Chemistry in Enviro-HIRLAM

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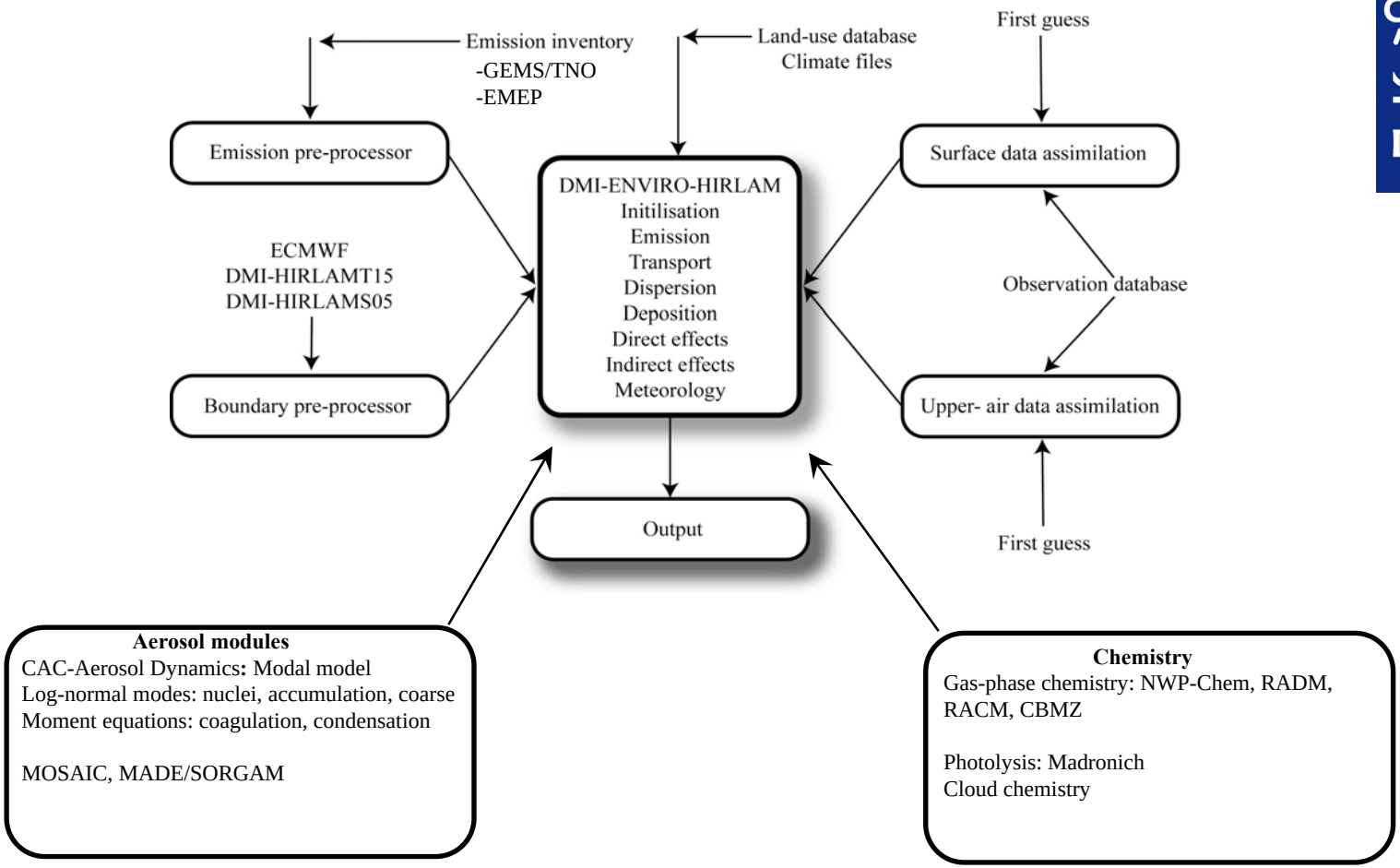
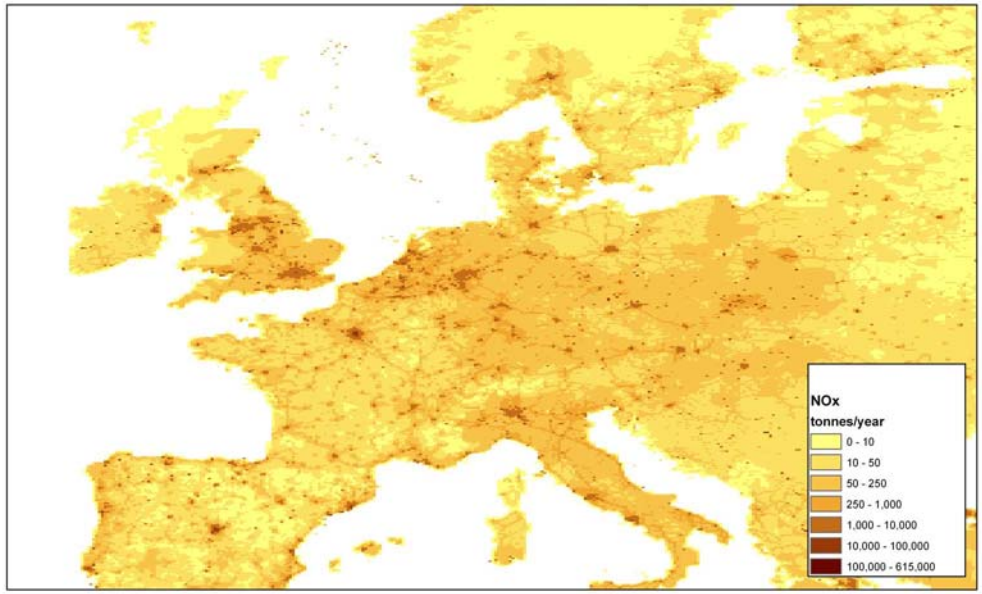

Emission inventory
-GEMS/TNO
-EMEP
Land-use database
Climate files
First guess
Emission pre-processor
DMI-ENVIRO-HIRLAM
Initilisation
Emission
Transport
Dispersion
Deposition
Direct effects
Indirect effects
Meteorology
Surface data assimilation
ECMWF
DMI-HIRLAMT15
DMI-HIRLAMS05
Observation database
Boundary pre-processor
Upper- air data assimilation
Output
First guess
Aerosol modules
CAC-Aerosol Dynamics: Modal model
Log-normal modes: nuclei, accumulation, coarse
Moment equations: coagulation, condensation
MOSAIC, MADE/SORGAM
Chemistry
Gas-phase chemistry: NWP-Chem, RADM, RACM, CBMZ
Photolysis: Madronich
Cloud chemistry

Emission pre-processing

GEMS-TNO emission inventory; 0.125 x 0.0625
(*Visschedijk, et al., 2007*)



NO_x emissions; ship tracks not included here

Emission pre-processing

GEMS-TNO species:
SO_2, NO_x, NH_3, CO, NMVOC's, CH_4, $PM_{2.5}$, PM_{10}

10 SNAP codes:

- Energy transformations
- Small combustion plants
- Industrial conbustion
- Industrial processes
- Fossil fuel production
- Solvent and product use
- Road transport
- Non-road transport and mobile machinery
- Waste disposal
- Agriculture

Emission processing

- Eulerian point sources (and areal sources)
- Well mixed grid cells
- Location of emission point, volume
- $\psi_i^{t+1} = \psi_i^{t-1} + 2\Delta t Q_i$
- Dependence on resolution

Emission processing

Pre-processing of inventory:

- Read inventory
- Unpack temporal variations
- VOC splitting (Theloke and Friedrich (2007))
- Lumping follows the chemistry scheme chosen (NWP-Chem)
- Unit conversions
- Mass conservative interpolation to model grid
- Handles SNAP codes

Currently, output read from external file during initilization

The NWP-Chem mechanism: Lumped tropospheric mechanism based on newest chemical knowledge

Developed for online coupled models

cpu-time economical

low memory requirements

Covers most important chemical processes responsible for air pollution and aerosol formation in meso-scale models

Advectied species: no, no2, so2, co, hc, hcho, o3, ho2, hno3, h2o2, h2, h2so4, op, ho, od, ro2, rooh

Rates and coefficients in NWP-Chem-gas is estimate based on lumping and optimization procedures.

Chemical reactions →QSSA.

NWP-Chem is tested against the RACM+ELCID mch. at different standard marine, rural and plume scenarios.

The Quasi Steady State Approximation (*Hesstvedt, et al., 1978*)

$$d\psi_i/dt = P_i - L_i\,\psi_i$$

Each equation assumed independent

For $L_i\Delta t > 10$ specie lifetime shorter than time step ->
Steady state solution: $\psi_i(t + \Delta t) = P_i(t)/ L_i(t)$

For $L_i\Delta t < 0.01$ the Euler forward algorithm is stable ->
$\psi_i(t + \Delta t) = \psi_i(t) + \Delta t\,(P_i - L_i\,\psi_i(t))$

For $0.01 < L_i\Delta t < 10$ P_i and L_i are assumed constant over a time step -> first order equation, constant coefficients ->

$$\psi_i(t + \Delta t) = P_i/L_i + (\psi_i(t) - L_i/P_i)\exp(- L_i\Delta t)$$

Lumping follows *Gross et al., 2005*

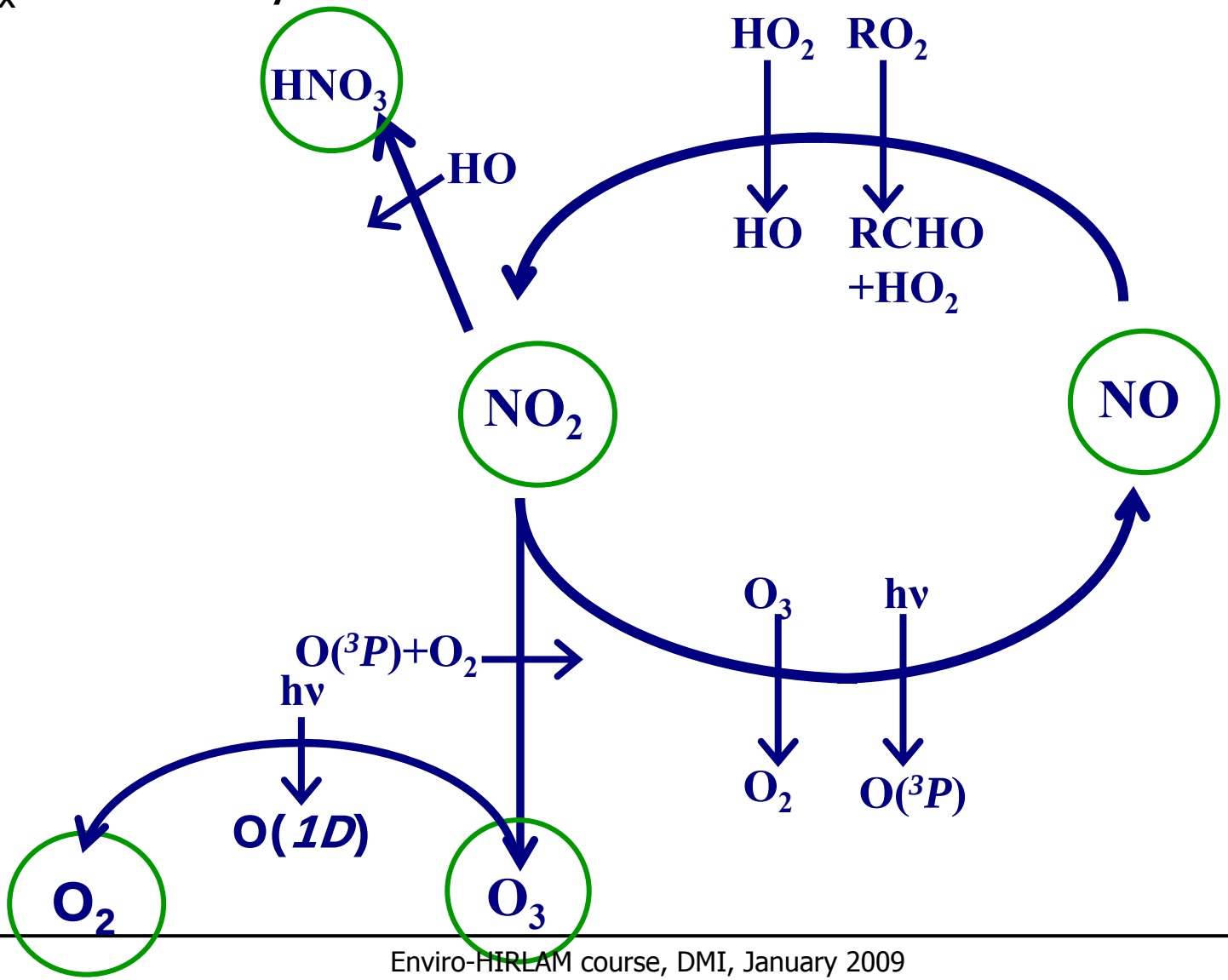
E.g. $[NO_x] = [NO] + [NO_2]$; $[O_3NO] = [O_3] - [NO]$

Photolysis reactions:

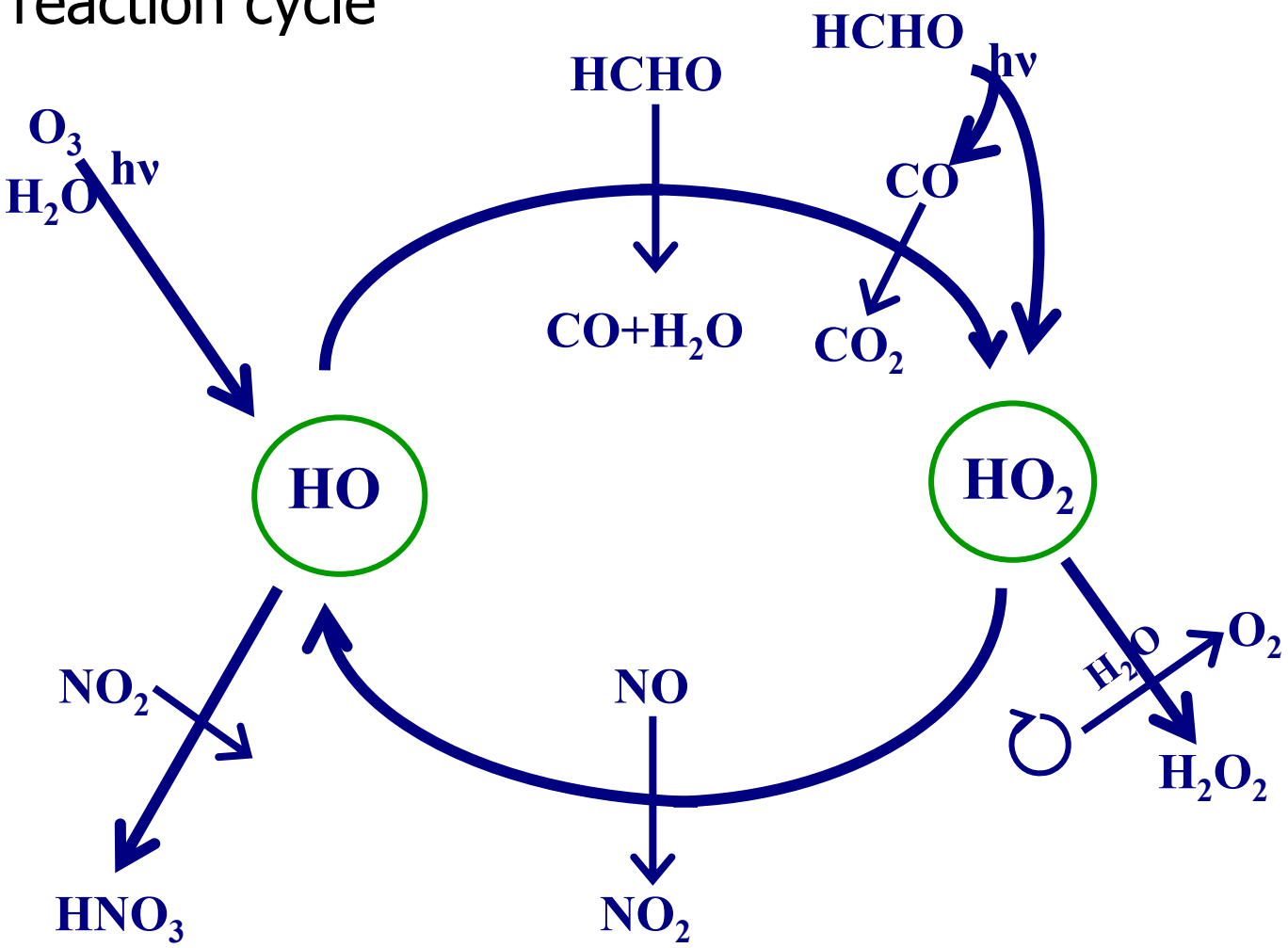
$NO_2 + hv \rightarrow O(^3P) + NO$
$O_3 + hv \rightarrow O(^2D) + O_2$
$HCHO + hv \rightarrow 2\ HO_2 + CO$
$HCHO + hv \rightarrow H_2 + CO$

Reaction rates are prescribed and follows *Poppe et al., 1996*

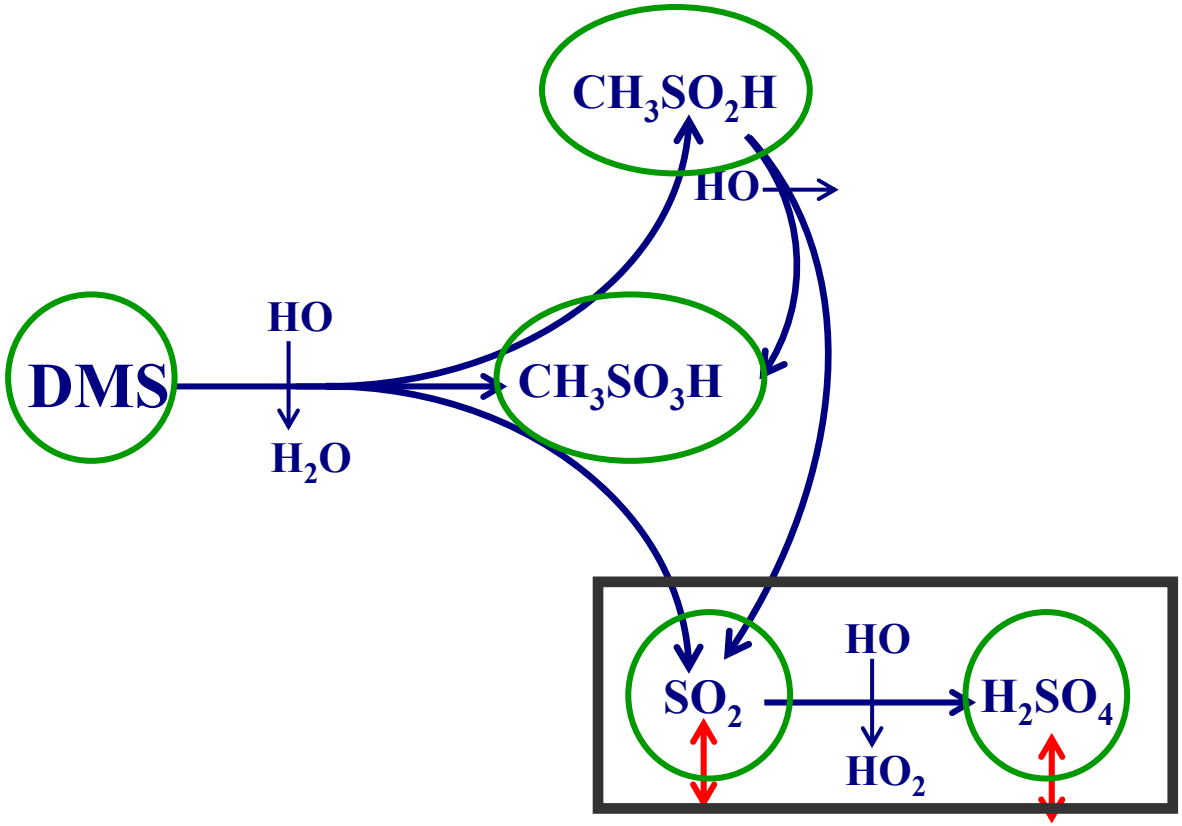
NO_x reaction cycle



HO_x reaction cycle

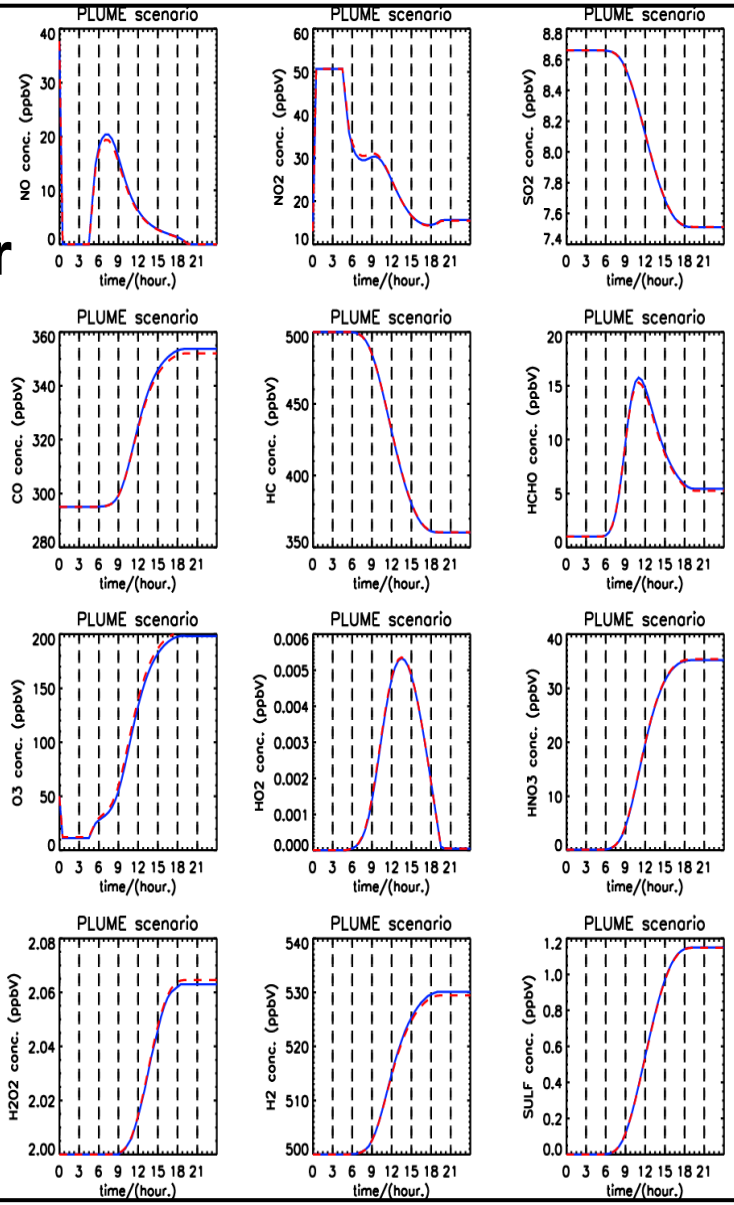


Sulfur chemistry:



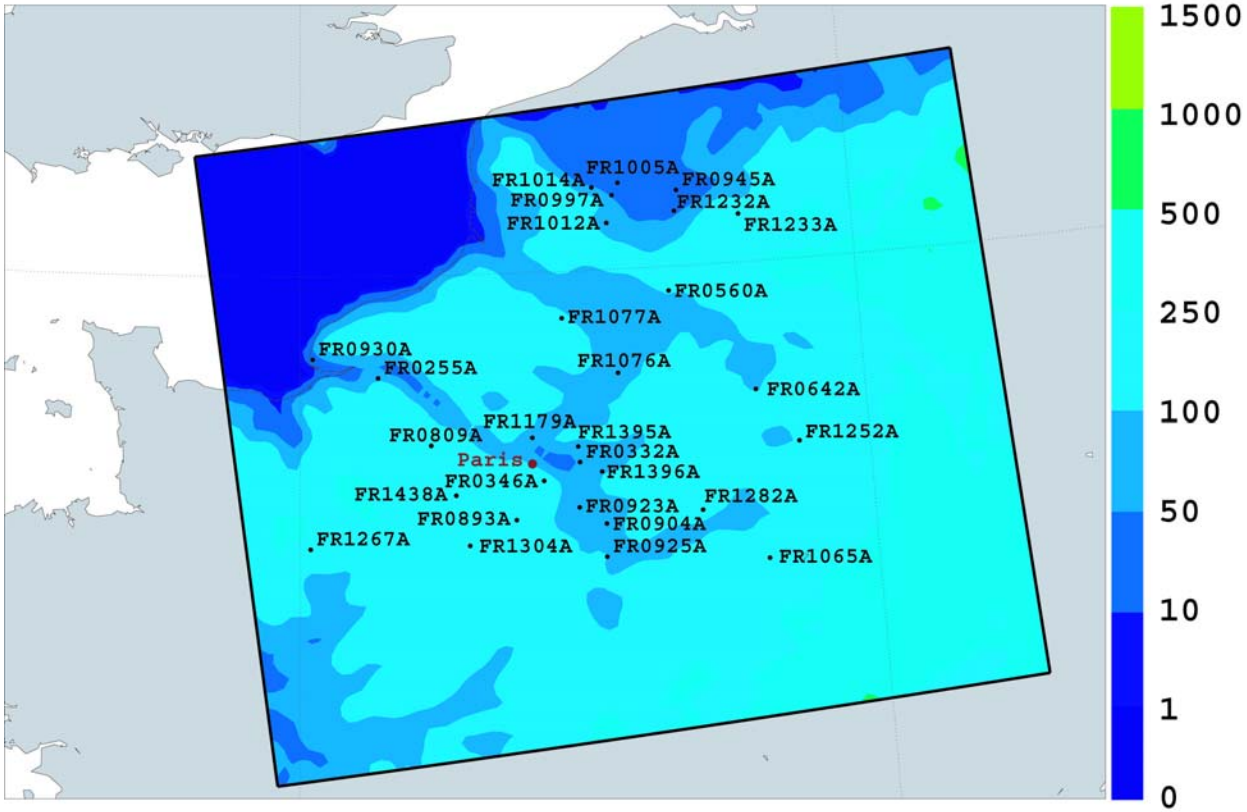
Testing of NWP-Chem:

0D comparison to other schemes



3D testing: full chemistry, aerosol dynamics and equilibration

Compare NO2 to AIRBASE measurements near Paris



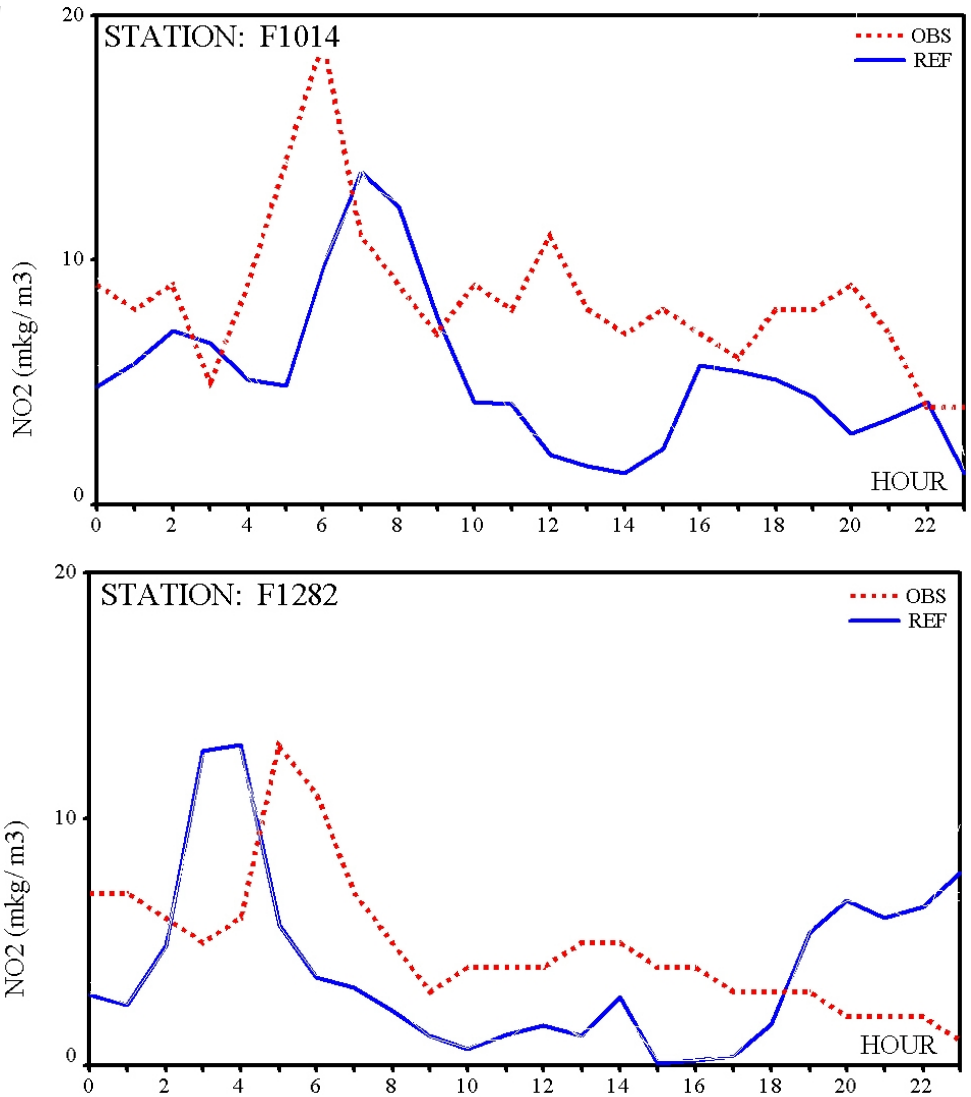
Model area (geopotential height (meters)) along with measurement stations

3D testing

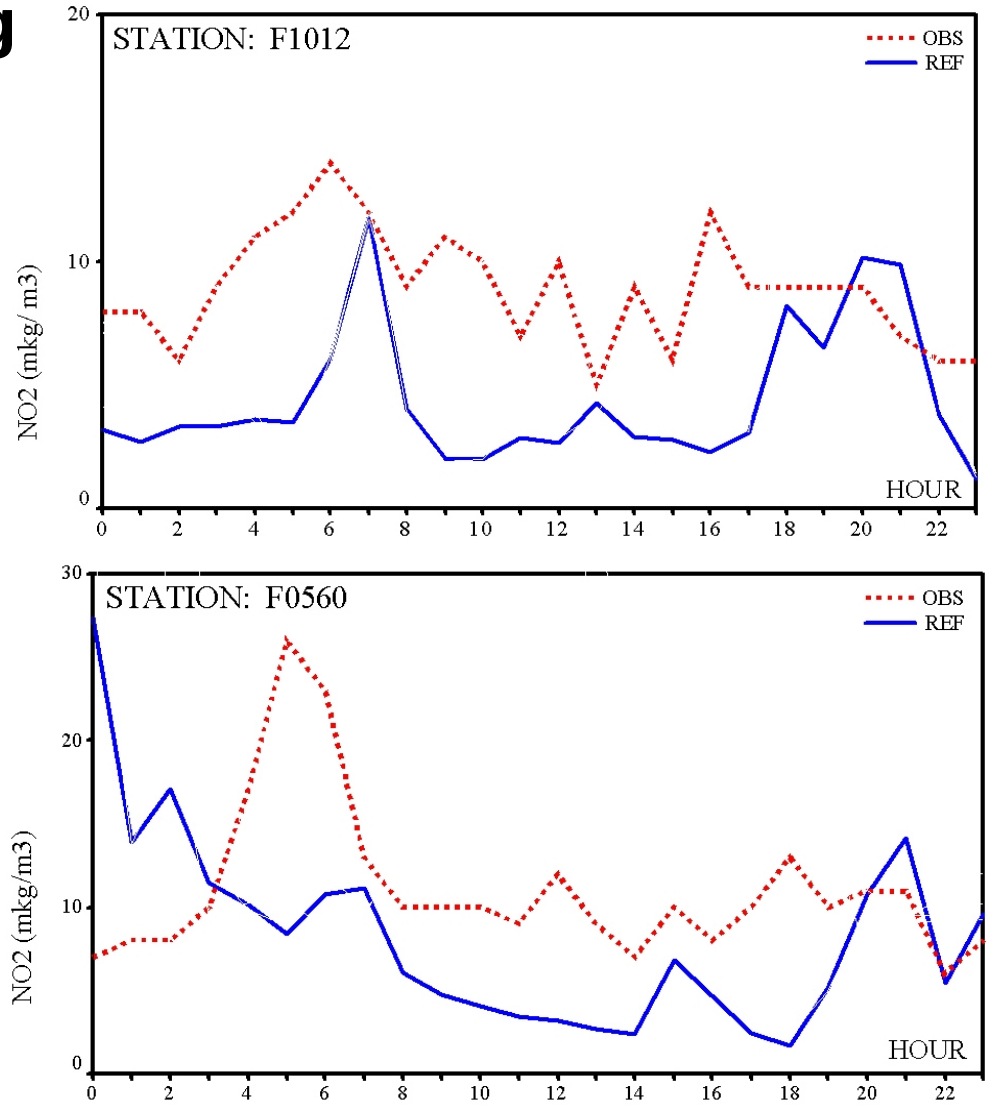
Simulation specifics

- Initialized 00 UTC 29 June 2005 + 48 h
- 24 hour spin-up
- Meteorological boundaries from DMI-HIRLAM-S05
- Inflow neglected
- 248 meas. Stations were available
- Urban stations disregarded;
- Recast to 50 x 50 km grid; 3 stations per grid cell
- Some stations had missing values
- 27 evenly spaced stations remained

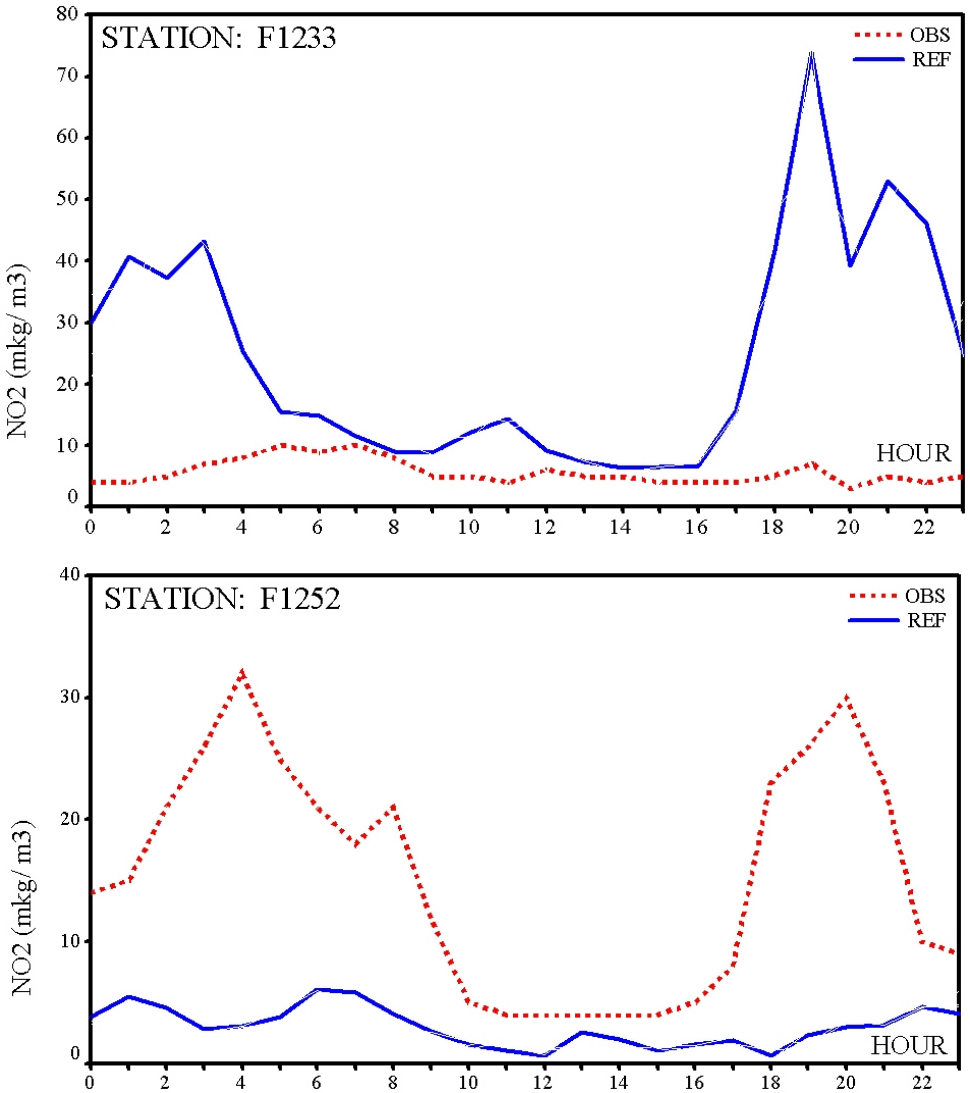
3D testing


STATION: F1014
OBS
REF
NO2 (mkg/m3)
HOUR
0
10
20
0 2 4 6 8 10 12 14 16 18 20 22
STATION: F1282
OBS
REF
NO2 (mkg/m3)
HOUR
0
10
20
0 2 4 6 8 10 12 14 16 18 20 22

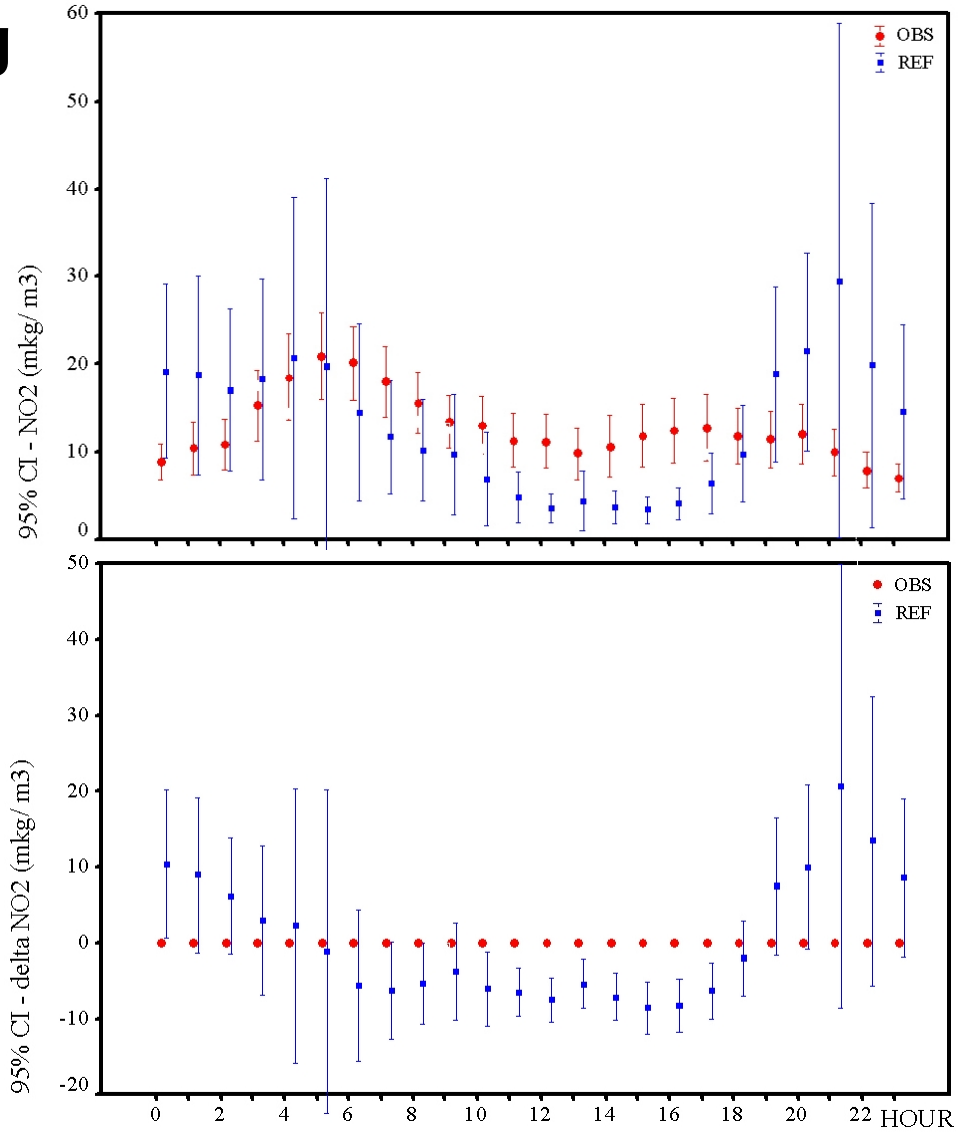
3D testing


STATION: F1012
OBS
REF
NO2 (mkg/ m3)
HOUR
0
10
20
0 2 4 6 8 10 12 14 16 18 20 22
STATION: F0560
OBS
REF
NO2 (mkg/m3)
HOUR
0
10
20
30
0 2 4 6 8 10 12 14 16 18 20 22

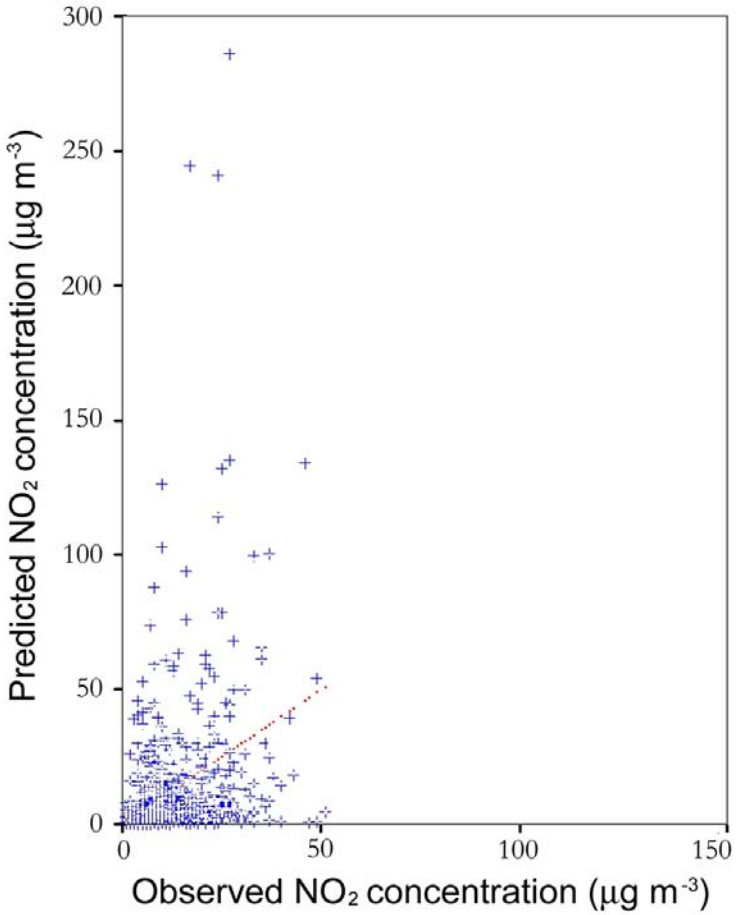
3D testing


STATION: F1233
OBS
REF
NO2 (mkg/ m3)
HOUR
0
10
20
30
40
50
60
70
80
0
2
4
6
8
10
12
14
16
18
20
22
STATION: F1252
OBS
REF
NO2 (mkg/ m3)
HOUR
0
10
20
30
40
0
2
4
6
8
10
12
14
16
18
20
22

3D testing



3D testing



Number of points: 648

Global stats: NMSE=1.2, BIAS=0.34 µg m^{-3}, FBIAS=0.02, R=0.38

Conclusions

NWP-Chem is the default scheme in Enviro-HIRLAM

It is cpu-time and memory economical

NWP-Chem performs well compared to more elaborate schemes in 0D simulations covering free tropospheric, tropos. background and plume scenarios.

The 3D vewrsion performs satisfactory w.r.t NO_2 in the case Considered

However, the full 3D version has only been tested in a single case