Multiscale Atmospheric Chemistry Modelling

GEM-AQ Status and new developments

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Supported by

- Canadian Foundation for Climate and Atmospheric Sciences
- Canadian Foundation for Innovation
- Canadian Space Agency
- Environment Canada
- Transport Canada

Objectives

- Develop stratospheric, tropospheric and air quality chemistry package on-line in GEM
- Chemical weather modelling
  - Air quality and free troposphere chemistry
  - Dynamics and chemistry in the UTLS region
- Carry out model evaluation and applications
- Develop adjoint and tangent linear chemistry for data assimilation
- Prepare a database of initial chemical conditions

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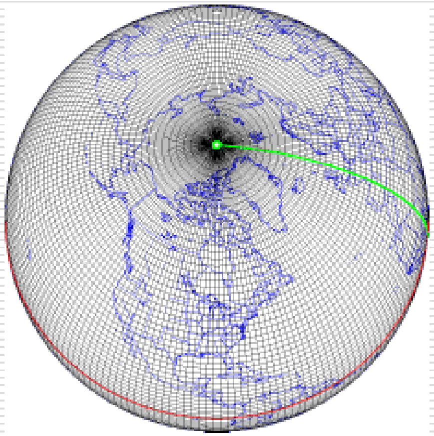
GEM modelling platform

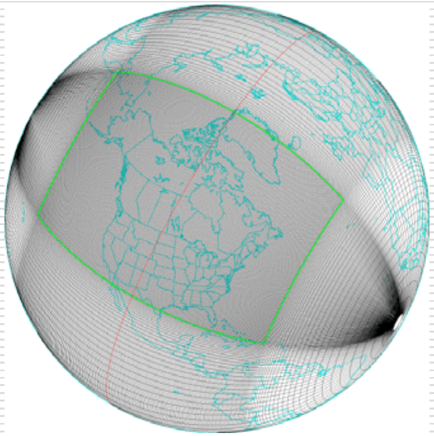
- Global Environmental Multiscale model (Côté at al., 1998)
- Model grid
  - ~35km global uniform - operational
  - ~15km global variable – operational
  - 1.5°x1.5° – global uniform – chemical runs
  - LAM domains i.e. Order of several to 1km
- 4D-VAR objective analysis
- Operational - top at 10mb (~30km) – 58 hybrid levels
- Research - top at 0.1 mb (~60km) – 80 hybrid levels
- Physics - MesoGlobal package
  - Hines non-orographic GWD
  - radiation code – Li and Barker (2003)
    - from surface to model top
    - correlated k-distribution scheme
    - treats short and long waves
    - can deal interactively with H_2O, O_3, CO_2, N_2O, CH_4, and four CFCs
- Stratospheric, tropospheric and air quality chemistry

GEM – dynamical core

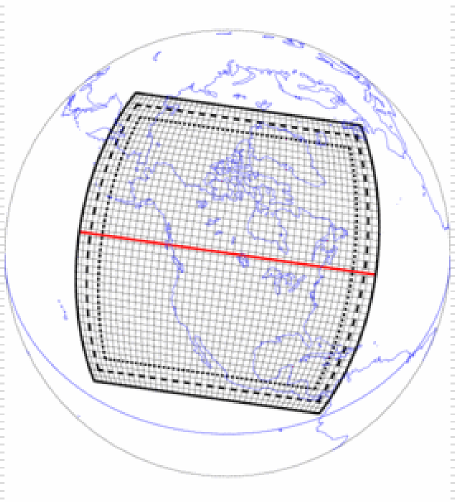
- Two time level semi-Lagrangian advection semi-implicit scheme
- Variable-resolution on an Arakawa C grid in the horizontal with second order accuracy
- Many grid configurations are possible



Global uniform



Global variable



Limited area

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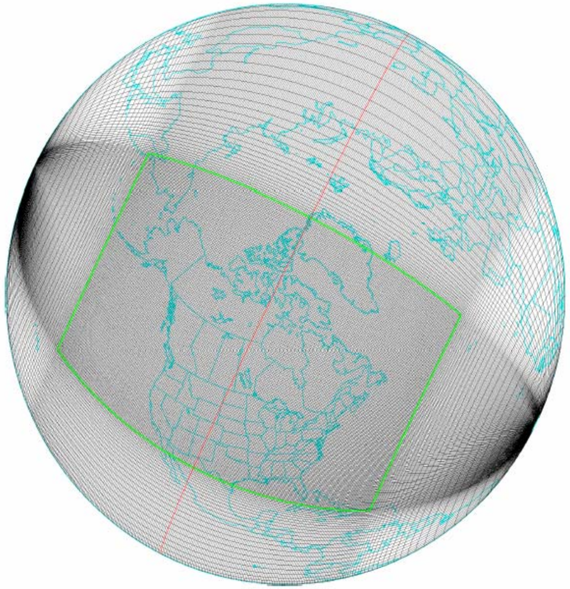
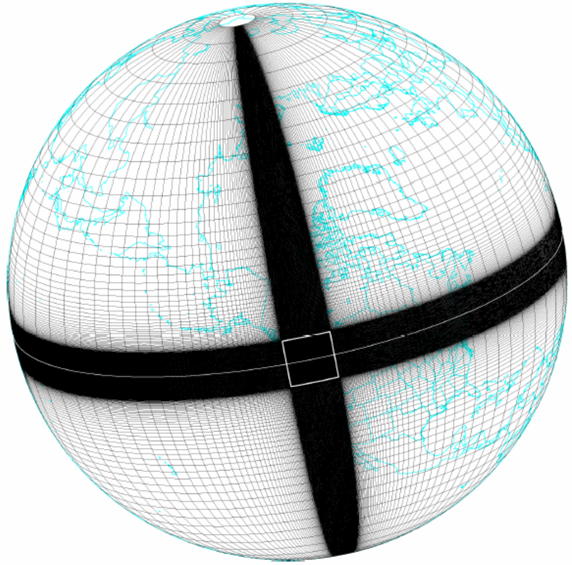
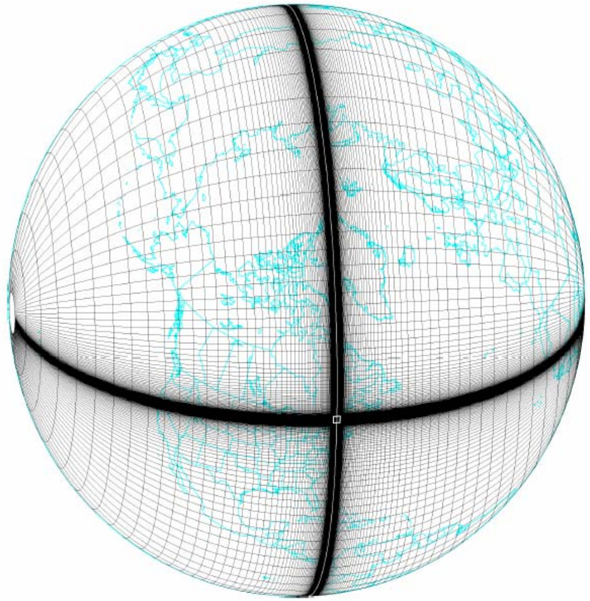
GEM Grids - example







- A variable resolution 255 x 289 horizontal grid; it has uniform 0.33° resolution over the 59.07° x 77.22° (180 x 235) central window.
- 427 x 414 *provincial* mesh having a 10° x 10° (304 x 304) window of uniform 0.033° resolution, centred on (122°W, 53.5°N).
- 584 x 569 *urban* mesh having a 150 km x 150 km (413 x 413) window of uniform 0.0033° resolution, centred on (73.5°W, 45.5°N).

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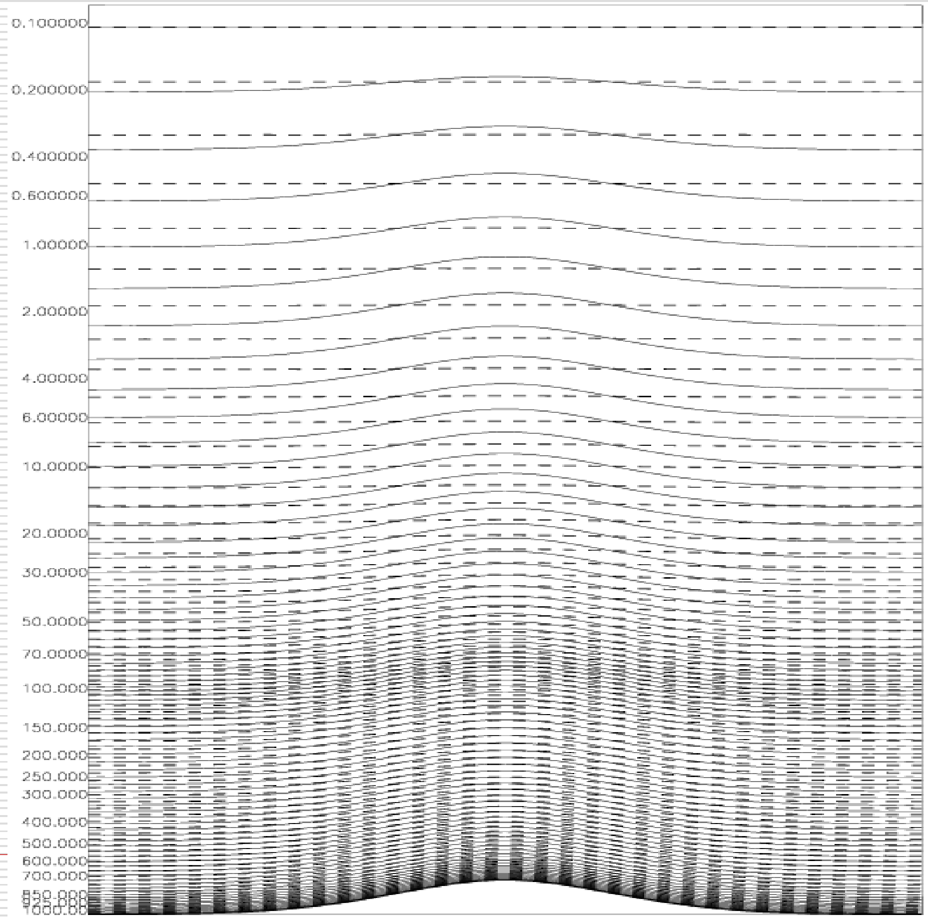
GEM dynamical core

- Non-staggered finite differences in the vertical with second order accuracy
- hybrid vertical coordinate (GEM V3.0 and higher) :

$$Z(\eta) = A(\eta) + B(\eta) Z_s$$



——— sigma

- - - - - - - hybrid

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GEM vertical coordinates

- GEM hybrid vertical coordinate system, where local pressure is:

$$P(\eta) = A(\eta) + B(\eta) \times P_{surface} \quad \text{and} \quad A(\eta) = P_{ref}[\eta - B(\eta)], P_{ref} = 800mb$$

$$\text{with } B(\eta) = \left(\frac{\eta - \eta_{top}}{1 - \eta_{top}} \right)^{rcoef}, rcoef \geq 1$$

- When rcoef=1, system reverts to essentially sigma coordinates

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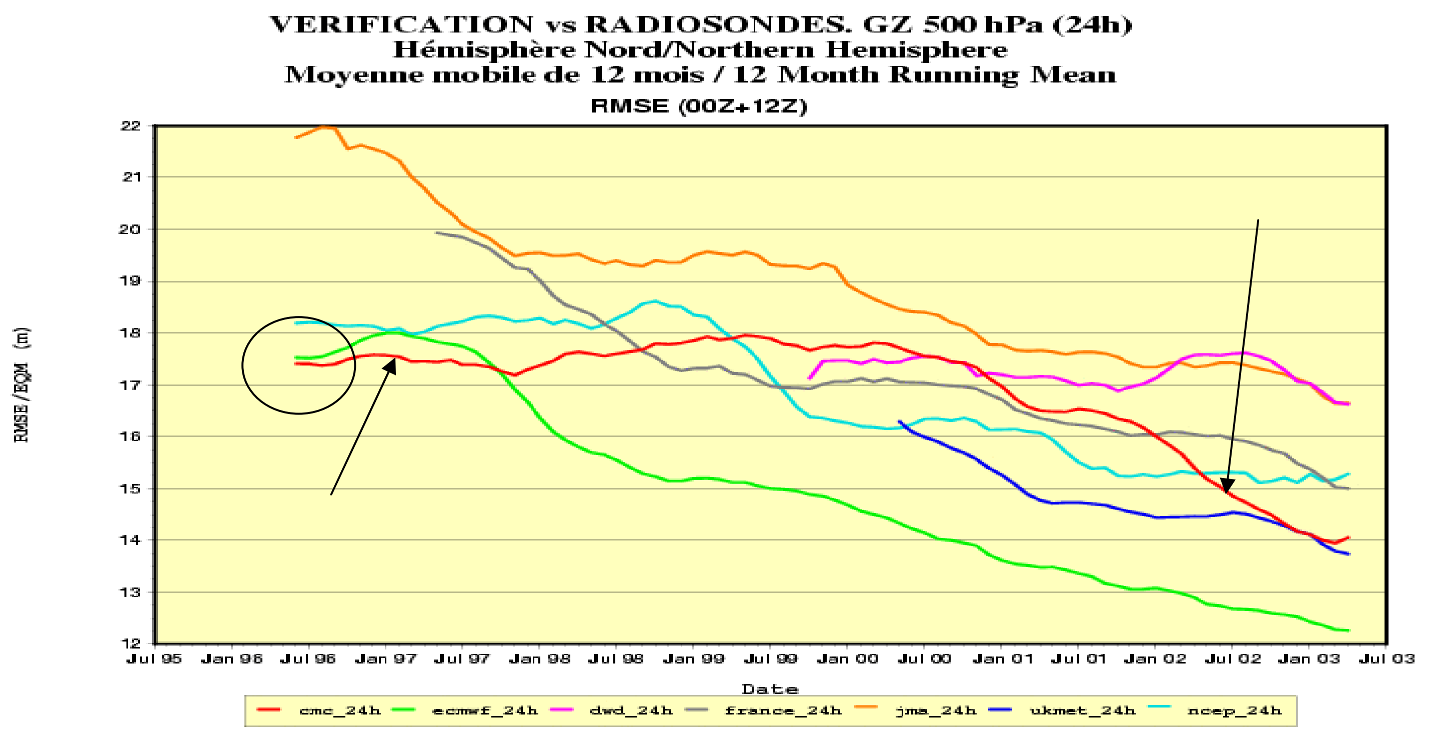
GEM skill score



CMC NCEP UK MetOffice ECMWF

GEM-Chemistry Modules

- Tracer transport – native to GEM
- Tracer convection
- Tracer vertical diffusion

- Emissions
  - Anthropogenic
  - Biogenic
  - Biomass burning
  - Lightning NOx
  - Aviation emissions

GEM-Chemistry Modules

- Gas phase chemistry
  - Trop. 50 species, ~130 reactions
  - Trop+strat 75 species, ~200 reactions
  - Fast Newton solver
- Photodissociation rates (J values)
  - from Messy
  - table look-up
- Heterogeneous chemistry (PSC…)
- Aerosol chemistry and physics
  - 5 size-resolved aerosol types
  - 12 bins each – 60 tracers

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Ongoing model evaluation

- Urban
  - Pacific 2001 – Vancouver (10 & 2 km)
  - ESCOMPTE – 2001 Marseilles (3 & 1km)
  - Krakow – 2005 (2.5km)
- Regional
  - North America – surface ozone (PM2.5)
  - Brazil - TROCCINOX
  - Quebec fires 2002
  - ICARTT
  - EU heat wave - 2006

Ongoing model evaluation

- Global (1.5^ox1.5^o)
  - CO from Aura-MLS
  - CO from MOPITT
  - Ozone – GOME
  - Ozone – Logan climatology
  - Aerosols – AON/AERONET/AEROCAN
  - Composite data from aircraft (Emmons et al., 2000)
  - SCIAMACHY tropospheric column NO_2
  - ACE – biomass burning

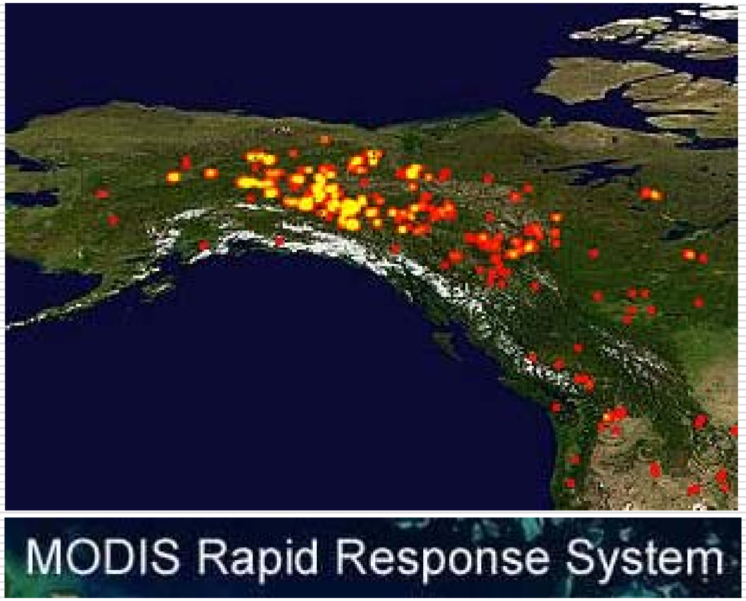
Alaskan and western Canadian wildfires in the summer 2004 GEM–AQ simulations and comparison with measurements

A. Lupu, J.W. Kaminski, L. Neary, J.C. McConnell, J. Jarosz,
C. Rinsland, P. Bernath, K.A. Walker, C. Boone,
N.T. O'Neill, E.J. Hyer, and J.S. Reid

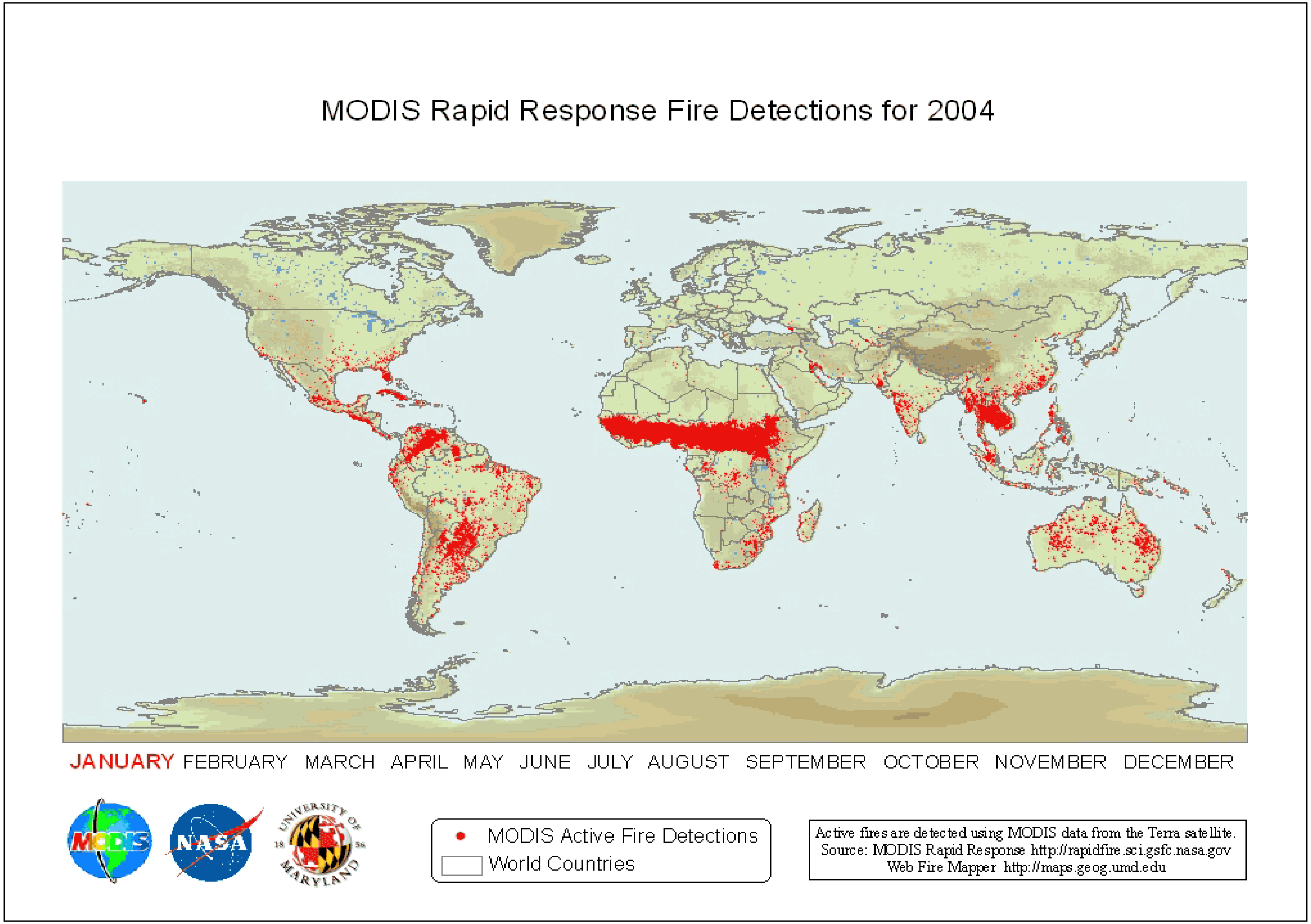
Alaska–Yukon Fires in June–July 2004

- Triggered by lightning in mid-June
- 2.6 million ha burned in Alaska
- 3.1 million ha burned in Canada
- Largest fire season on record in North America
- Lasted until the end of September

Global fire map for period 06/29–07/08



Fire Detection from Space



GEM−AQ Setup

BB emissions

- Monthly emissions at 1º spatial resolution from the Global Fire Emission Database version 2.0 − multiplied by 2 (MOPITT inversion studies)
- Distributed into daily emissions by using MODIS fire counts
- Emission factors from Andreae and Merlet, 2001 applied to amount of dry matter burned
- Species emitted: CO, NO, CH_3OH, HCOOH, C_2H_6, C_2H_4, C_2H_2, C_3H_8, HCHO, CH_3COOH, HCN, CH_3CN, SO_2, higher alkanes and alkenes, toluene and aromatics
- No aerosols

- 1.5º × 1.5º global uniform grid
- 28 hybrid levels up to 10 hPa
- 30-min time step
- Meteorology updated every 24 h
- Chemistry output every 1 h

Injection of emissions:

0−2 km:	30%
2−8 km:	60%
8−12 km:	10%

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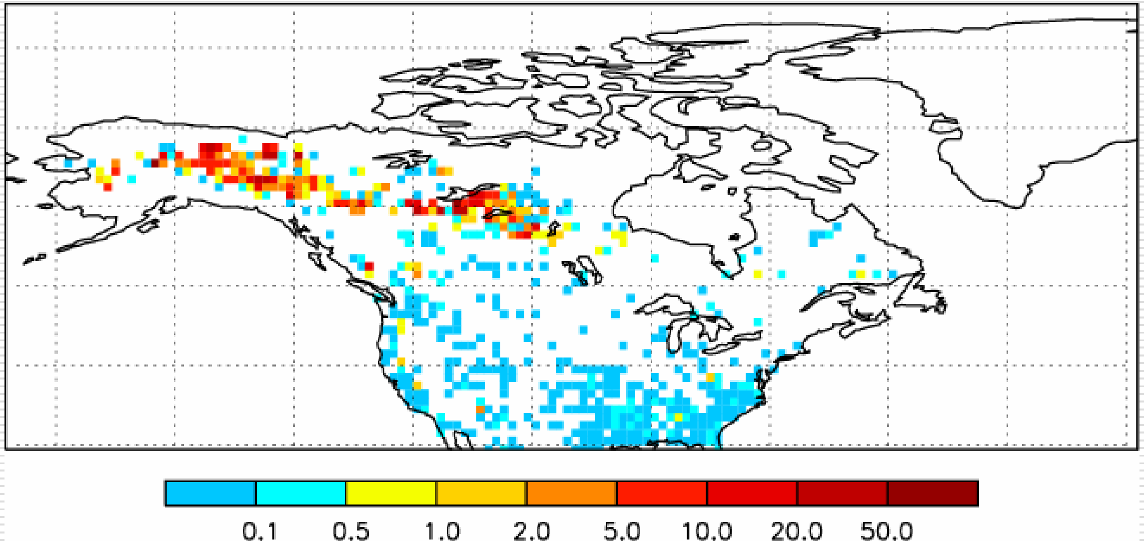
CO emissions for July 2004



CO emissions (g/m^2) from GFEDv2.
Total mass for Alaska + Canada is 6.2 Tg.

Quantifying Emissions

- Total direct carbon emissions

$$C_t = A \times B \times f_c \times \beta$$

A − burned area (ha)
B − average density of biomass (t / ha)
f_c − carbon fraction of biomass
β − fraction of biomass consumed (depends on type and intensity of fire and type of biomass)

- Species emissions

$$E_x = C_t \times EF_x$$

E_x − emission of species *x*
EF_x − emission factor (usually expressed as g species *x* / kg dry matter burned)

(Seiler & Crutzen, 1980; Andreae & Merlet, 2001)

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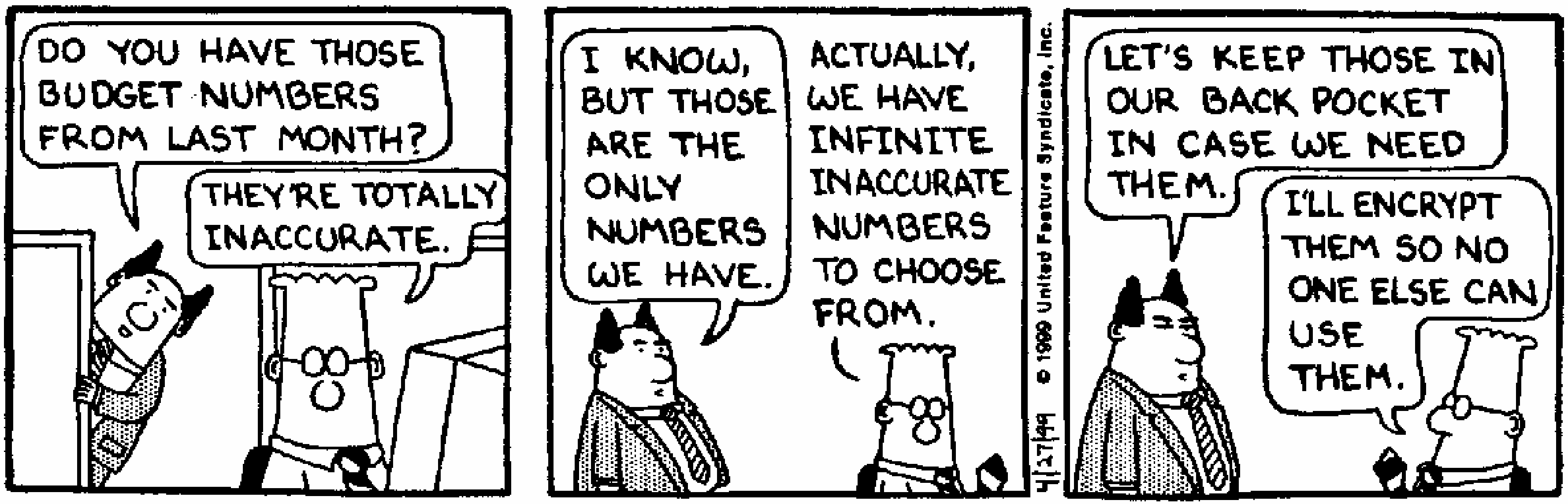
Uncertainties

- Fire Sampling: factor of 2−4
- Area burned: factor of 2
- Fuel Load: factor of 2−3
- Combustion factor: 20%
- Emission factor: 30-60%



Thanks: Jeff

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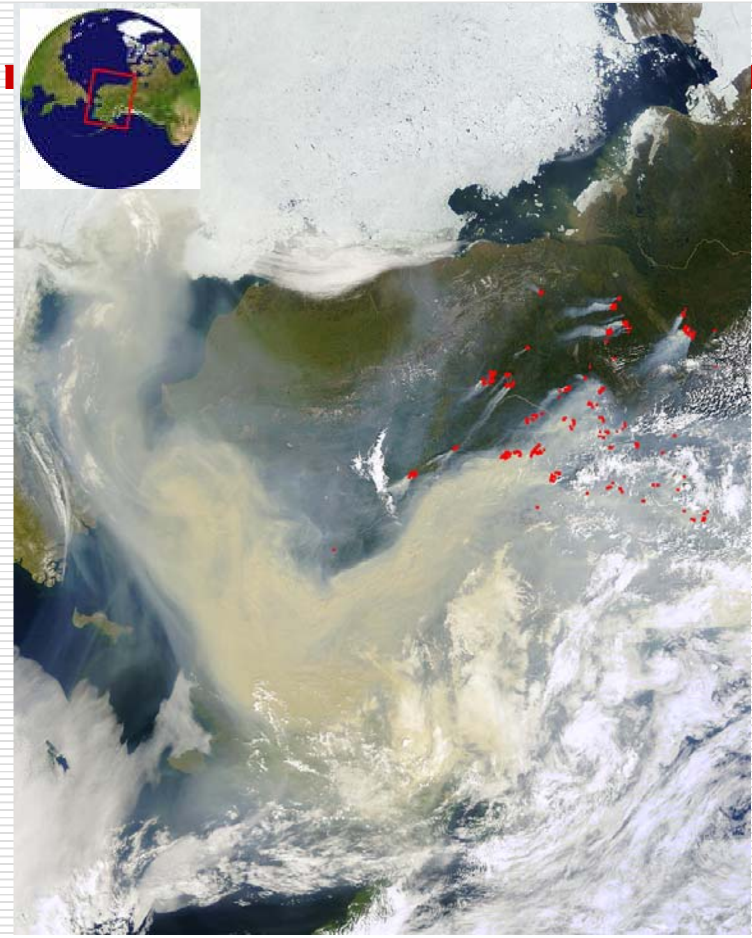
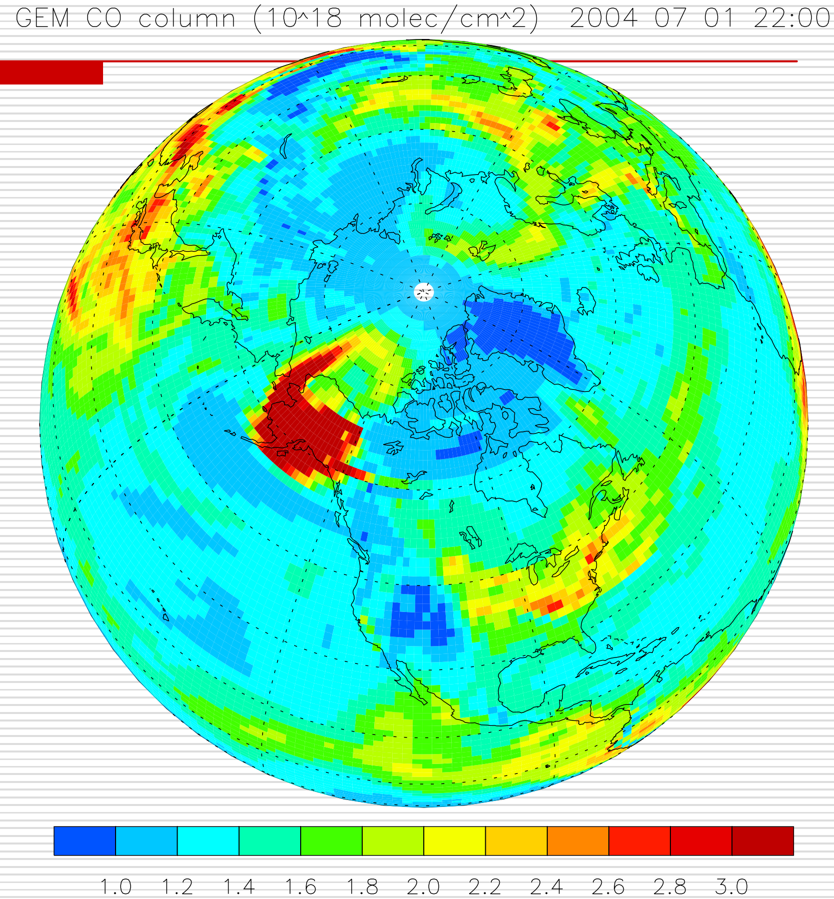
Smoke across Alaska – 1 July 2004, 2140 UTC



MODIS Rapid Response System



GEM−AQ CO column

GEM–AQ vs. TOMS AI

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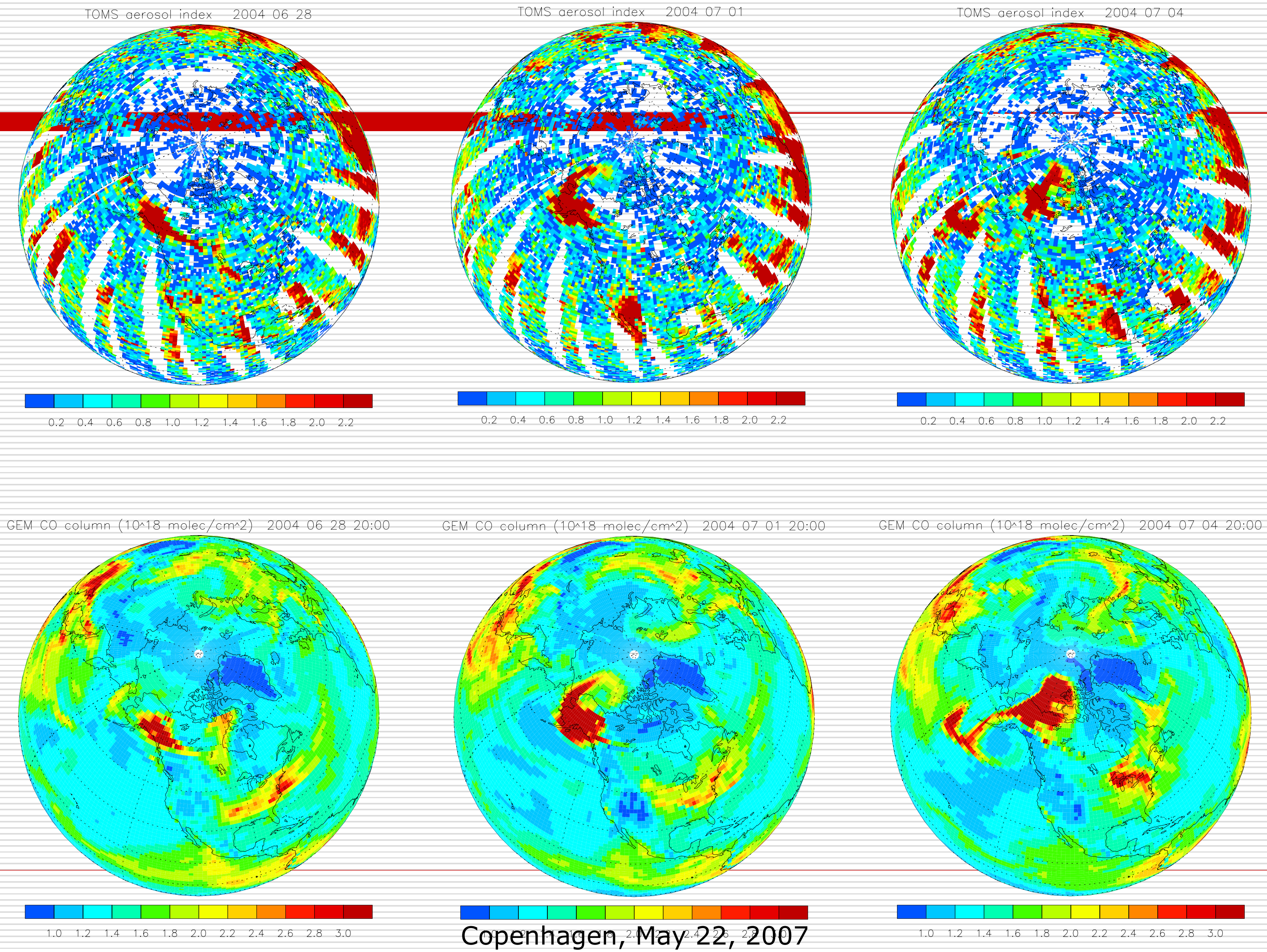
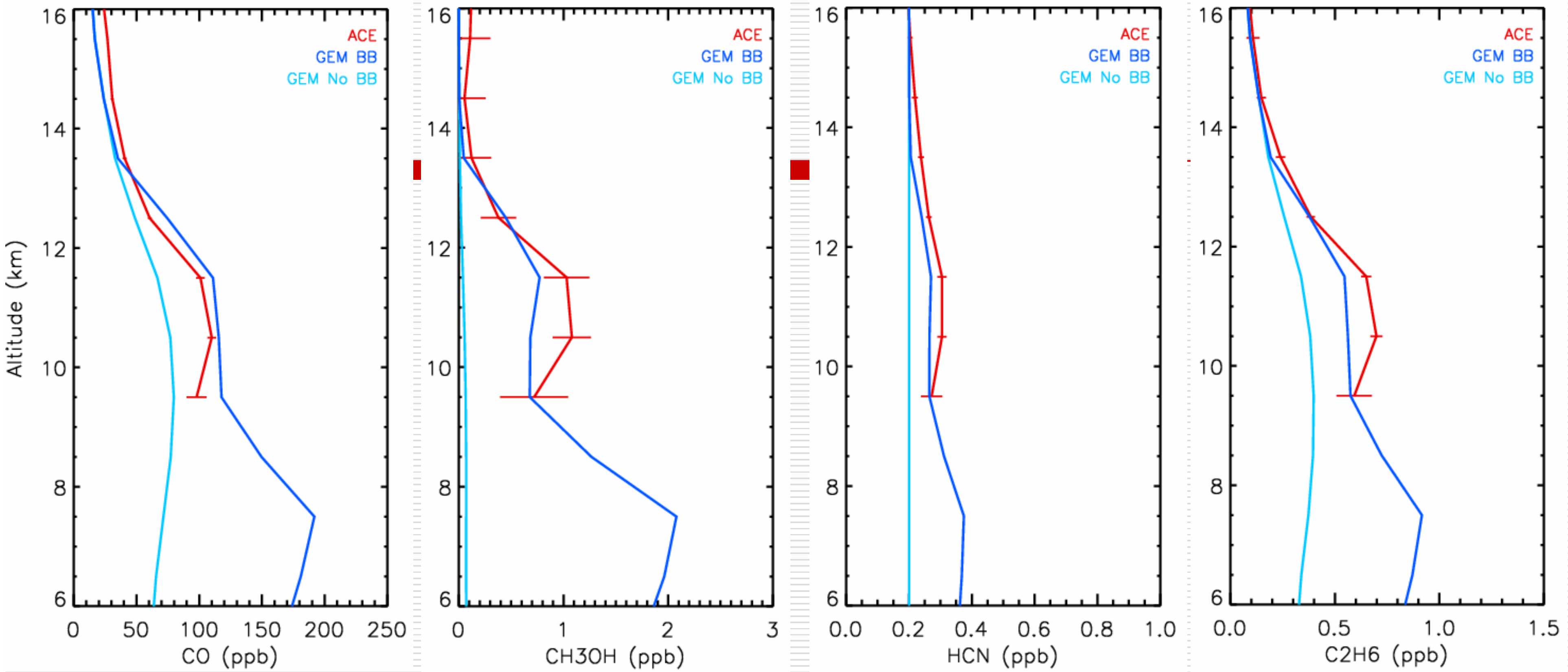


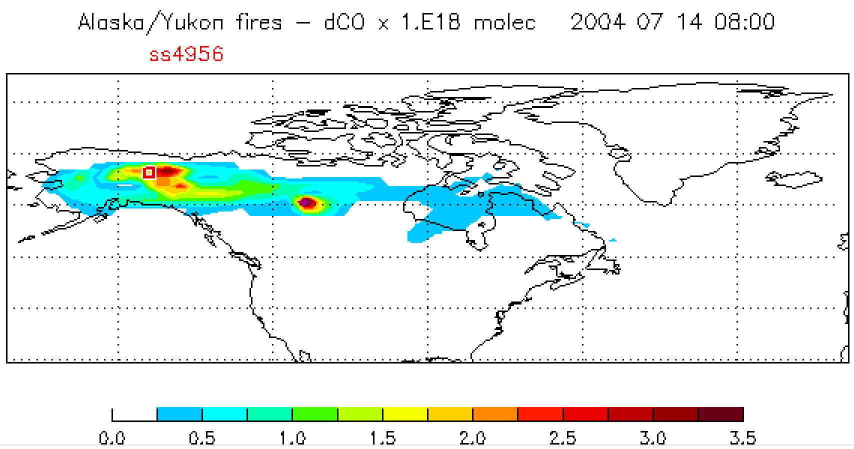
Copenhagen, May 22, 2007

ACE – Atmospheric Chemistry Experiment

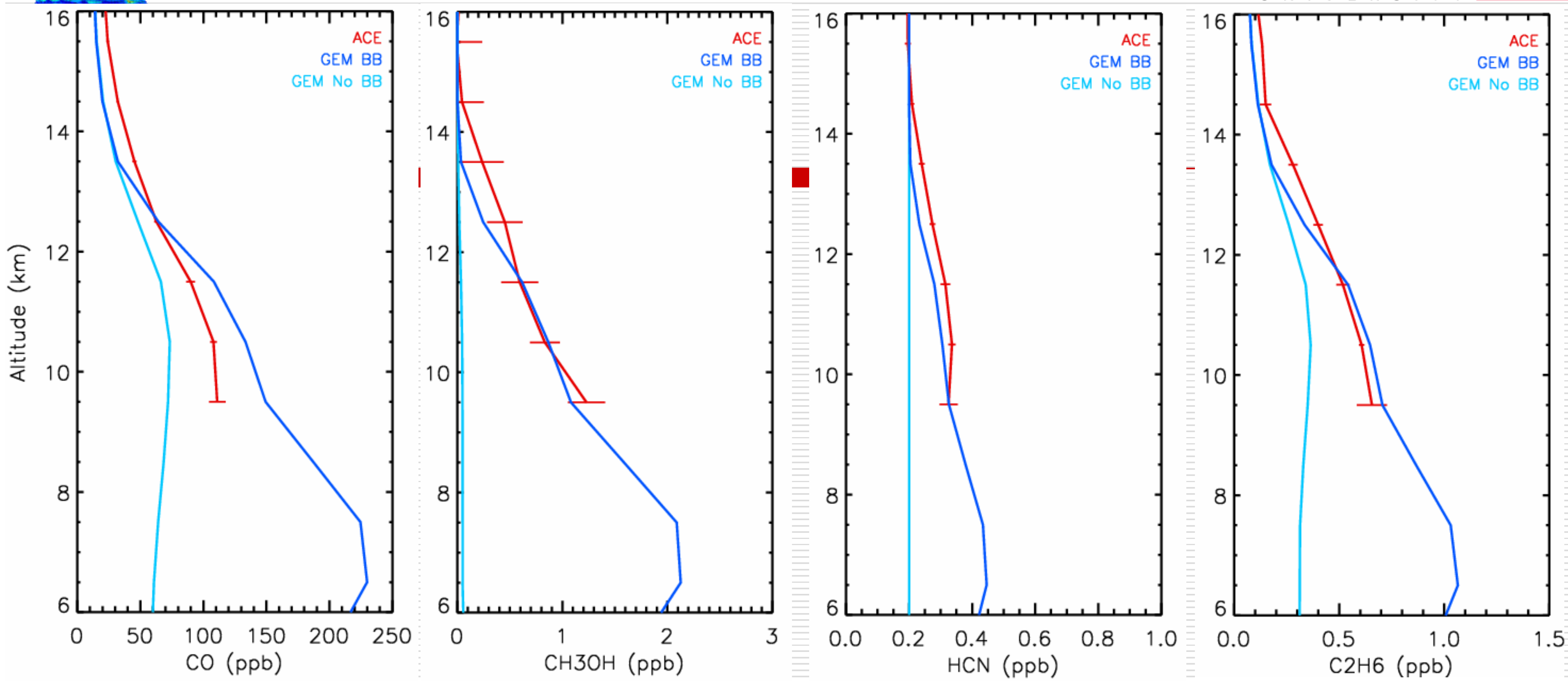
- ACE-FTS is an infrared Fourier transform spectrometer with high spectral resolution of 0.02 cm^{-1} from 750 to 4400 cm^{-1}
- onboard Canadian SCISAT-I satellite launched in August 2003 into a 74º inclined orbit at 650 km altitude
- species can be retrieved down to about 5 km

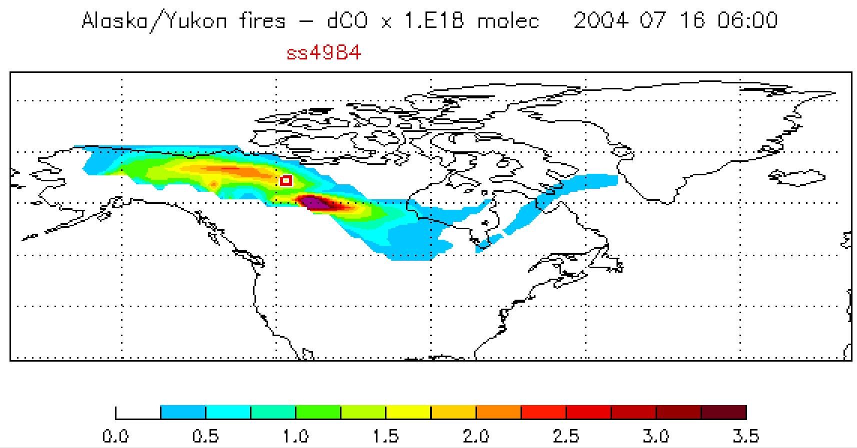
ACE occultation ss4956



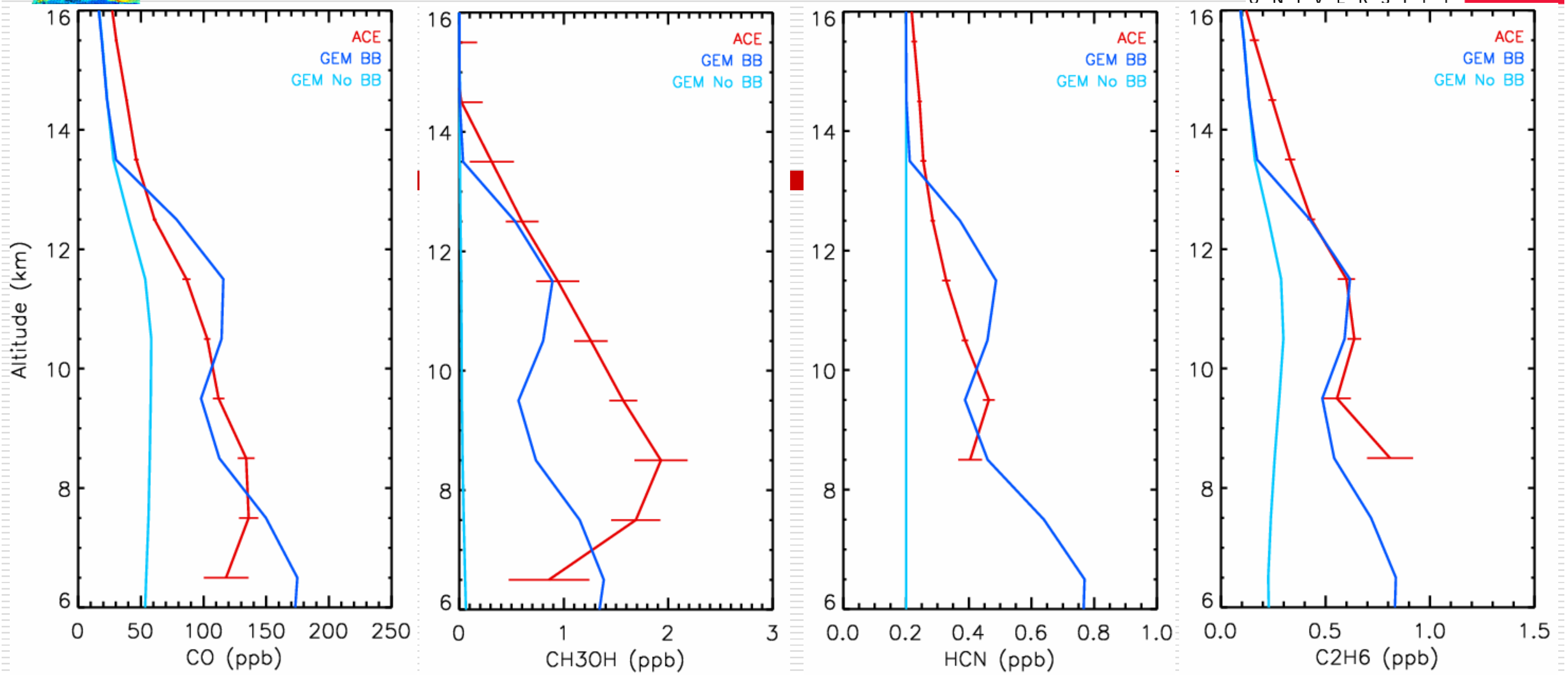


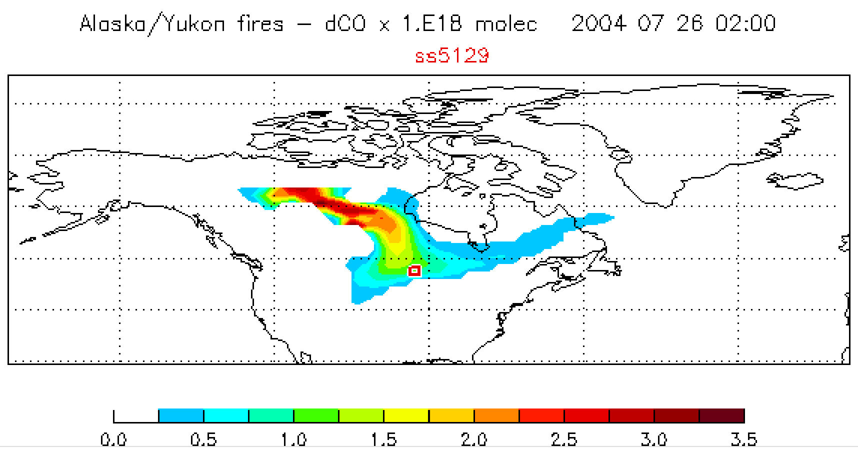
ACE occultation ss4984



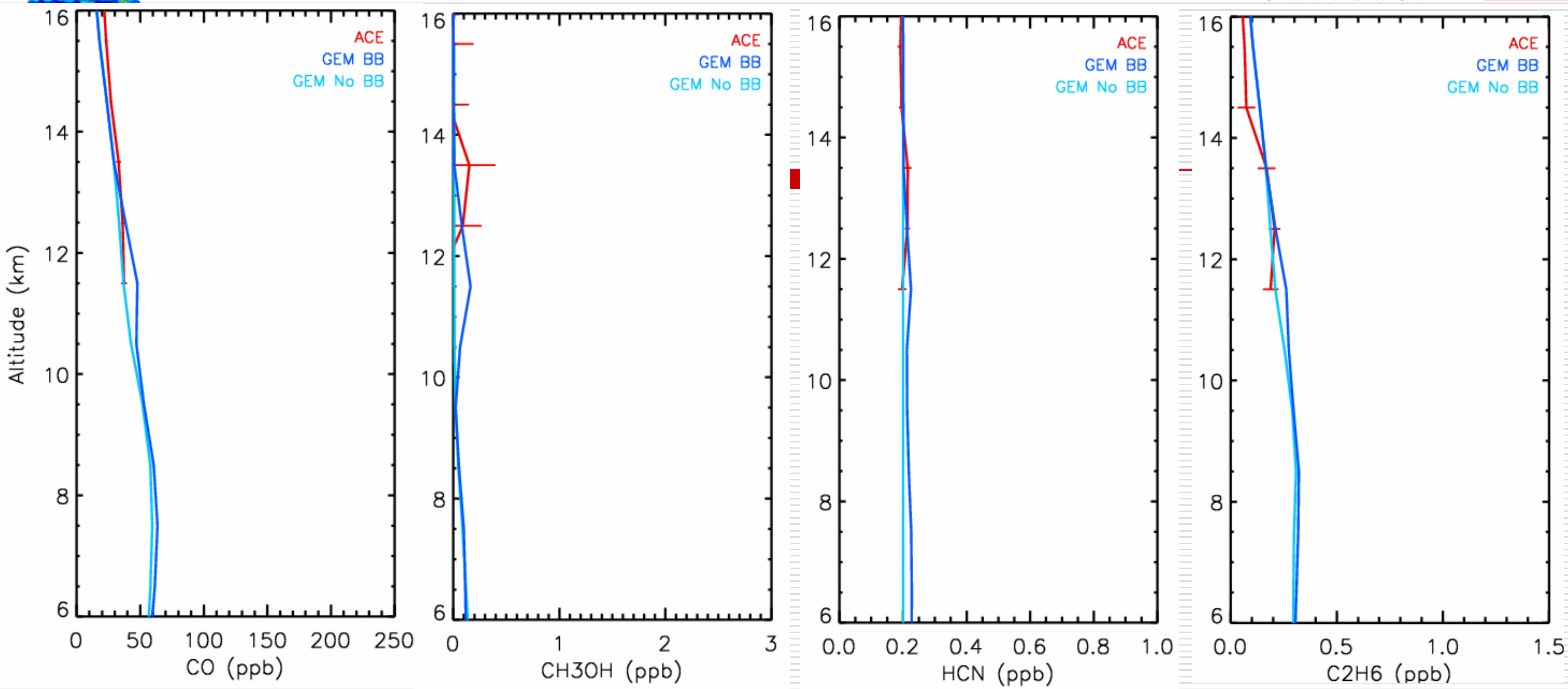


ACE occultation ss5129



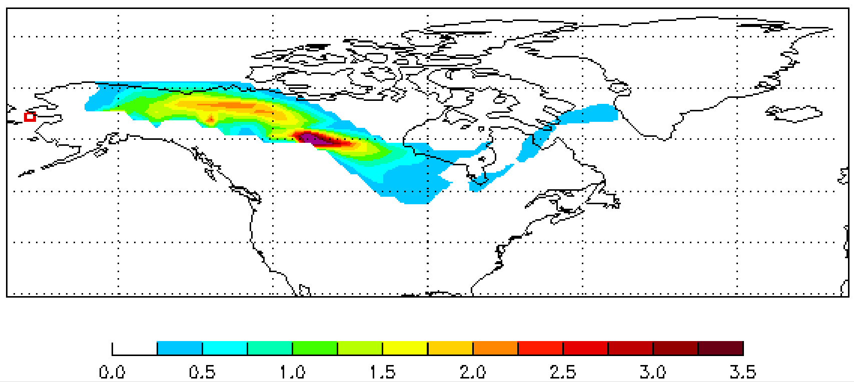


ACE occultation ss4986



Alaska/Yukon fires – dCO x 1.E18 molec 2004 07 16 09:00

ss4986



Conclusions A-Y Fires

- June-July 2004 fires seen in satellite and aircraft observations were reproduced spatially and temporally by GEM-AQ
- Sensitivity to injection heights: BB emissions have to be injected above the BL, pyroconvection
- Relative ratios of various species in the plume seem to show that the emission factors used are realistic
- There is uncertainty about the absolute value of emissions (e.g., CO from peat burning)

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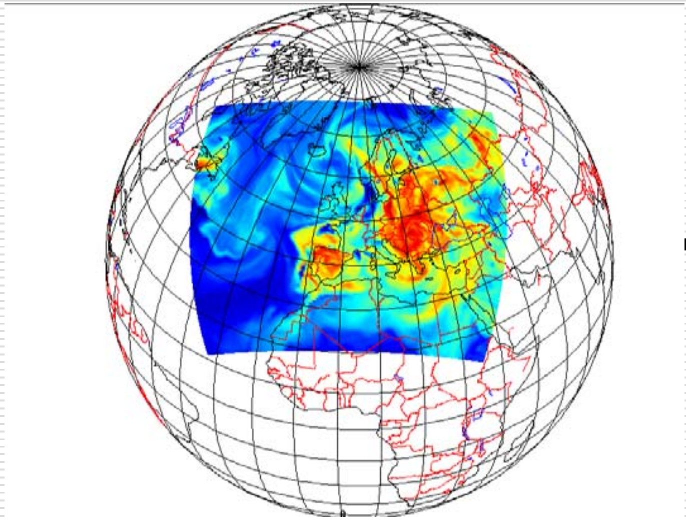
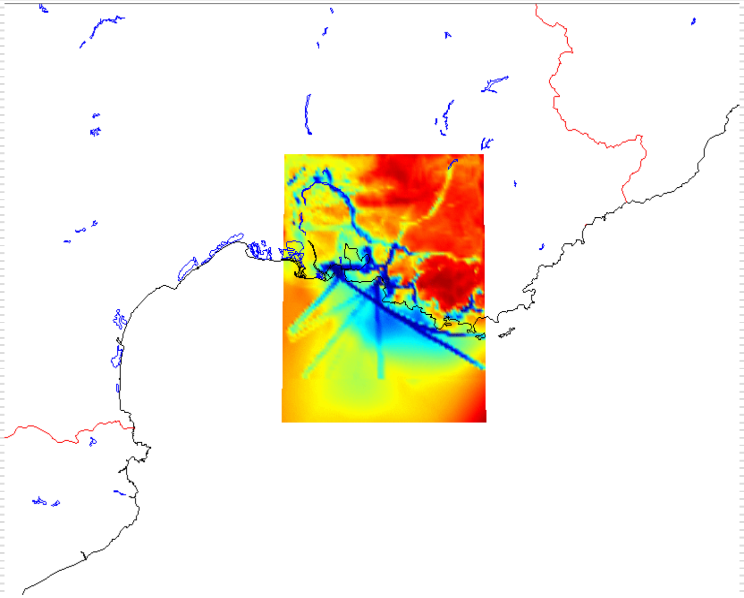
Limited Area Modelling

GEM-AQ



MC2-AQ
GEM/LAM-AQ



0.22° x 0.22° variable global

0.027° x 0.027°

ESCOMPTE Campaign - 2001

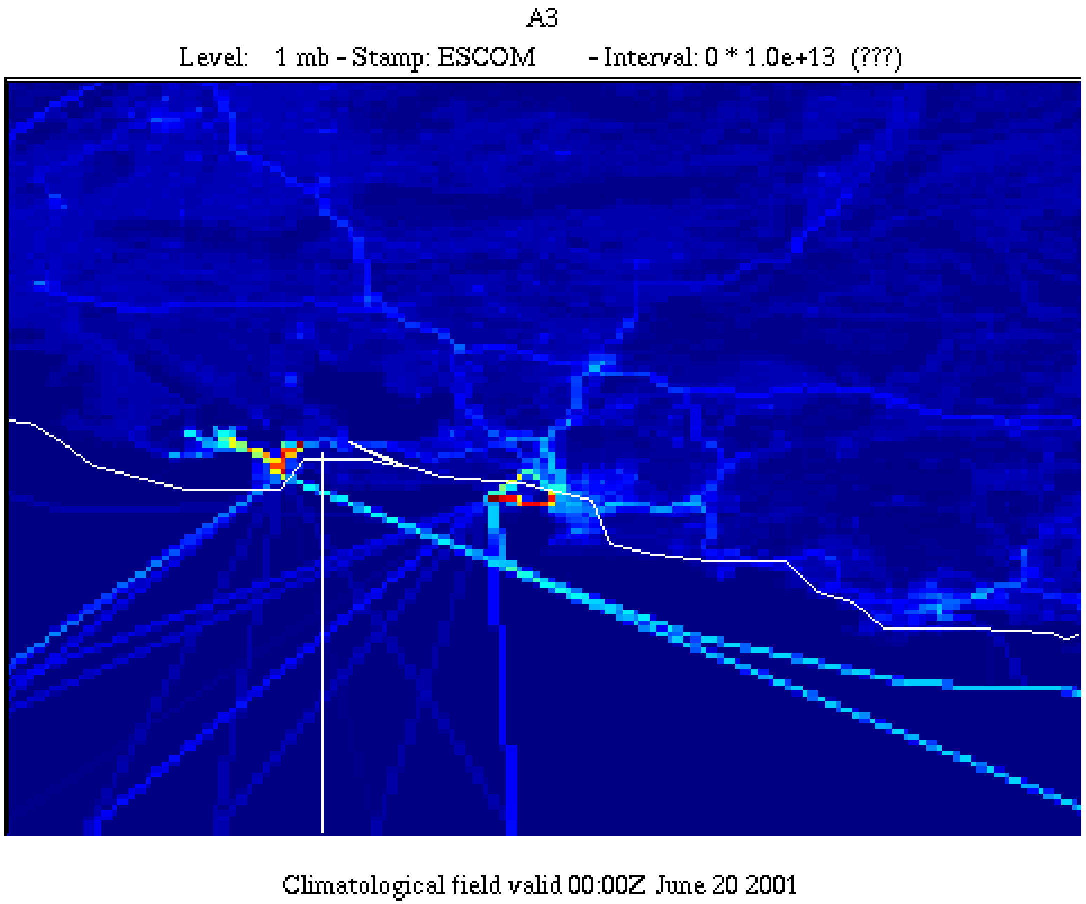
- The campaign covers 4 field experiments with different meteorological conditions in Southern France (around Marseille)

- Validation database for numerical air quality models
  - Detailed emissions inventory
  - Meteorological observations
  - Air pollutants concentrations
  - aircraft, ferry, remote sensing, constant density balloons and surface stations

- Pollutants concentrations are strongly influenced by complex circulation (land-sea breeze) and orographic effects (channelling plumes)

Escompte Emission Inventory NO surface emission - 1km

- Grid: UTM projection 140 x 140 grid points
- resolution: 1 km^2
- 21 inorganic and 126 organic species
- source types:
  - area emission
  - point source emission



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Stratospheric intrusion

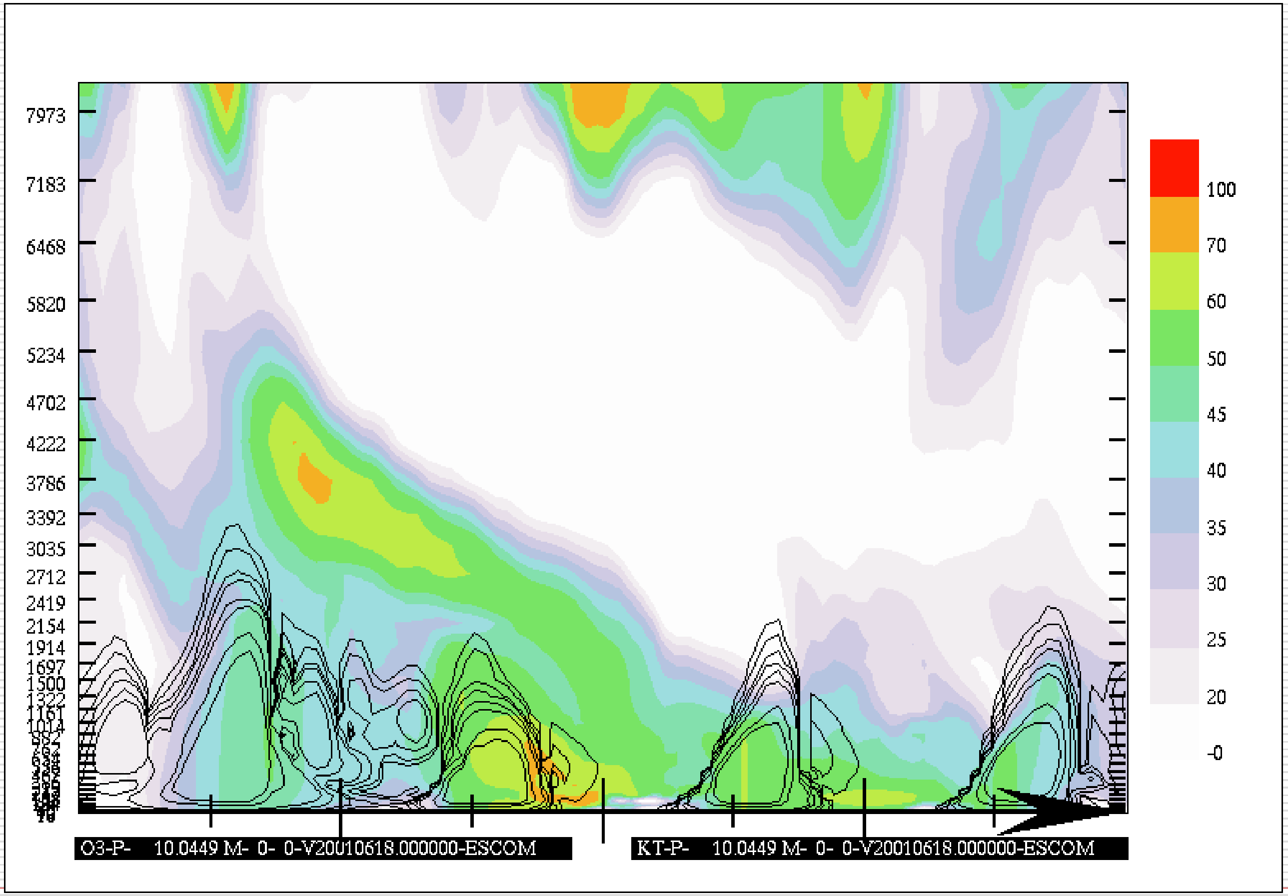

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Photo-oxidants formation and transport over Europe during the heat wave period in July 2006

Joanna Struzewska
Warsaw University of Technology, Warsaw, Poland

Jacek W. Kaminski
York University, Toronto, Canada

Copenhagen, May 22, 2007

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Heat wave development

- Based on weather services reports:
  - July 3rd - Heat wave in Western Europe (France)
  - July 4th - Hot air reached Central Europe
  - July 6th - Severe thunderstorms over Western Europe
  - July 7th - Hot air from over Africa passing towards Lithuania and Latvia
  - July 13th High air temperature across Europe – African air from the south-west and air from Asia from the east

Aim of the study

- Analysis of photochemical pollution during first heat wave period over Central Europe in July 2006 (July 3 – 14)
  - Analysis based on GEM-AQ model simulation over Europe
  - Meteorological situation over Europe used for the interpretation of air quality indices
- GEM-AQ model evaluation:
  - Meteorological and air quality measurements - 14 stations from Poland
  - Ozone measurements - 5 UK and 4 French stations (Airparif)
  - 2 stations from Lithuania
  - Station type: rural / background

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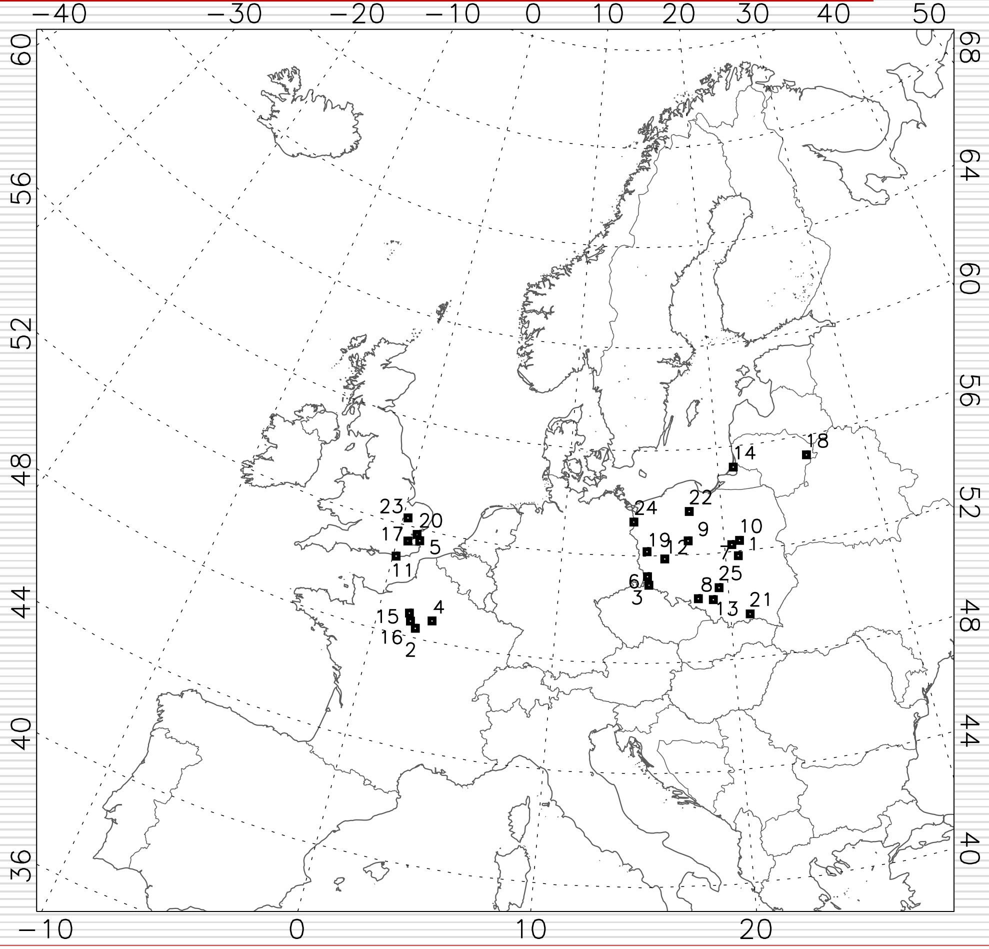
AQ Stations



Station names

1 – Belsk
2 – Bois–Herpin
3 – Czerniawa
4 – Est–Saints
5 – Harwell
6 – Jeleniow
7 – Kampinos
8 – KedzierzynKozle
9 – Krzyzowka
10 – Legionowo
11 – Lullington–Heat
12 – Mscigniew
13 – Olkusz
14 – Preila
15 – Purnay–le–templ
16 – Ramboulliet
17 – Rochester
18 – Rugsteliskes
19 – Smolary_Bytnickie
20 – St–Osyth
21 – Szymbark
22 – Tuchola
23 – Wicken–Fen
24 – Widuchowa
25 – Zloty_Potok

GEM-AQ experiment setup

- Grid: global variable resolution mode
  - 0.135 deg (~15 km) over Europe (core)
  - 400 x 350 (core)
- Time span: 3 - 14 of July 2006
- Time step: 450 s.
- Modelling strategy
  - OA every 6 hours used to produce trial fields
  - Chemical initial conditions from 5-year run with GEM-AQ, 1.5x1.5 deg. uniform resolution

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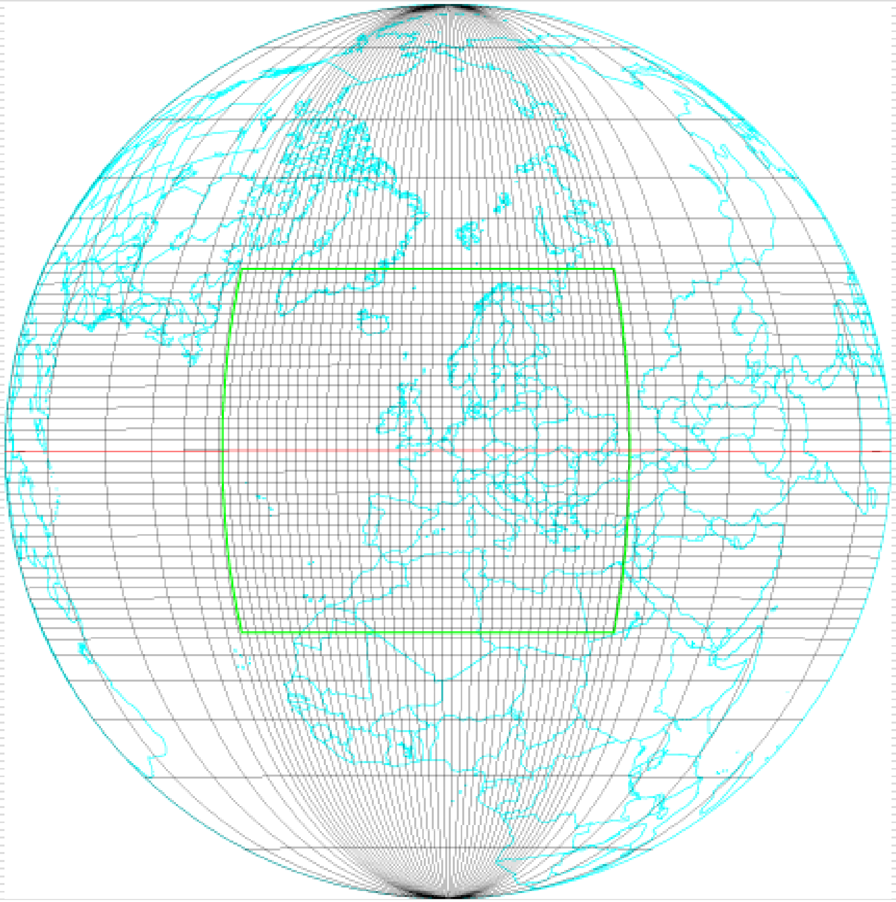
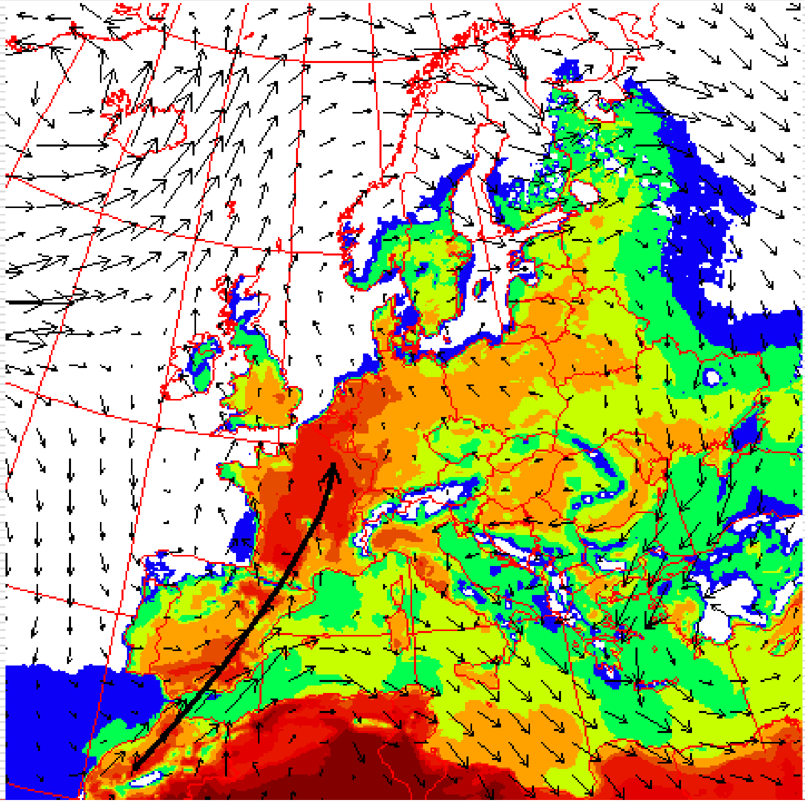
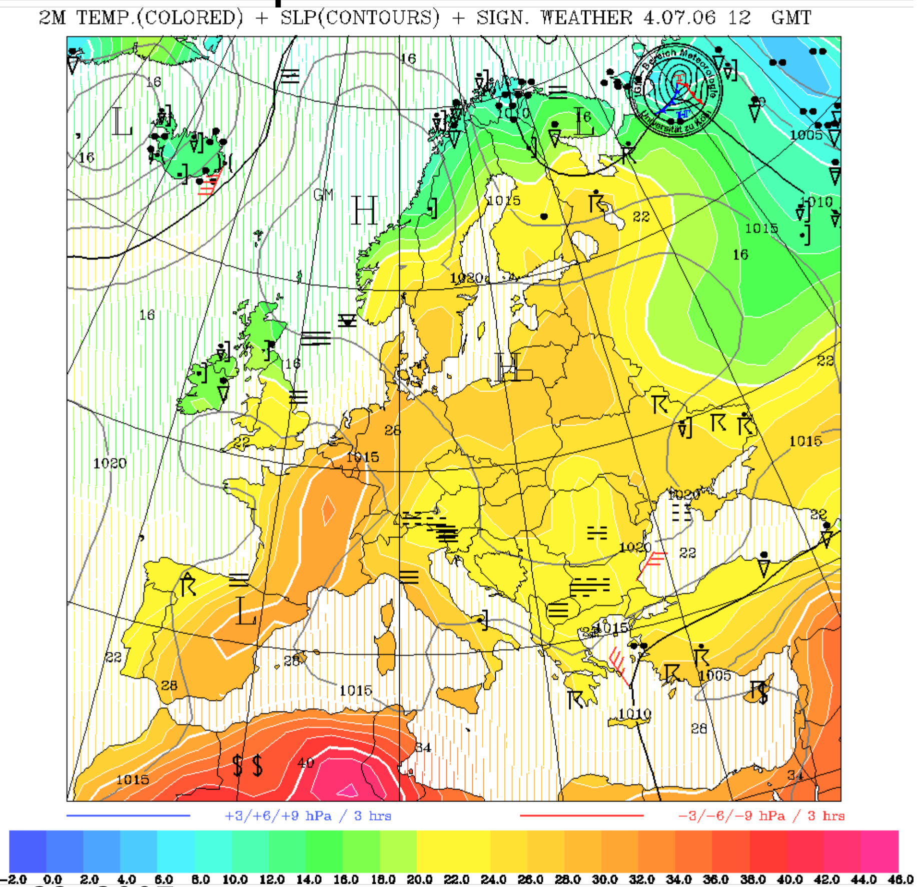
GEM-AQ – global variable grid



Synoptic situation July 4th

- Low pressure system forced transport of hot air masses towards Western Europe





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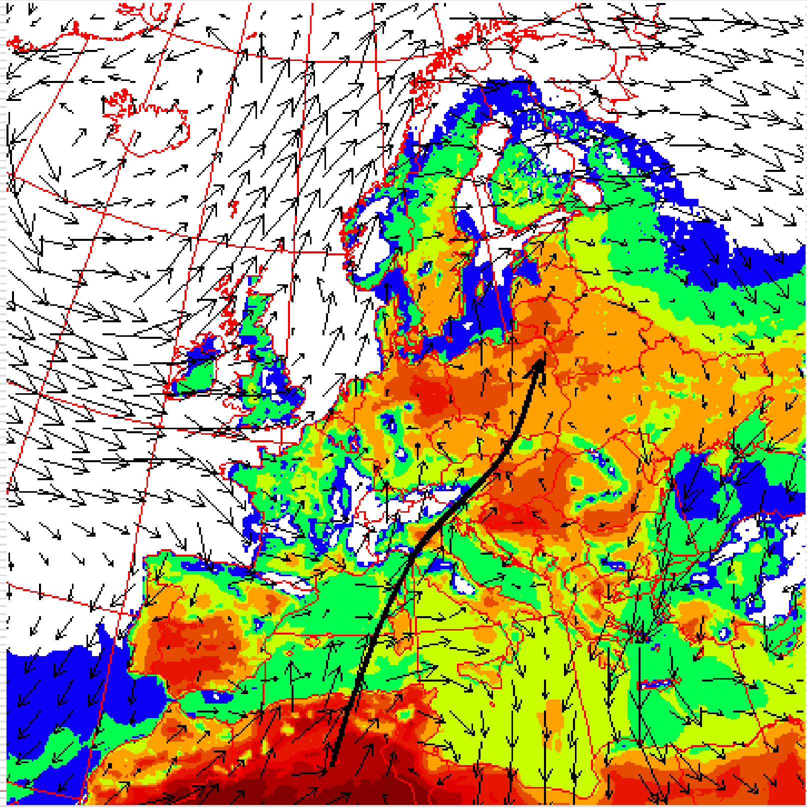
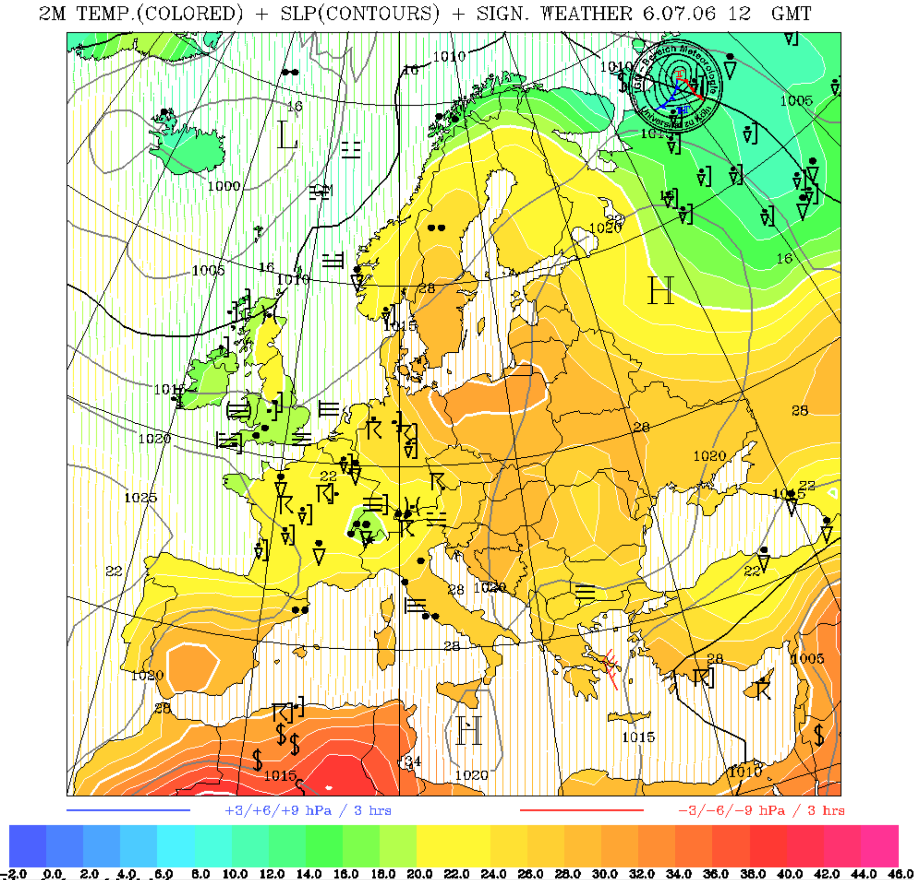
Synoptic situation July 6th

- Mutual location of pressure systems over Africa and Central Europe allowed for transport of hot air masses to the north





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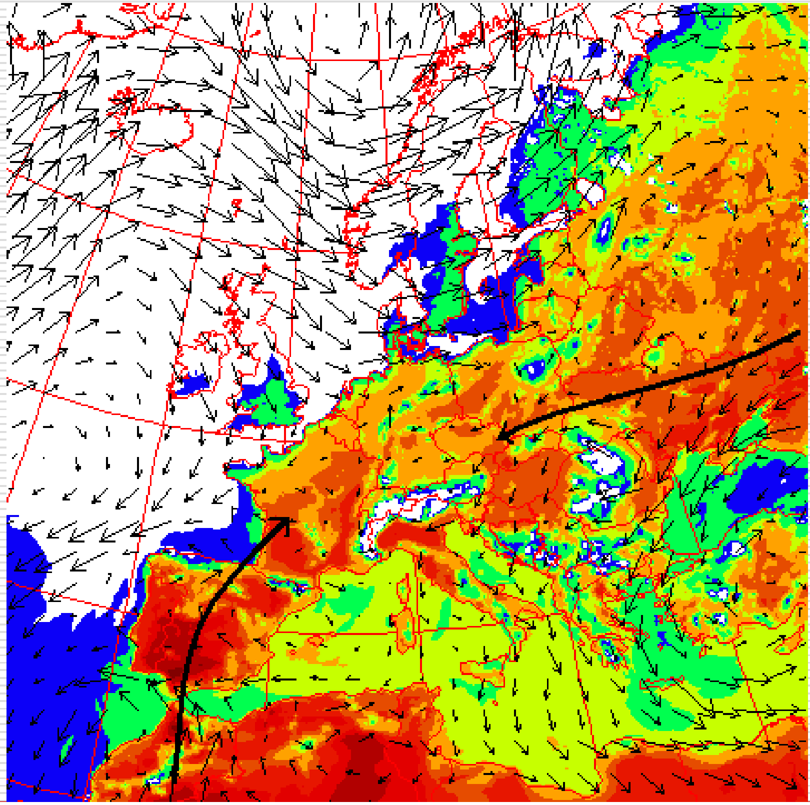
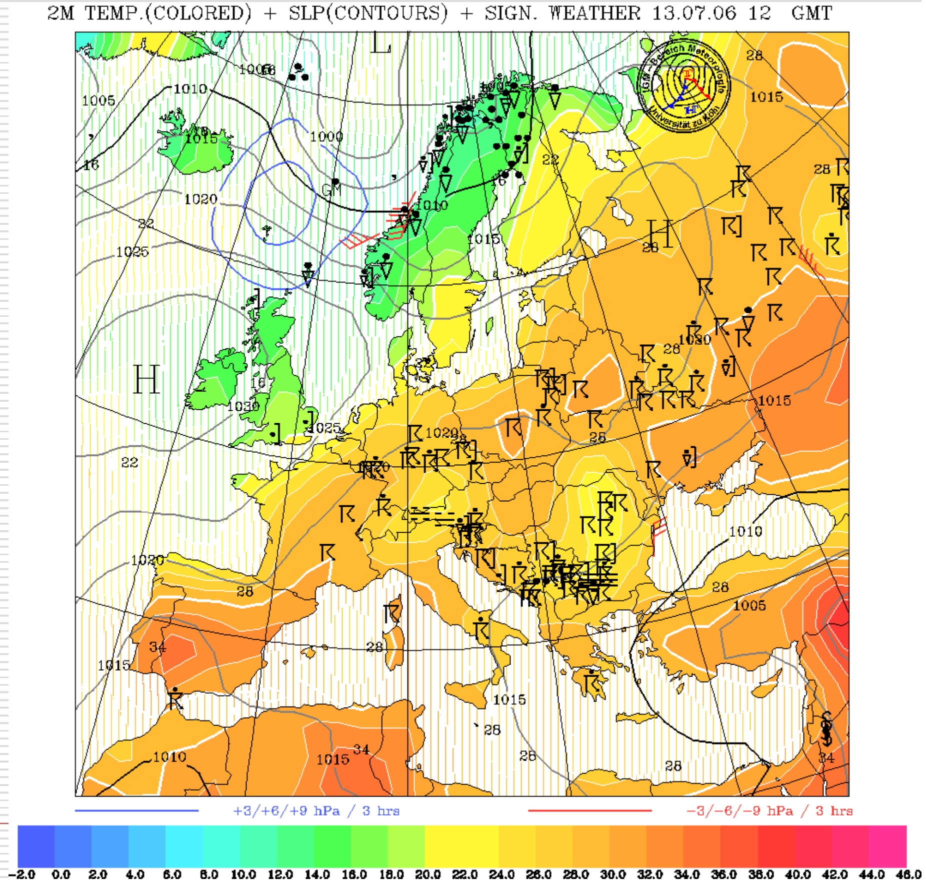
Synoptic situation July 13th

- Circulation patterns causing the transport of hot air masses towards Europe from the south and east





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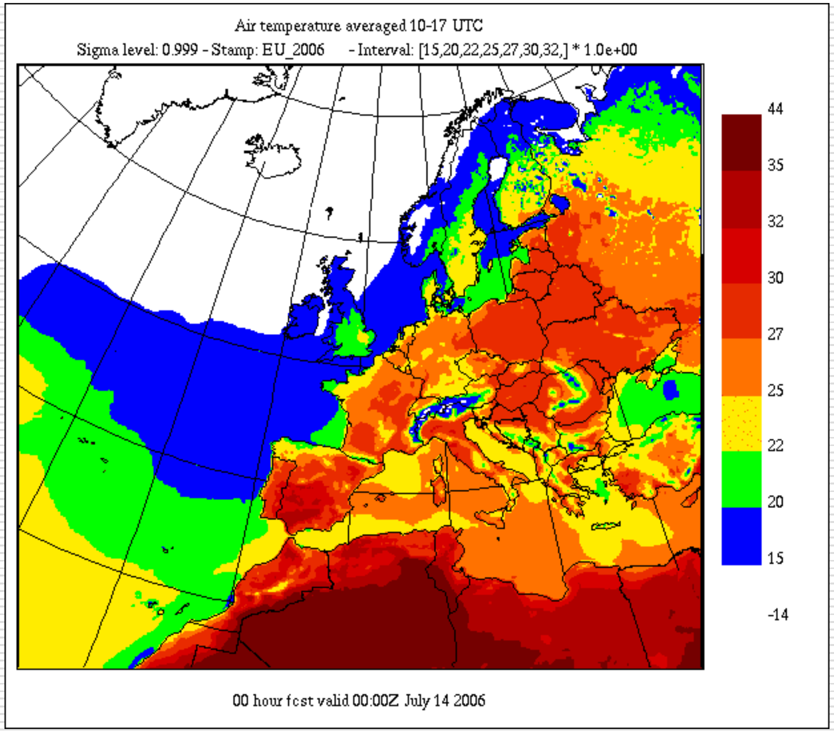
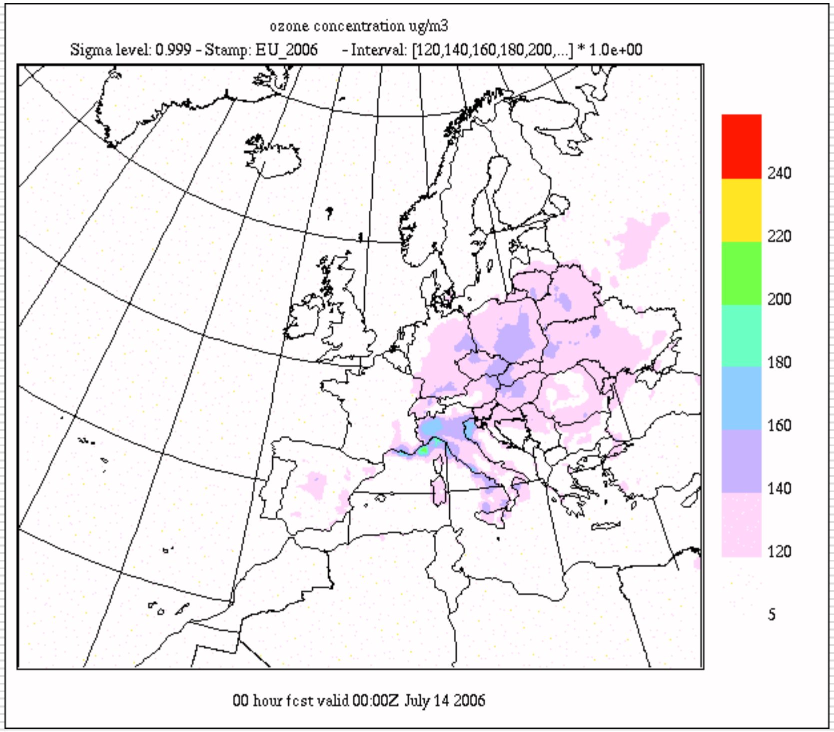
8-hour average temperature and O_3





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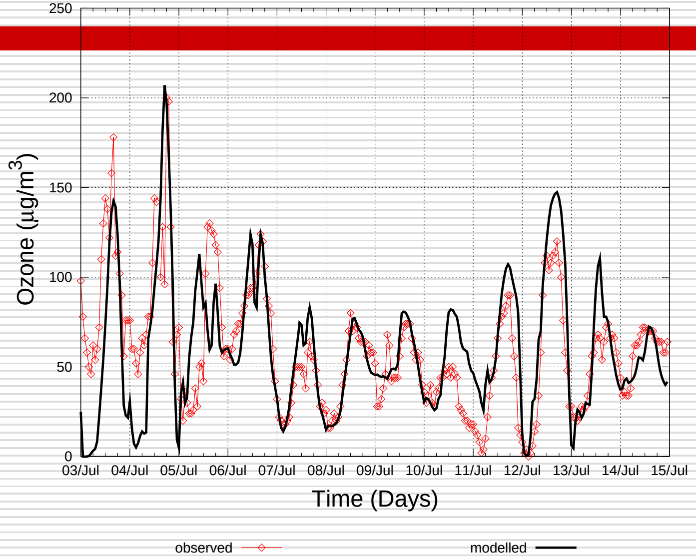
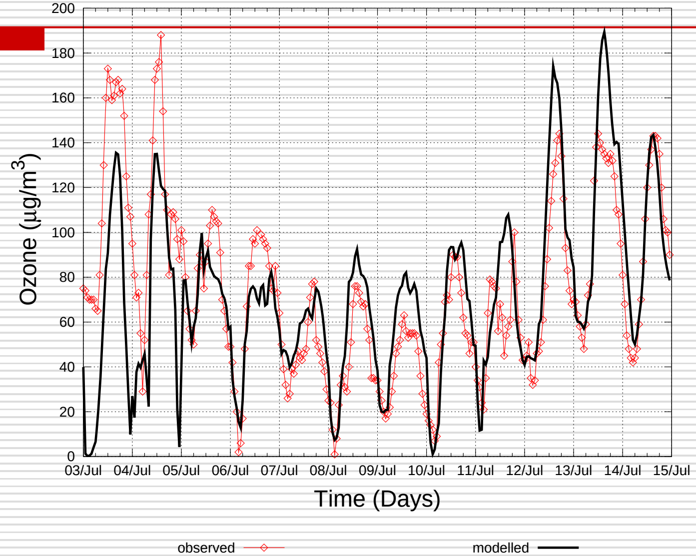
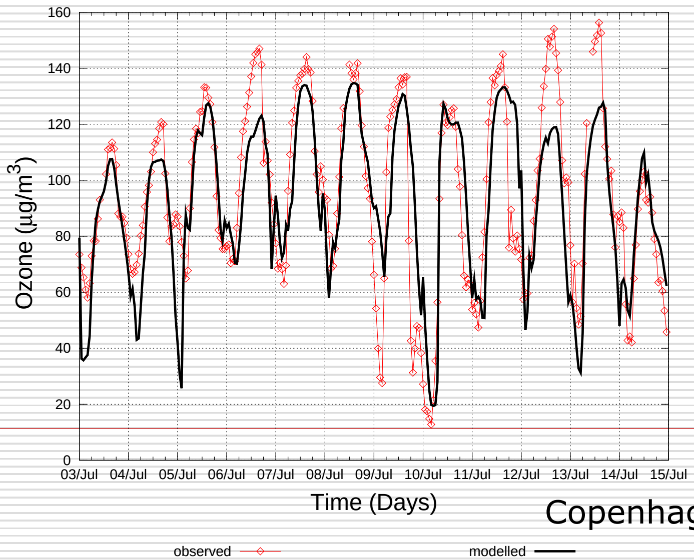
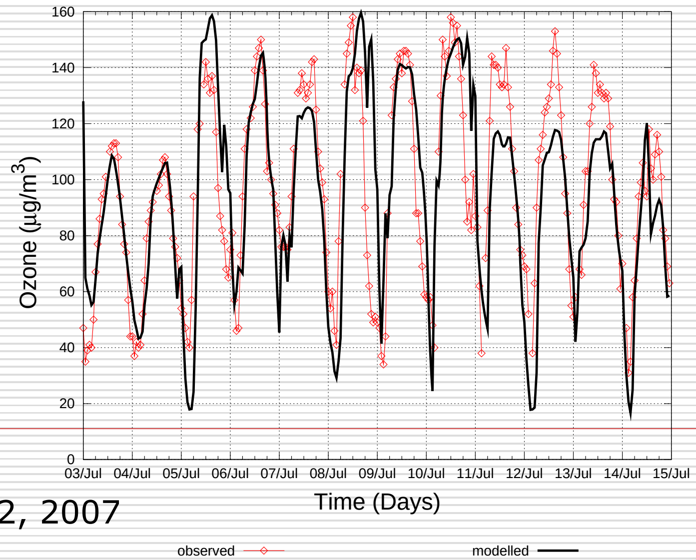
Ozone @ F and PL stations



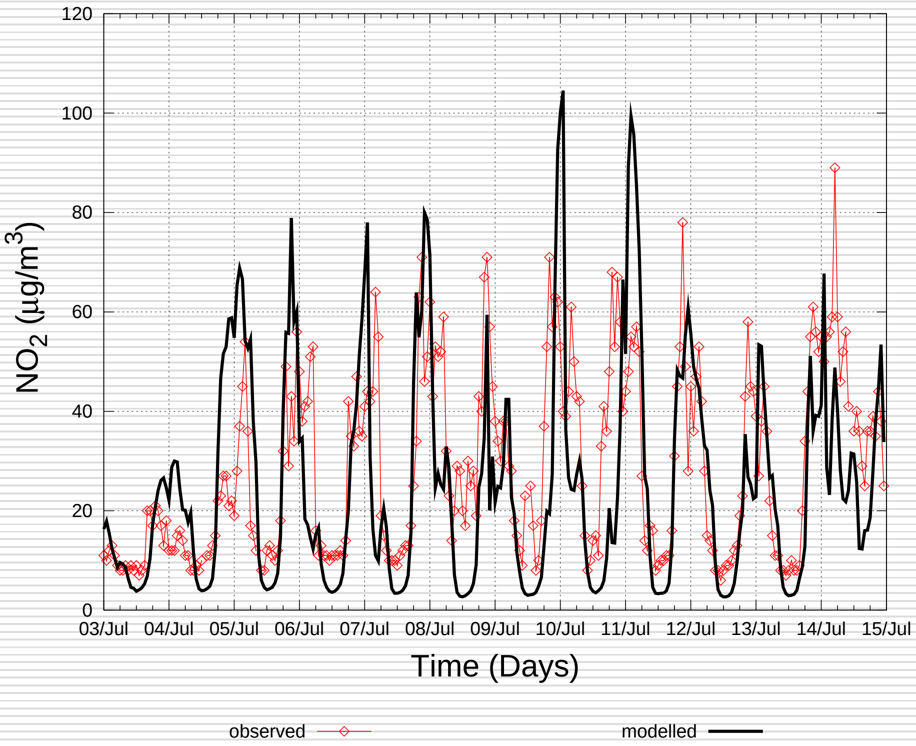


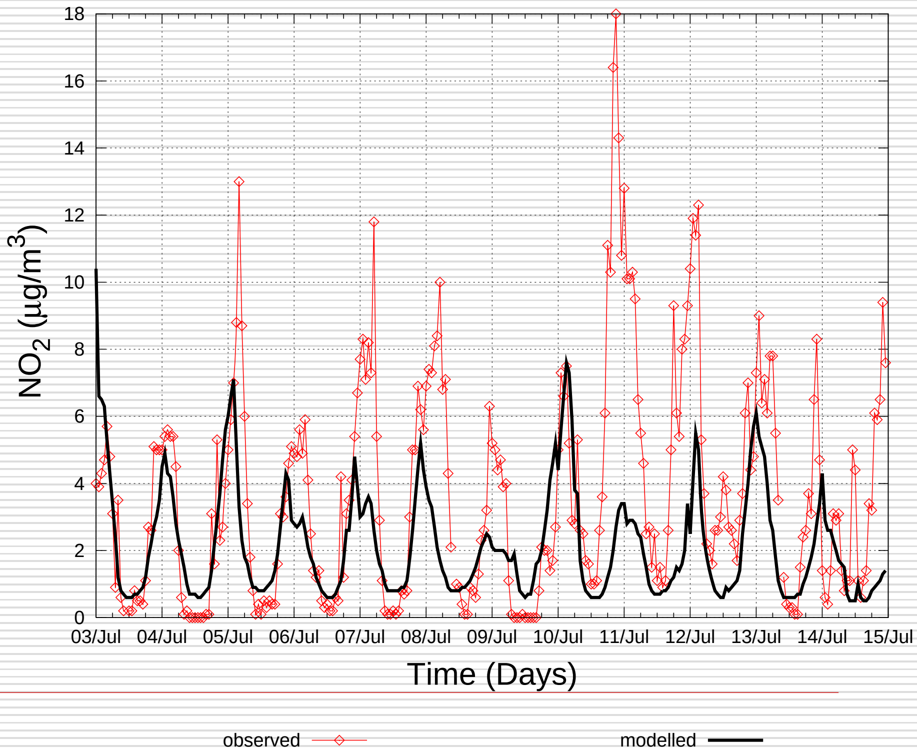


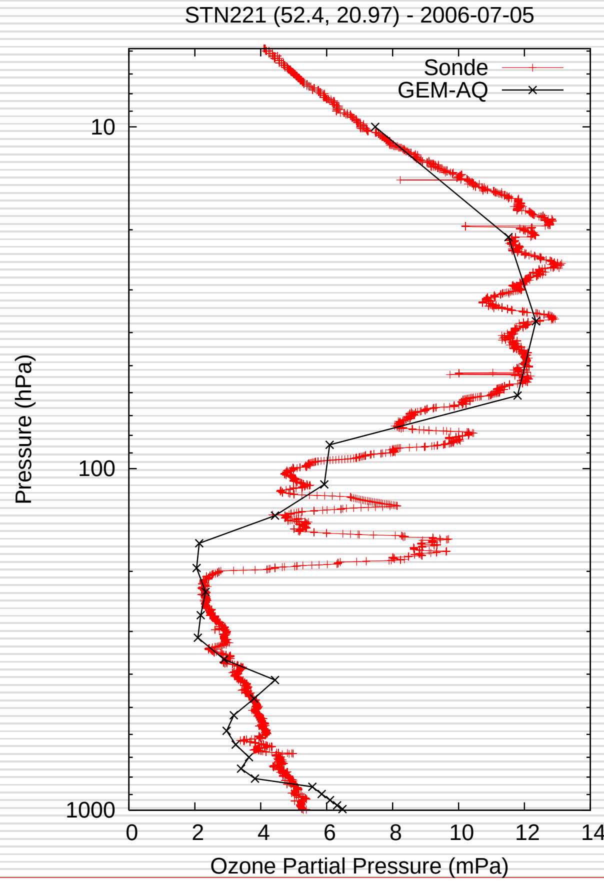


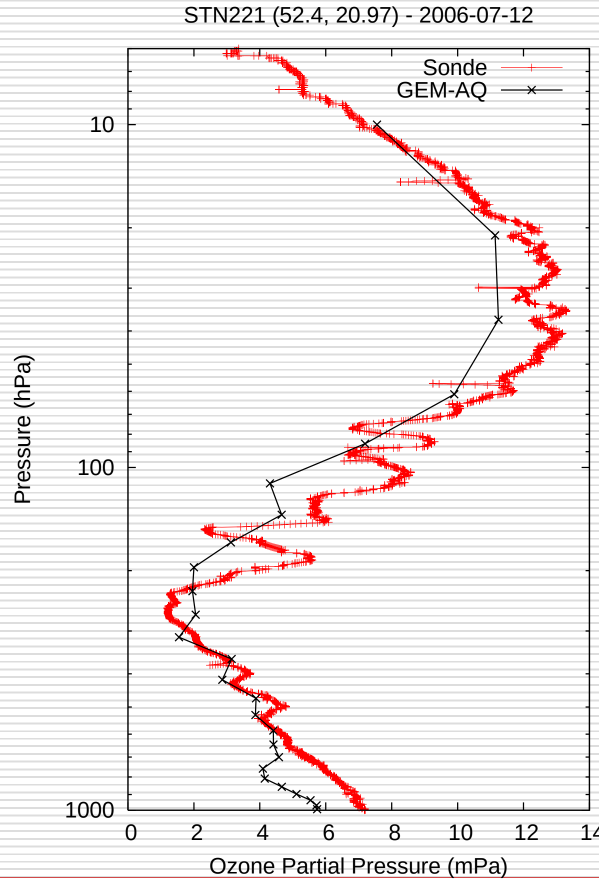
AMDAL

NO2 @ PL stations






STN221 (52.4, 20.97) - 2006-07-05
Sonde
GEM-AQ
Pressure (hPa)
10
100
1000
0
2
4
6
8
10
12
14
Ozone Partial Pressure (mPa)


STN221 (52.4, 20.97) - 2006-07-12
Sonde
GEM-AQ
Pressure (hPa)
10
100
1000
0
2
4
6
8
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Ozone Partial Pressure (mPa)

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Summary

- The on-line GEM-AQ model reproduced correctly development of pressure systems and inflow of hot air masses towards Europe
  - Good agreement with surface synoptic maps and meteorological measurements
- Heat wave during the first week of July 2006 was connected with the development of low pressure system over France and favourable anticyclonic circulation over Central Europe

Summary

- The GEM-AQ model reproduced high ozone concentrations during heat wave period
- Good agreement with O_3 measurements (rural-background station type)
  - Ozone variability better reproduced for UK and French monitoring stations
    - Emission data might be less accurate for Central-Eastern Europe
    - Biogenic emission used for this study might not be representative for heat wave period
  - For some Polish stations ozone concentrations slightly overestimated especially during nighttime

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The final challenges

- OSSE - Observation Simulation System Experiment
- Instrument design and location/orbit selection
- Application of weather prediction and atmospheric chemistry to other environments

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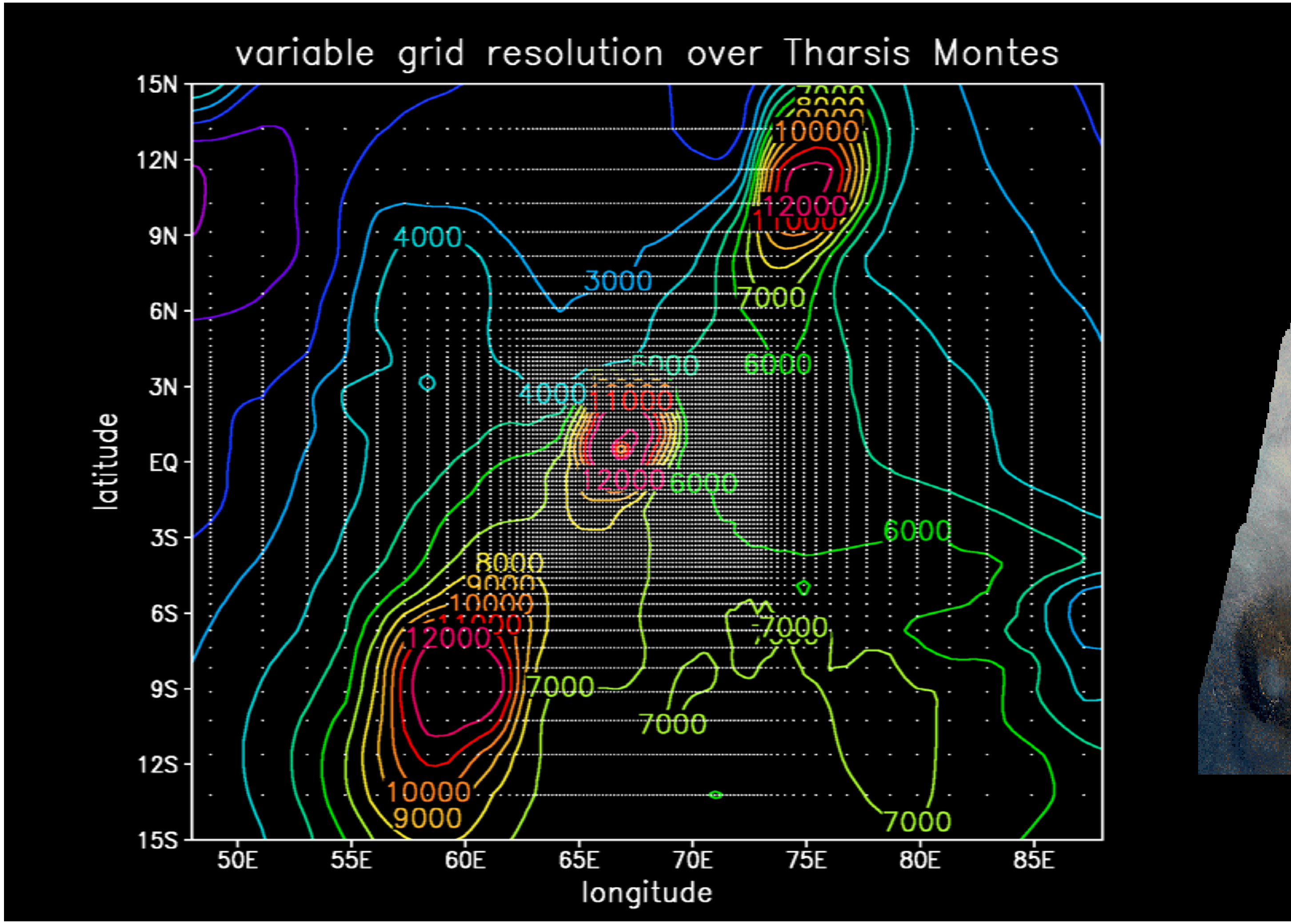
variable grid resolution over Tharsis Montes
latitude
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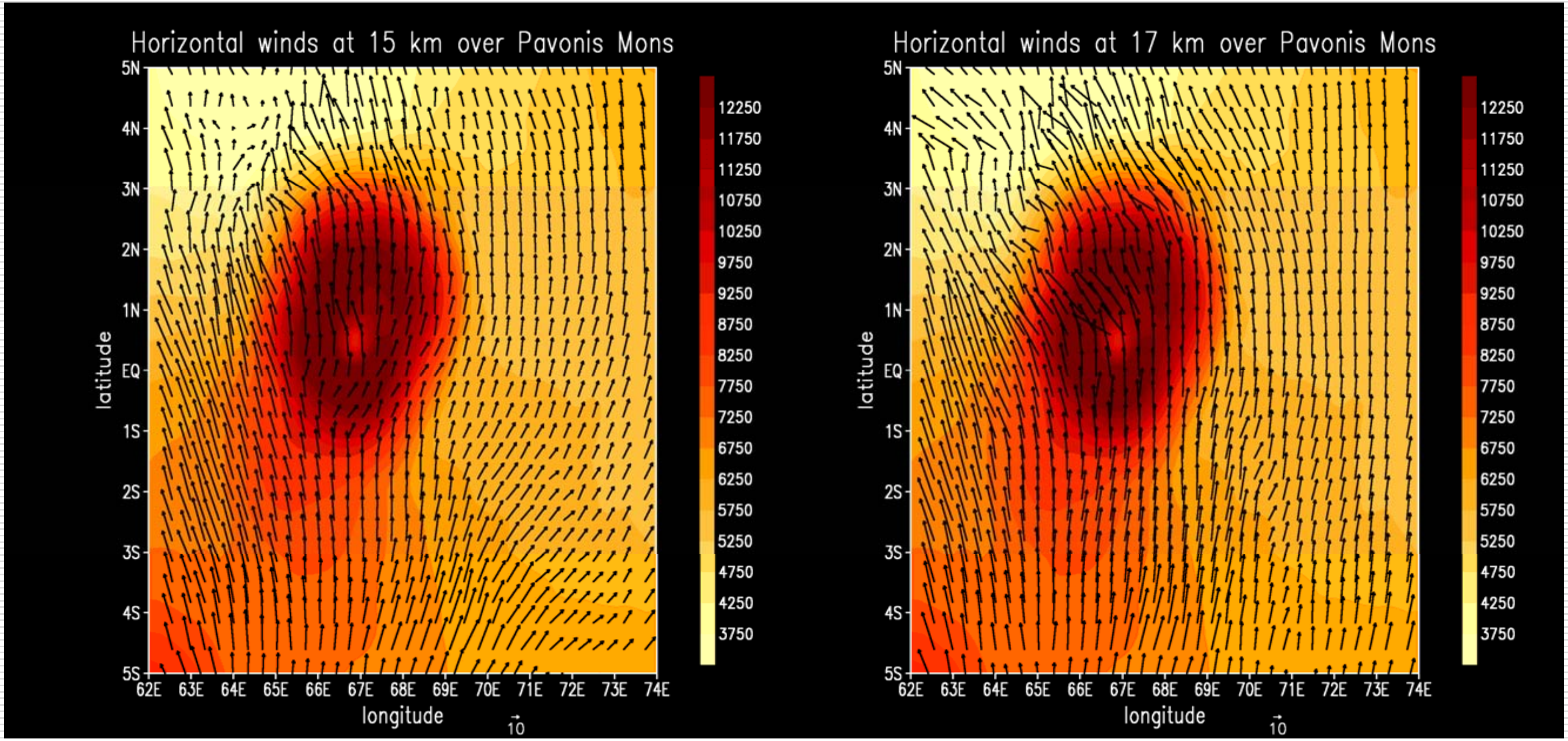
High resolution wind simulation



Global Multiscale Mars Model (GM3)