-gas is estimated based on lumping and optimization procedures.
- Chemical reactions →QSSA.
- Equilibrium systems → Mass-Flux Iteration method.
- NWP-Chem-gas are tested against the RACM+ELCID mch. at different standard marine, rural and plume scenarios.

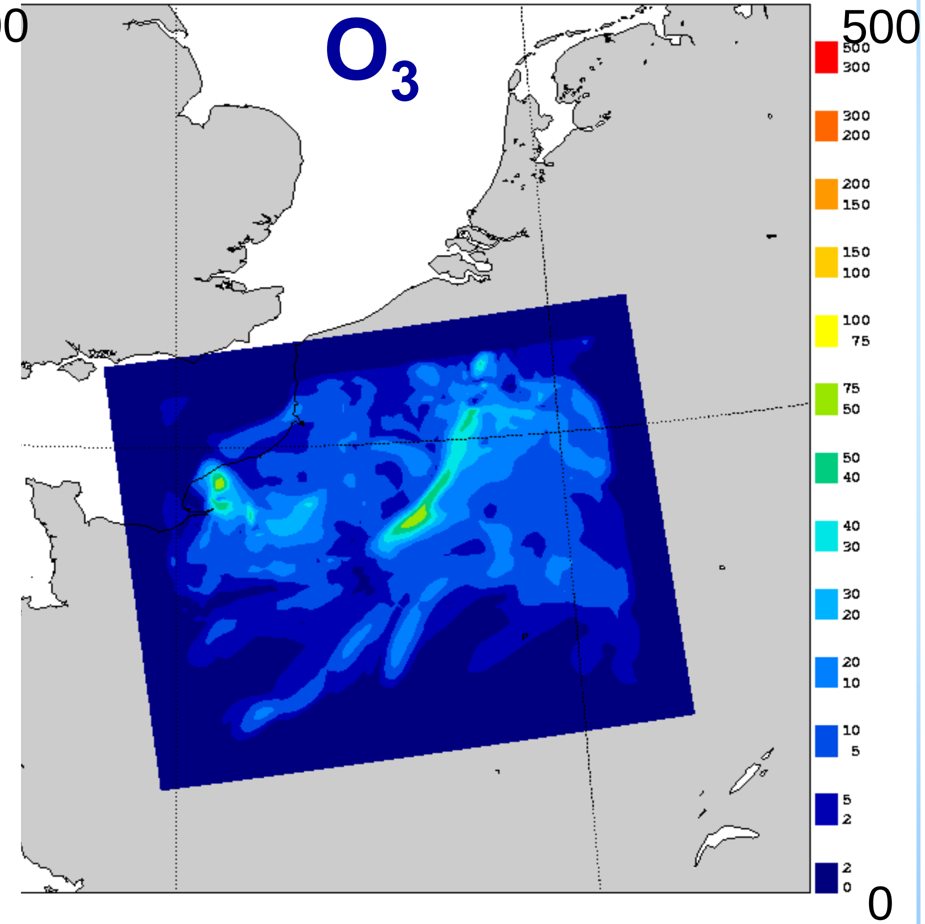

PLUME scenario
O3 conc. (ppbV)
200
150
100
50
PLUME scenario
HO2 conc. (ppbV)
0.04
0.03
0.02
0.01
0.00
PLUME scenario
NO conc. (ppbV)
0.5
0.4
0.3
0.2
0.1
0.0
12 36 60 84 108 132 156 180
time/(hour.)
PLUME scenario
NO2 conc. (ppbV)
3
2
1
0
12 36 60 84 108 132 156 180
time/(hour.)
RACM/GEAR
NWP-Chem-Gas/GEAR
NWP-Chem/QSSA



PLUME scenario
SO2 conc. (ppbV)
PLUME scenario
SULF conc. (ppbV)
PLUME scenario
HC conc. (ppbV)
time/(hour.)
PLUME scenario
HCHO conc. (ppbV)
time/(hour.)
RACM/GEAR
NWP-Chem-Gas/GEAR
NWP-Chem/QSSA

00 UTC June 29 – 00 UTC June 30, 2005.
Concentration (µg/m³)





Aerosol dynamic model in Enviro-HIRLAM
Ref. Gross and Baklanov, 2004

The aerosol dynamic model is base on the modal description of the particle distributions suggested by Whitby et al. (1997), i.e. lognormal distributions are used for particle size in each mode.

Analytical solutions are found using the suggestions by Whitby et al. (1997) and Binkowski et al. (2000). These solutions are used in the model.

The present model has three modes: nuclei, accumulation and coarse.

Aerosol dynamic model in Enviro-HIRLAM, Cont.

The following aerosol physical processes are solved

Accumulation mode (j):

- primary condensation growth, G(j),
- intramodal coagulation, C(j→j),
- intermodal transfer of moment from nuclei to accum. mode, C(i→j),
- emission, E(k,j)

$$d\, M(k,j)/dt = G(j) - C(j \rightarrow j) + C(i \rightarrow j) + E(j)$$

Nuclei mode (i):

- homogeneous nucleation, N(i), (present only binary),
- condensation growth, G(i),
- intramodal coagulation C(i→i)
- intermodal loss of nuclei particles to accumulation mode, C(i→j),

$$d\, M(i)/dt = N(i) + G(i) + C(i \rightarrow i) + C(i \rightarrow j)$$

Analytical solutions are found using the suggestions by *Whitby et al. (1997)* and *Binkowski et al. (2000)*, and these solutions are used in the model.

Enviro-HIRLAM, model examples

- Domain ~ 500 x 400 km around Paris, France.
- Resolution: horizontal 0.05º x 0.05º, vertical 40 levels
- Sim.: 00 UTC June 29 – 00 UTC June 30, 2005. Δt = 300 sec.
- Meteorological cond.: low winds, convective clouds, little precip.

- Reference run: - feedbacks. Perturbed run: + 2nd indirect effect.
- Second indirect effect based on modified version of STRACO, where the autoconversion from Rasch-Kristjansson has been implemented.

- All presented 2D fields are the lowest model level.

Second indirect effect

Microphysics of clouds, its interacting with aerosols, CCN/IN growing, washout and rainout → precipitation

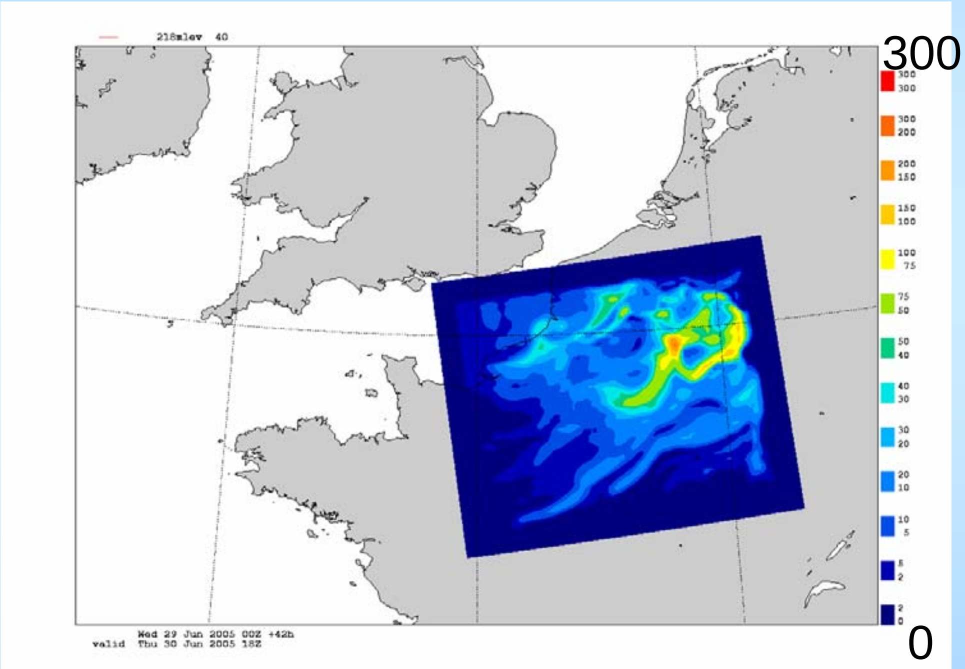
That means it affects: cloud LWC, lifetime, and precipitation

Processes needed to describe is effect: in-/below-cloud scavenging, droplet sedimentation

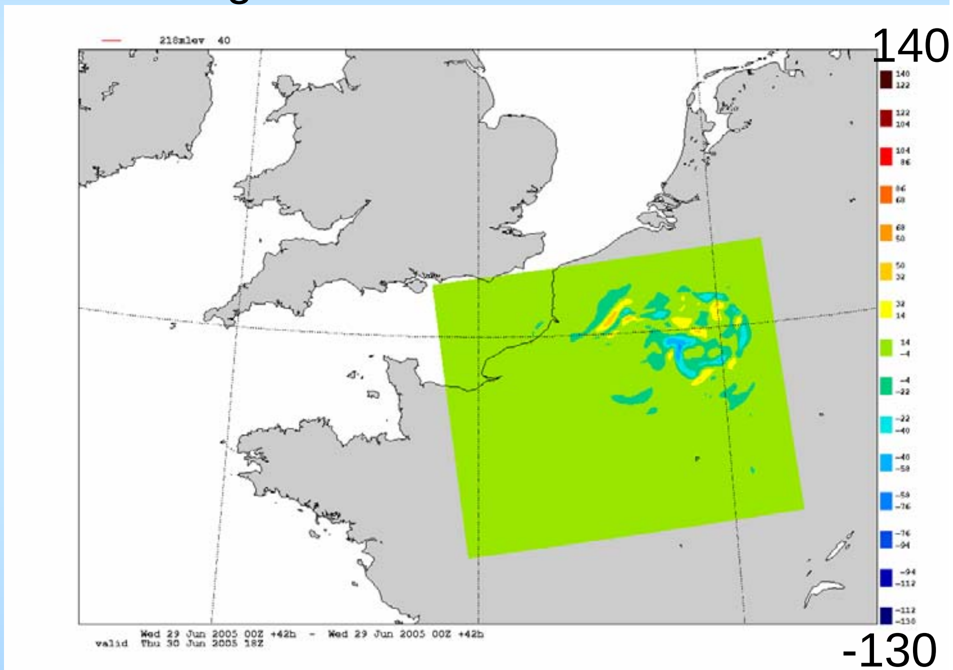
Key variables: scavenging efficiency, precipitation rate, sedimentation rate

O_3 concentration ($\mu g/m^3$) at 18 UTC

Reference



Including second indirect effect



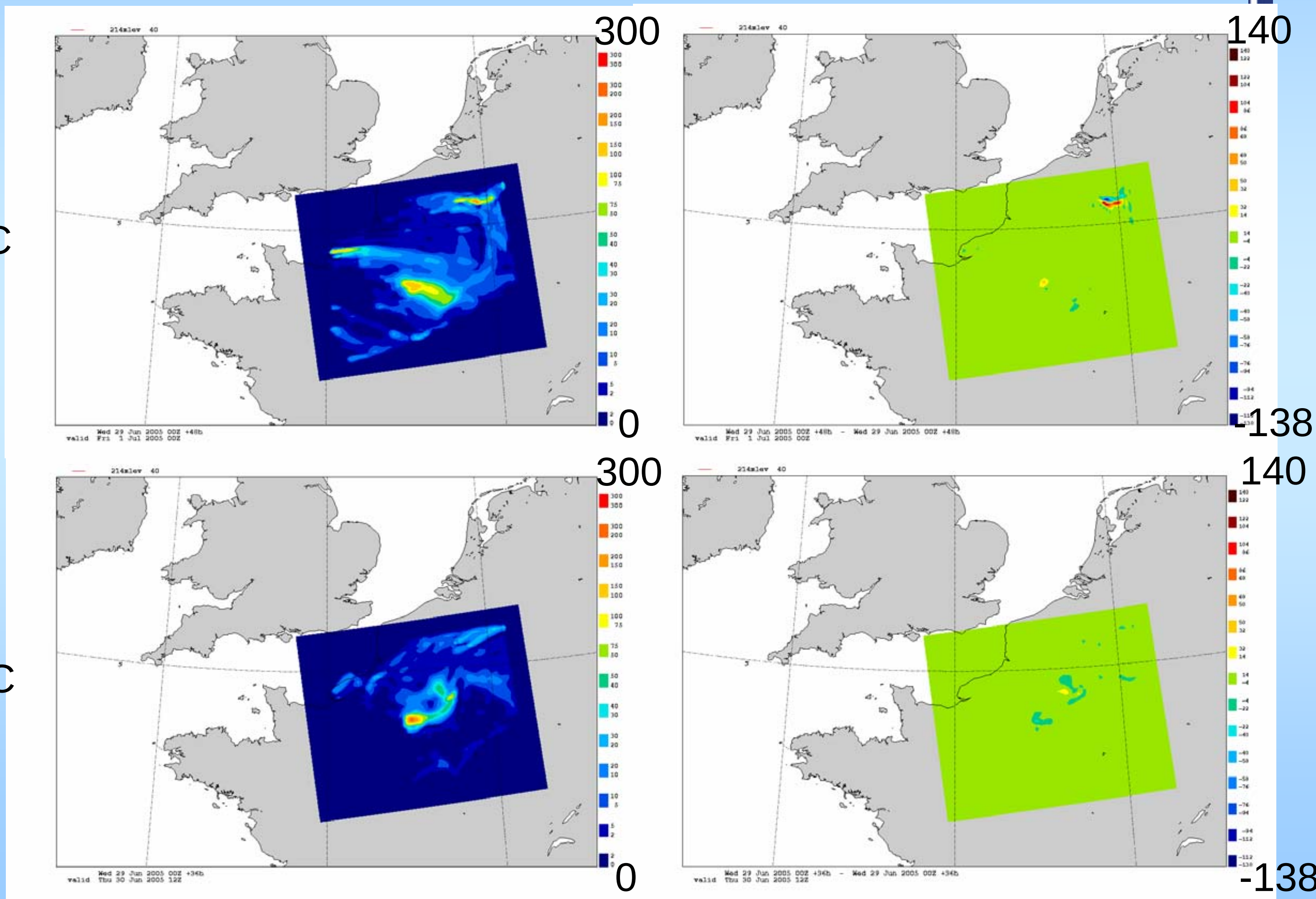
Changes in O_3 conc. happened primarily in upper right hand quadrant.

NO_2 concentrations ($\mu g/m^3$)

Reference | Including second indirect effect

00 UTC

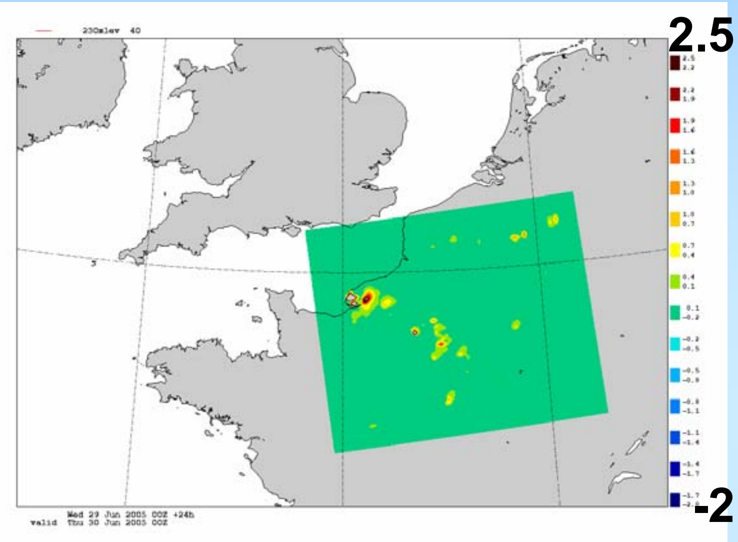
12 UTC

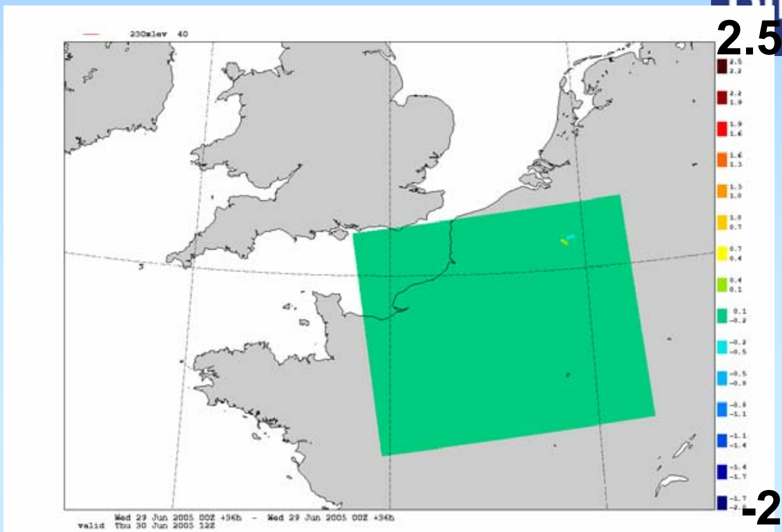


H_2SO_4 concentrations (µg/m^3)

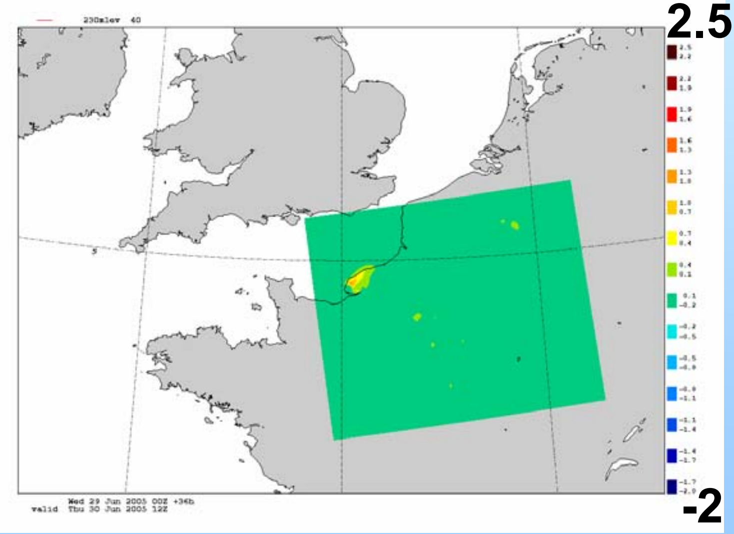
Reference | Including second indirect effect

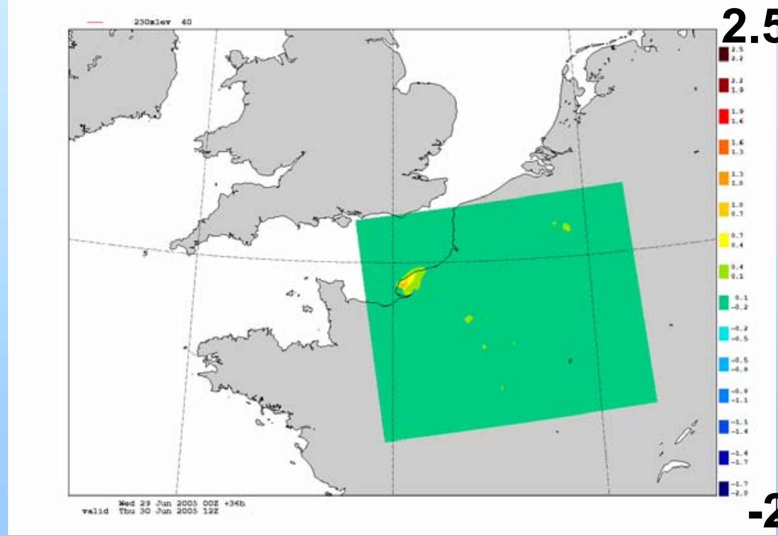
00 UTC



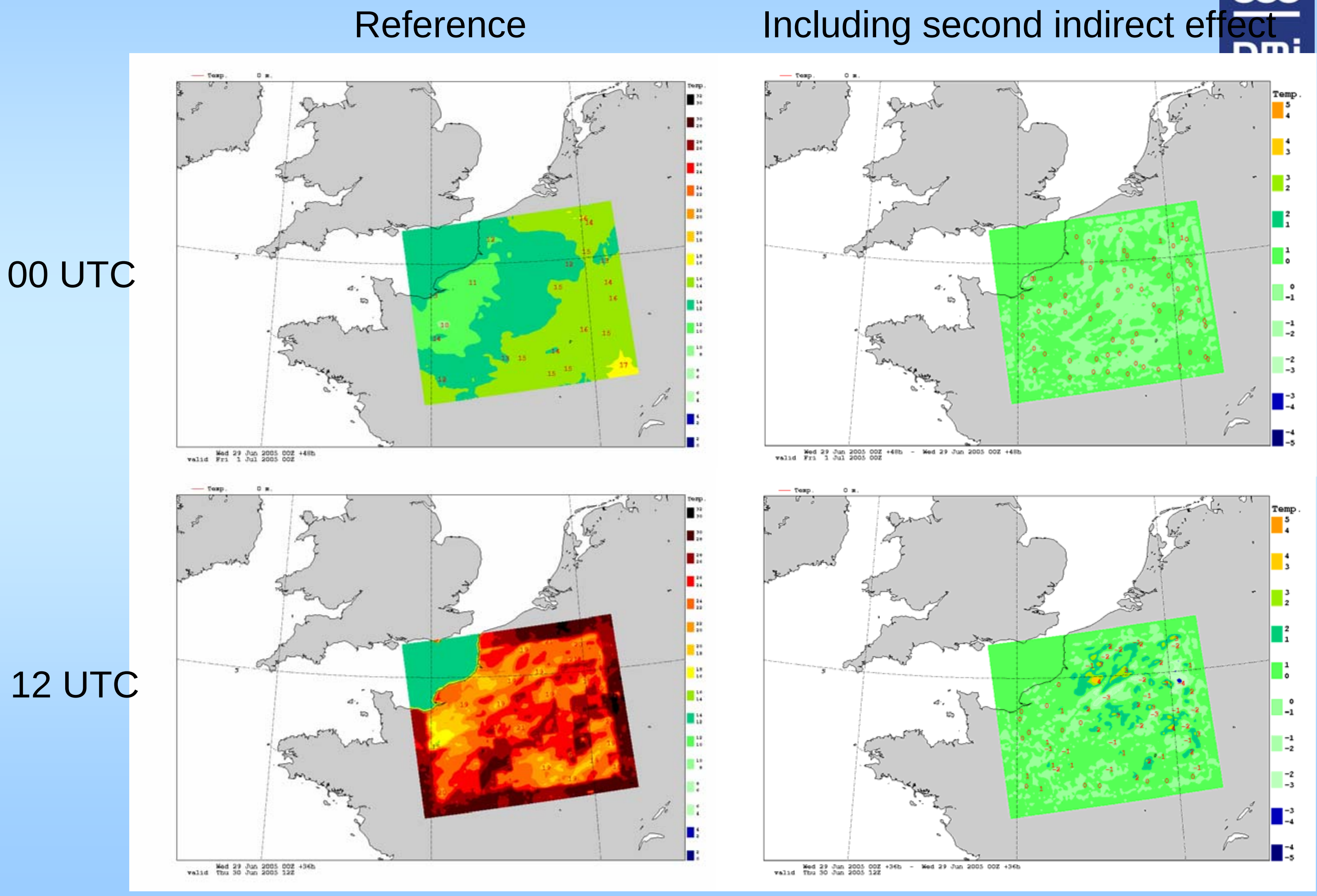


12 UTC





Surface temperature (C)



Temperature changes are up to 4º C

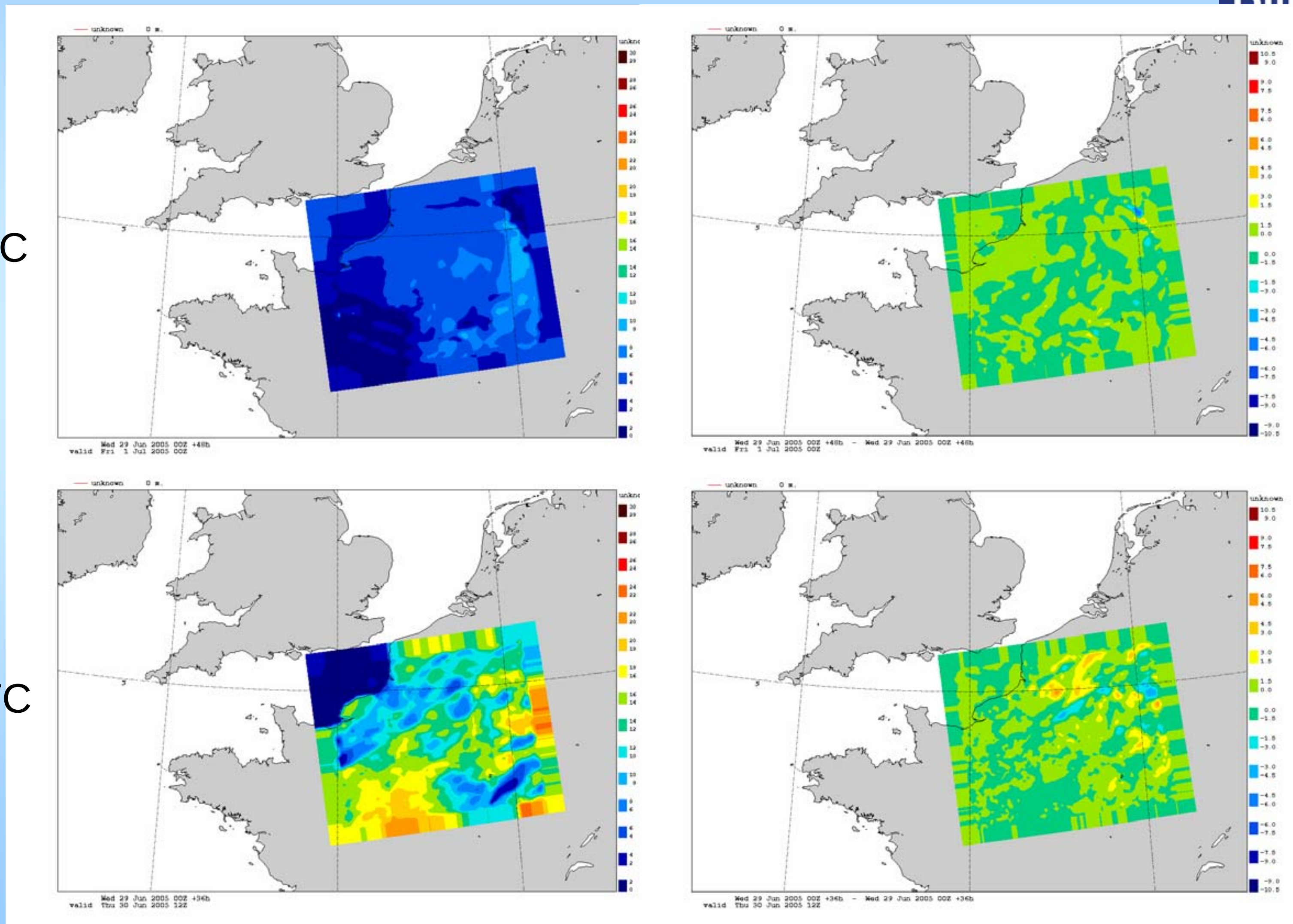
PBL height *(m) X 0.01*

Reference

Including second indirect effect

00 UTC

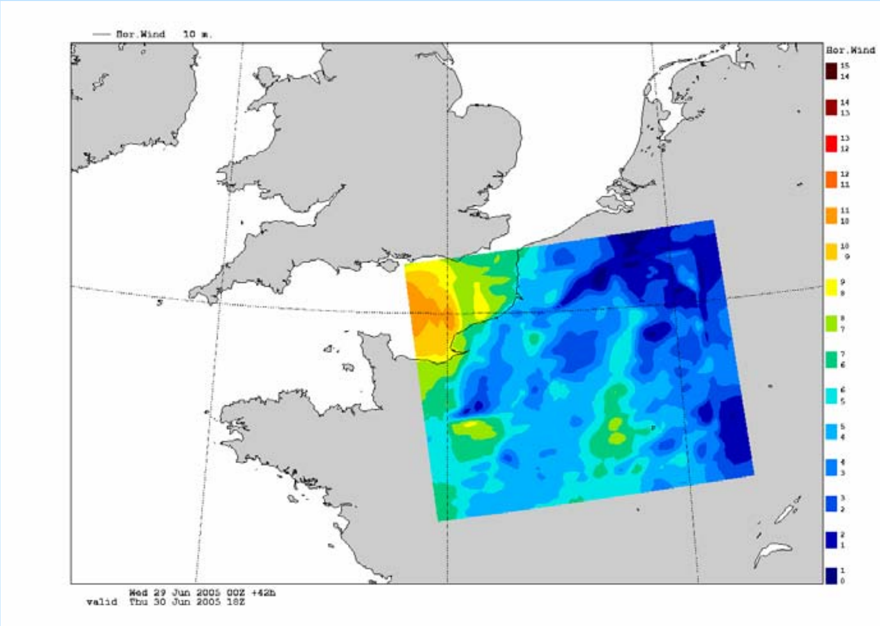
12 UTC



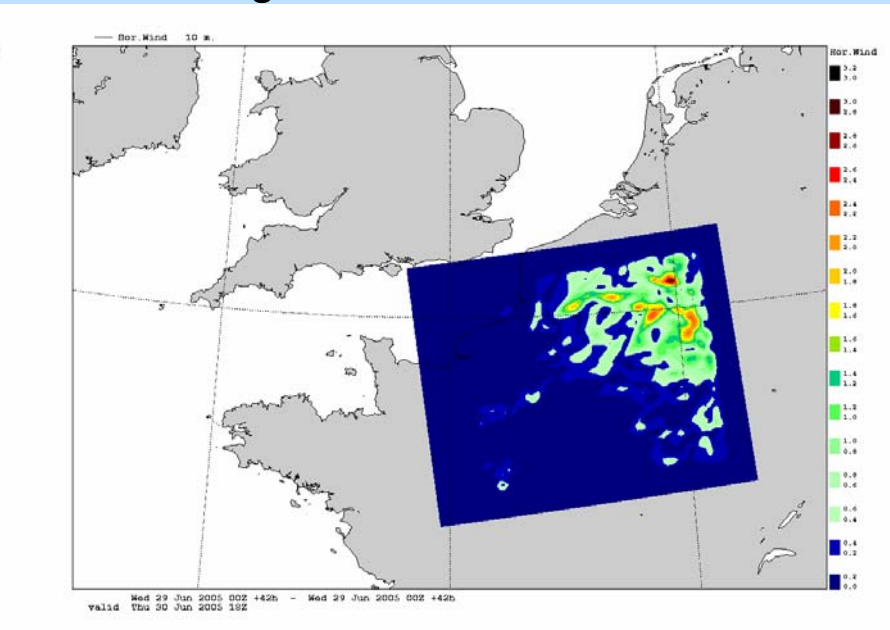
Changes in PBL height quite large (up to 600 m)

10 meter wind (m/s) at 18 UTC

Reference

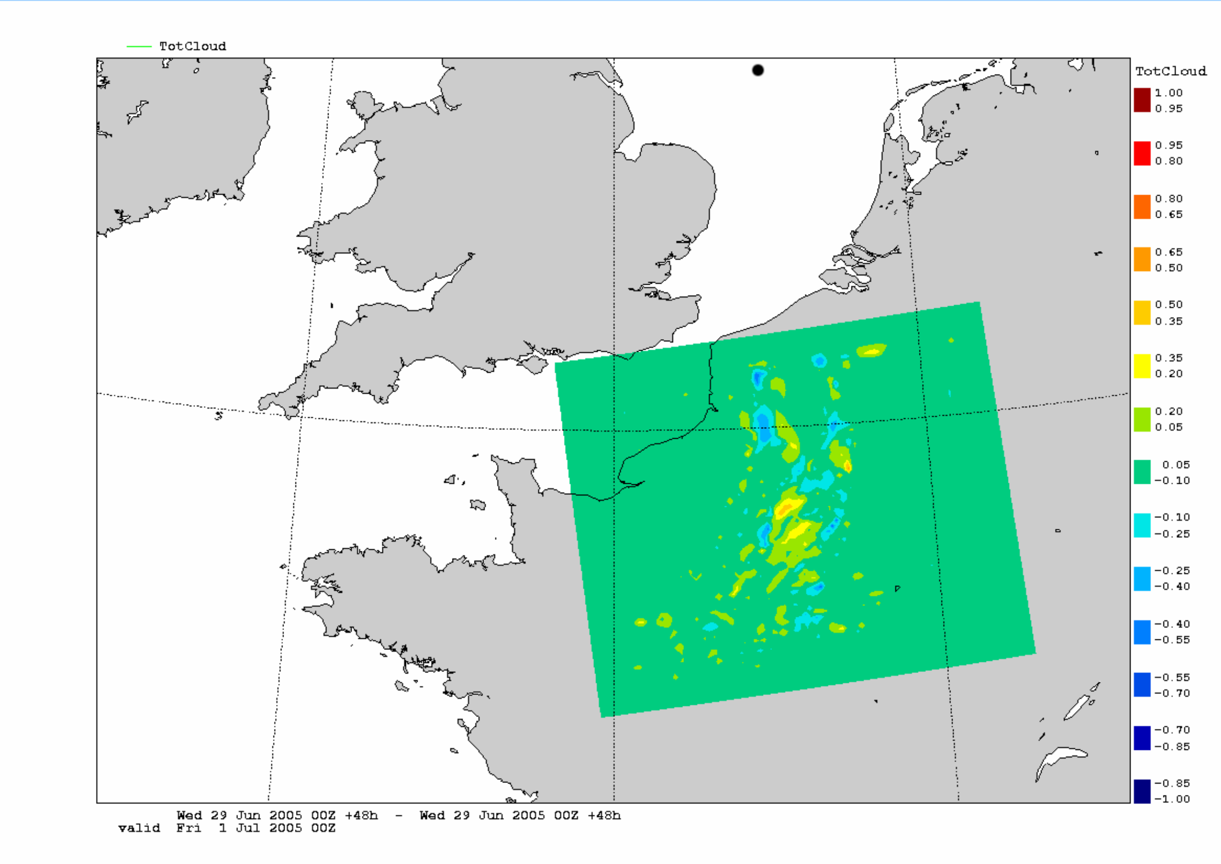


Including second indirect effect



wind changes up to 3m/s

Change in total cloud cover at 00 UTC (%)



Changes in cloud cover is accounted for by changes in low cloud and no change in high or medium Clouds: seems consistent, since there is no convection of the tracers.

Summary/Conclusion

- First test of Enviro-HIRLAM with fully coupled
  - chemistry,
  - aerosols dynamics, and
  - feedbacks.
- The test shows that feedbacks from the fully coupled system has an impact on
  - the chemistry,
  - the aerosols, and
  - Meteorology.

  Mainly emission driven.
- More tests and improvements of NWP-Chem mch. Is needed.
- More tests of Enviro-HIRLAM on larger area and against measurements is needed.

DMI super computer

Old

NEC SX-6

Theoretical peak: 0.5 Tflops

New

CRAY XT5

Theoretical peak: 35 Tflops

Future developments:

- Include ternary nucleation
- Add an aqua phase chemical mechanism
- Exchange the MFI with non-iterative scheme
- Improvements of the NWP-Chem mch.
- Develop a NWP-Chem-pollen mechanism

The influence of air pollution on the increase of allergy

- Investigations indicate that air pollution has a direct effect on the increasing number of people with allergy (Ishizaki, 1987).

- No correlation between the increasing number od people with allergy and the emissions of NO_X, SO_2 and atmospheruc dust (Behrendt et al., 1992; Ring et al., 2001; Sunyer et al., 2005).

- Gassner et al. (1987) have observed that their is a correlation between O_3 air pollution and pollen.

- Pollen is chemical effected by particles and NO_Xs.

Electron microscope picture of grass pollen before (a) and after (b) it has been polluted with aerosol particles

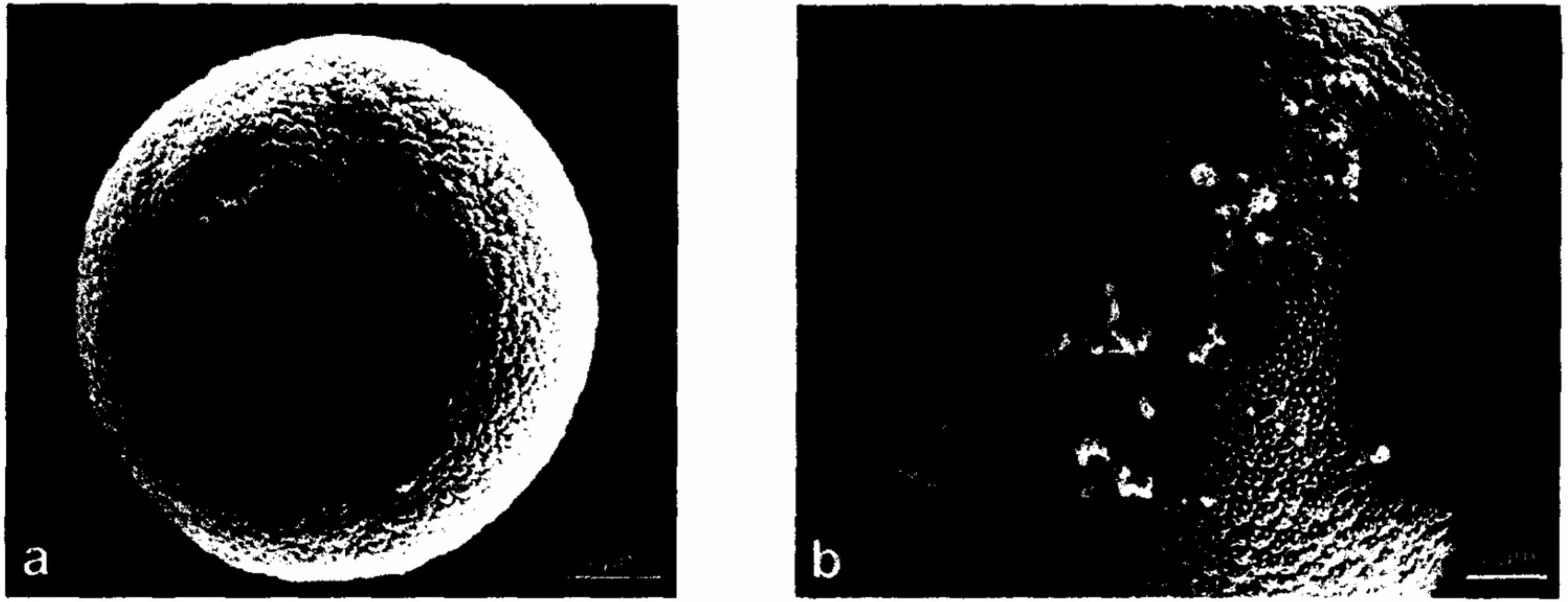


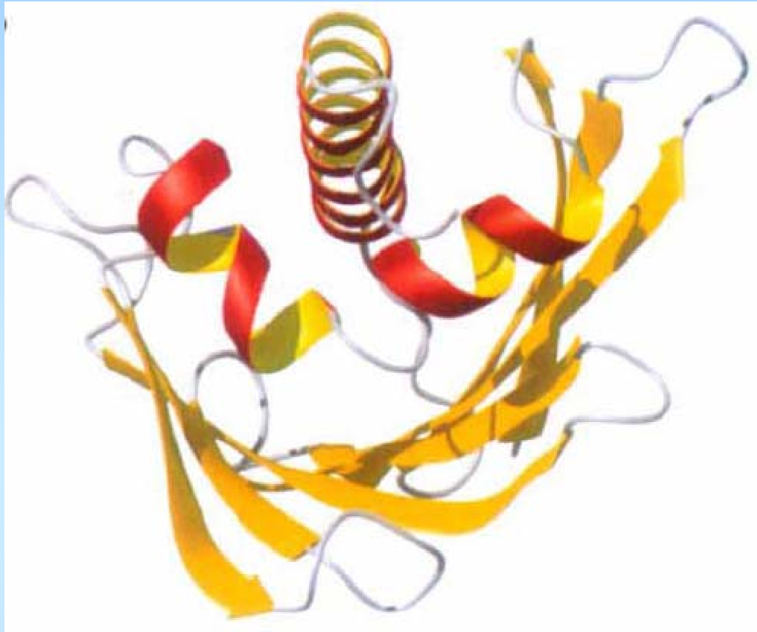
Fig. b: Pollen surface covered with aerosol particles.

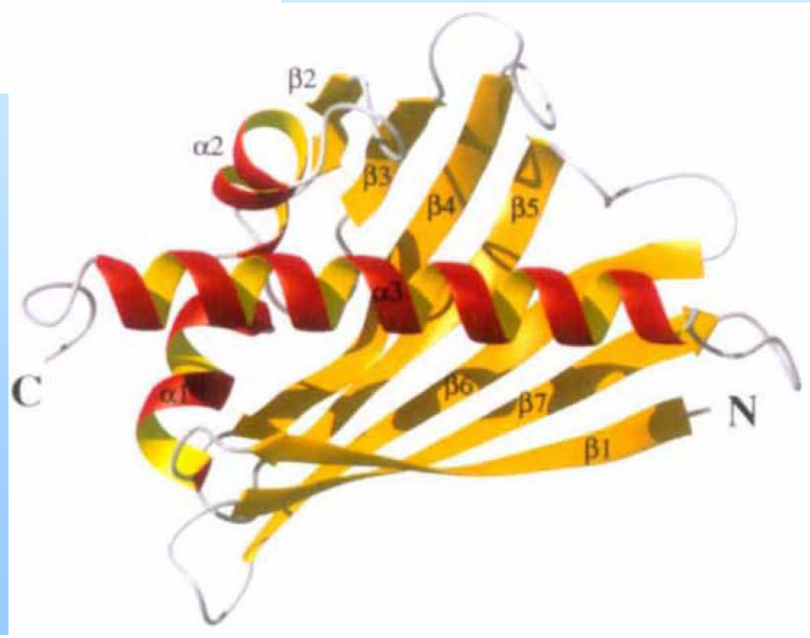
Hope we soon can ”estimate” the increase of proteins released from grass pollen when it is in a polluted environment.

Ex.: Birch pollen

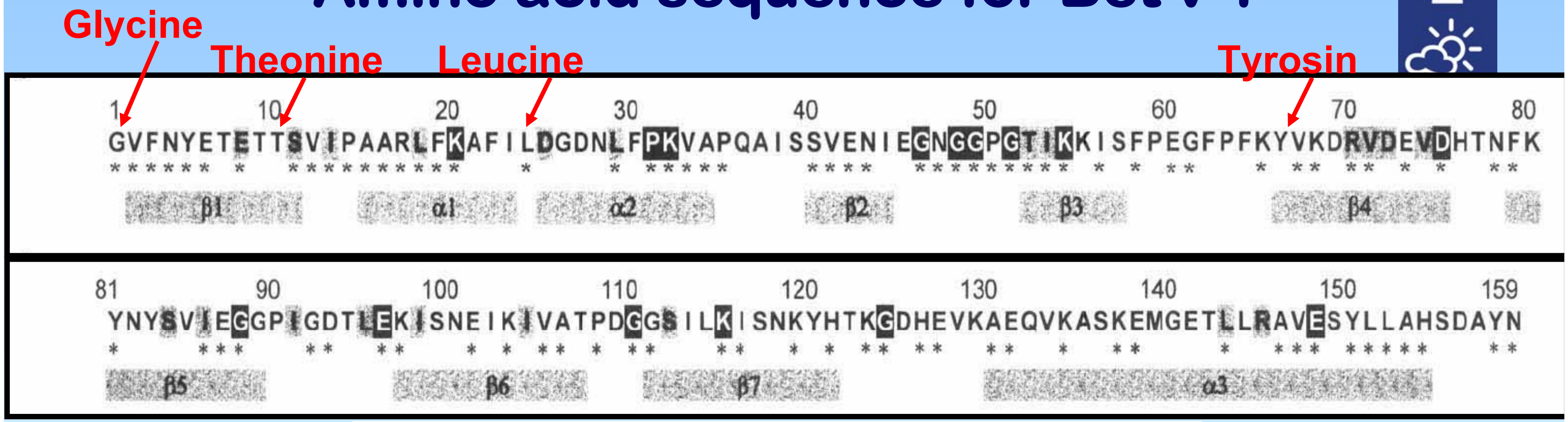
Allergens

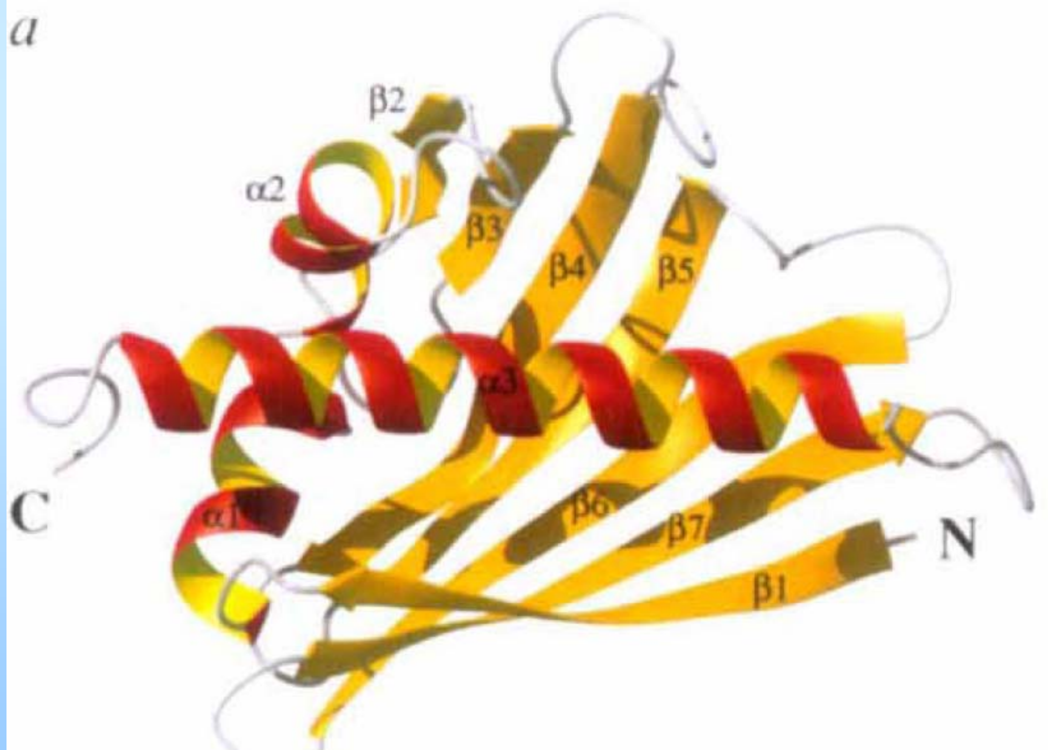
- Bet v 1
- Bet v 2
- Bet v 3
- Bet v 4
- Bet v 5
- Bet v 6
- Bet v 7



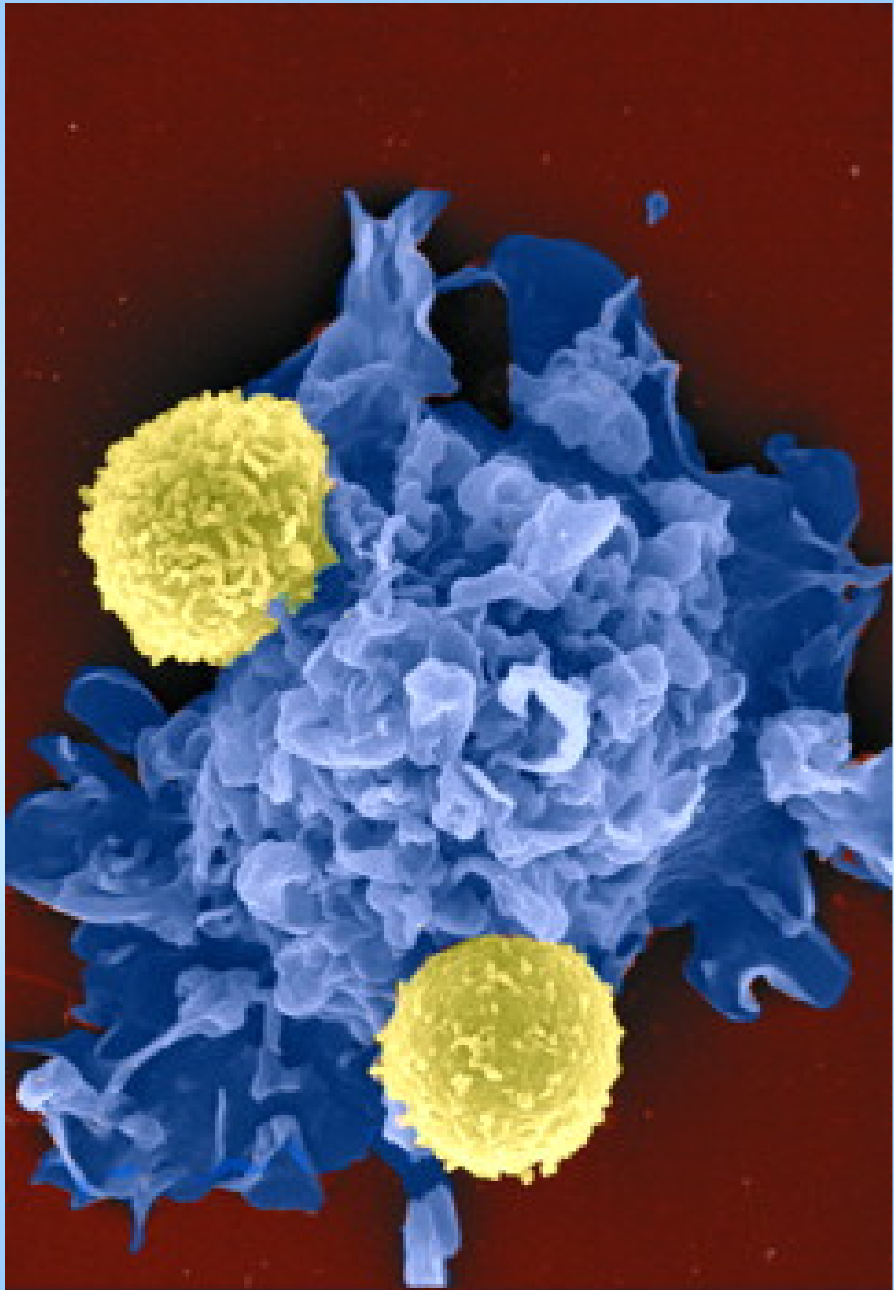


Amino acid sequence for Bet v 1





We will soon have the first estimated rate constant of birch pollen nitration



D cells (blue) exposed to lipids (yellow).

↓

makes

↓

An increasing Th2 response.

Research has shown that this exposure increases under air pollution.

The mechanism is unknown but it is assumed that air pollution stressing pollen which results in an increased activation of the lipids.

The allergic reaction of pollen on humans