The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization
IAEA International Atomic Energy Agency

2148-24

Fifth ICTP Workshop on the Theory and Use of Regional Climate Models

31 May - 11 June, 2010

Implementation of gas-phase chemistry within RegCM

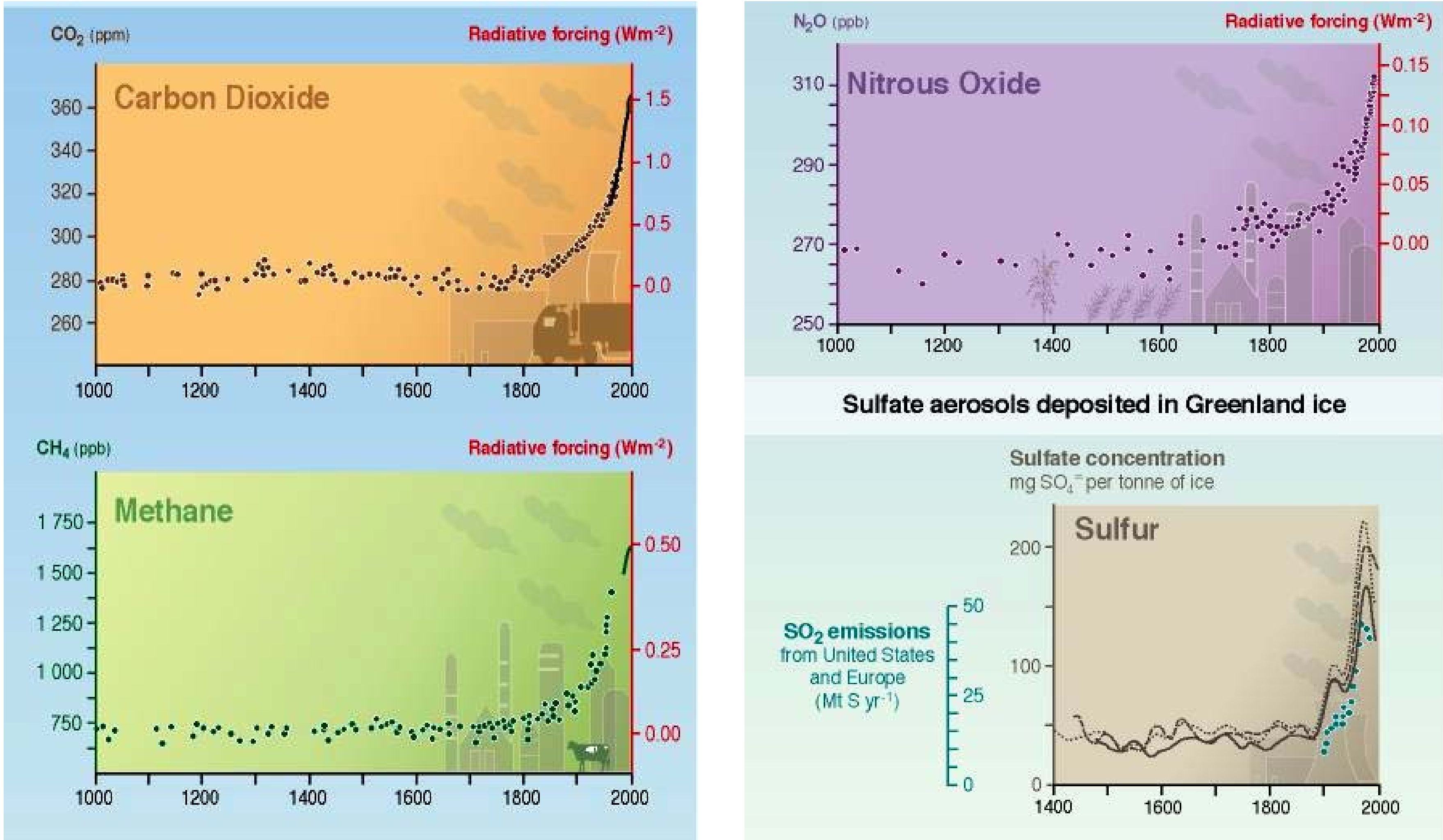
ZAKEY Ashraf Saber, Shalaby A., Steiner A., Stordal F. and Giorgi F.
Egyptian Meteorological Authority Air Pollution and Climate Dept
P.O.Box 11784, Qobry El-Qobba
El-Kalefa El-Mamoon Street
Cairo
EGYPT

Implementation of Gas-Phase chemistry in RegCM

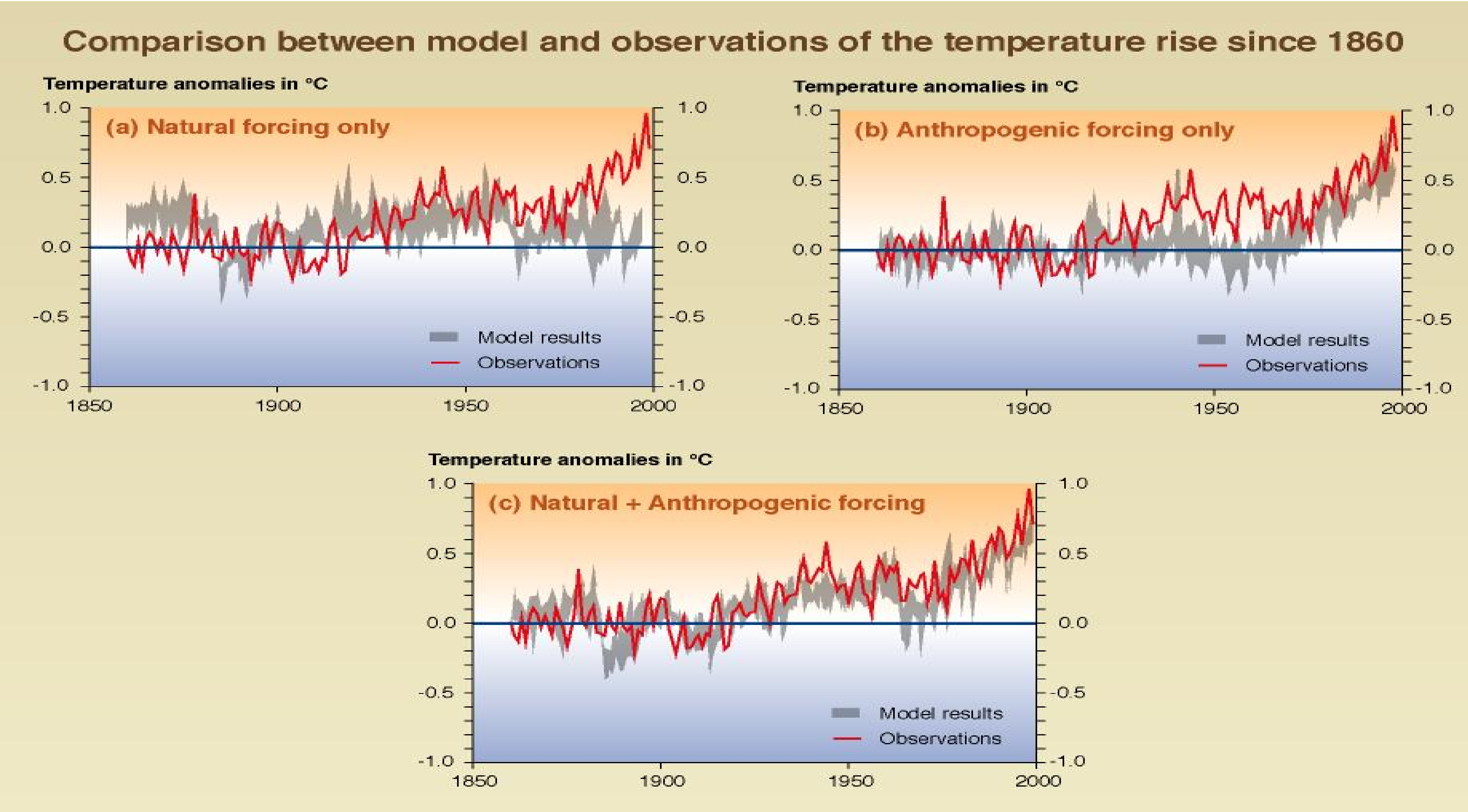
(Climate-Chemistry Interaction, CCI)

A. Zakey, A. Shalaby, A. Steiner, F. Stordal and F. Giorgi

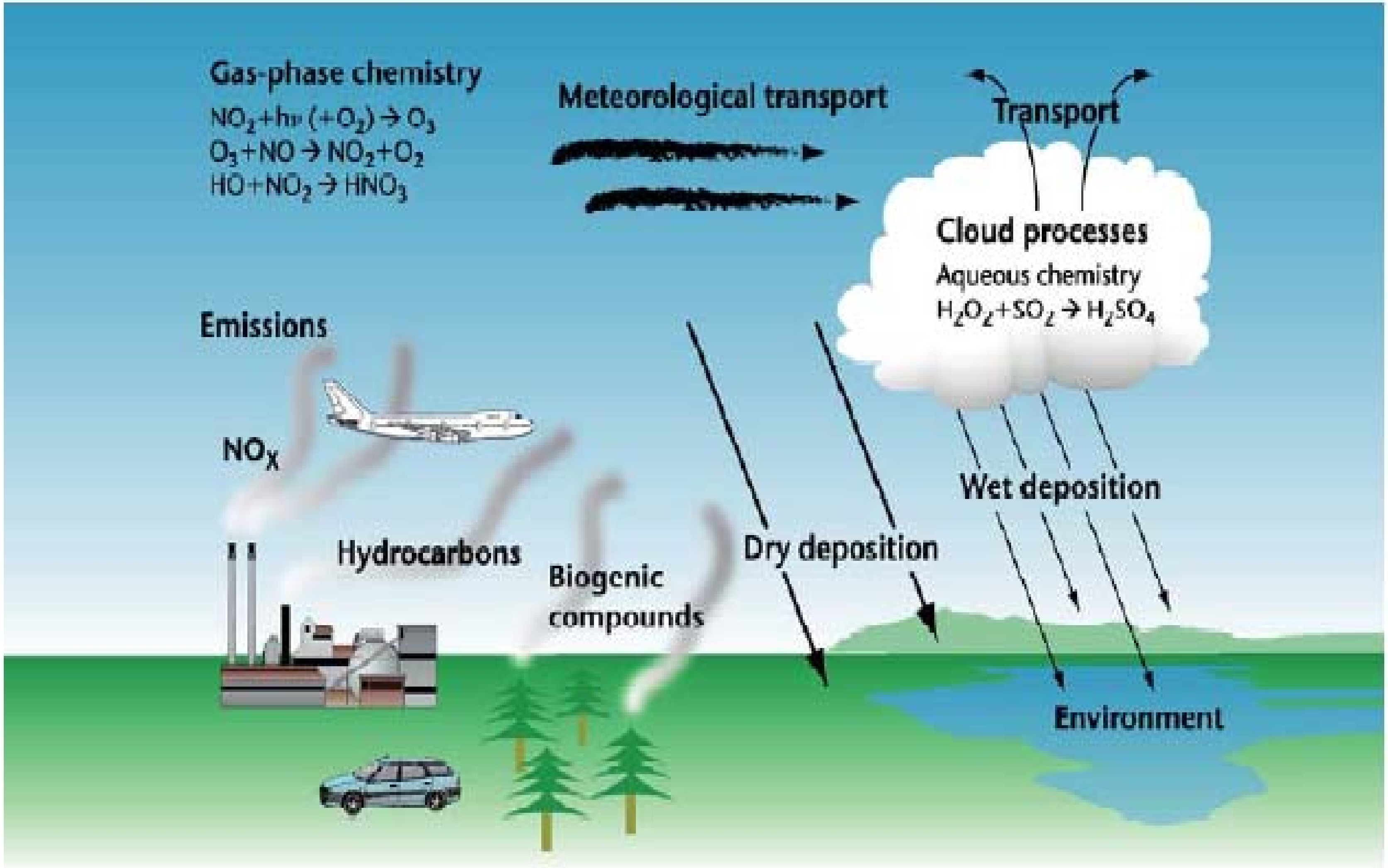
Human activities have changed the composition of the atmosphere since the pre- industrial

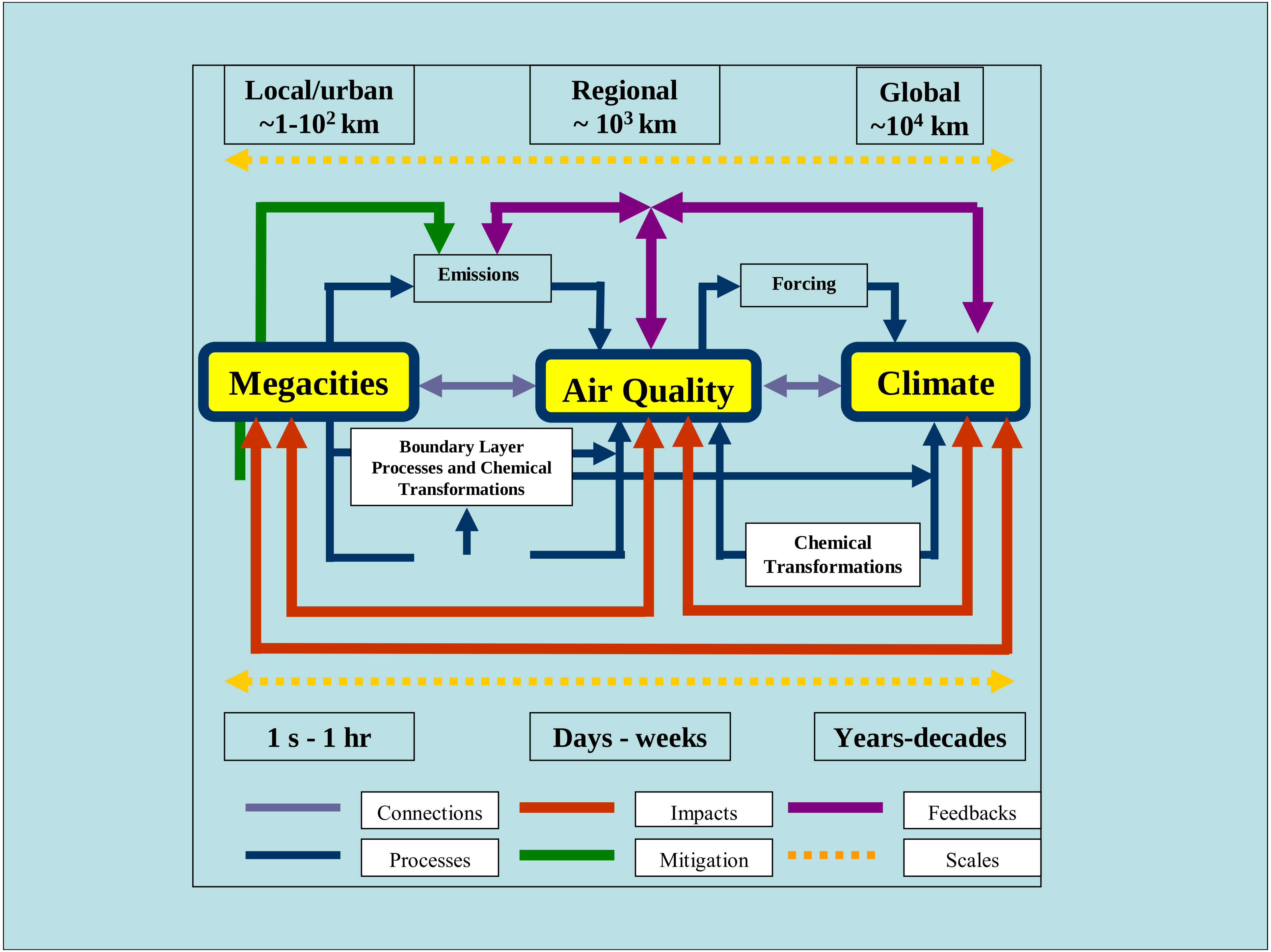


Most of the observed warming in the past 50 years is attributable to human activities



Atmospheric Chemistry Processes





Local/urban
~1-10^2 km
Regional
~ 10^3 km
Global
~10^4 km
Emissions
Forcing
Megacities
Air Quality
Climate
Boundary Layer
Processes and Chemical
Transformations
Chemical
Transformations
1 s - 1 hr
Days - weeks
Years-decades
Connections
Impacts
Feedbacks
Processes
Mitigation
Scales

Timescales of ozone chemistry

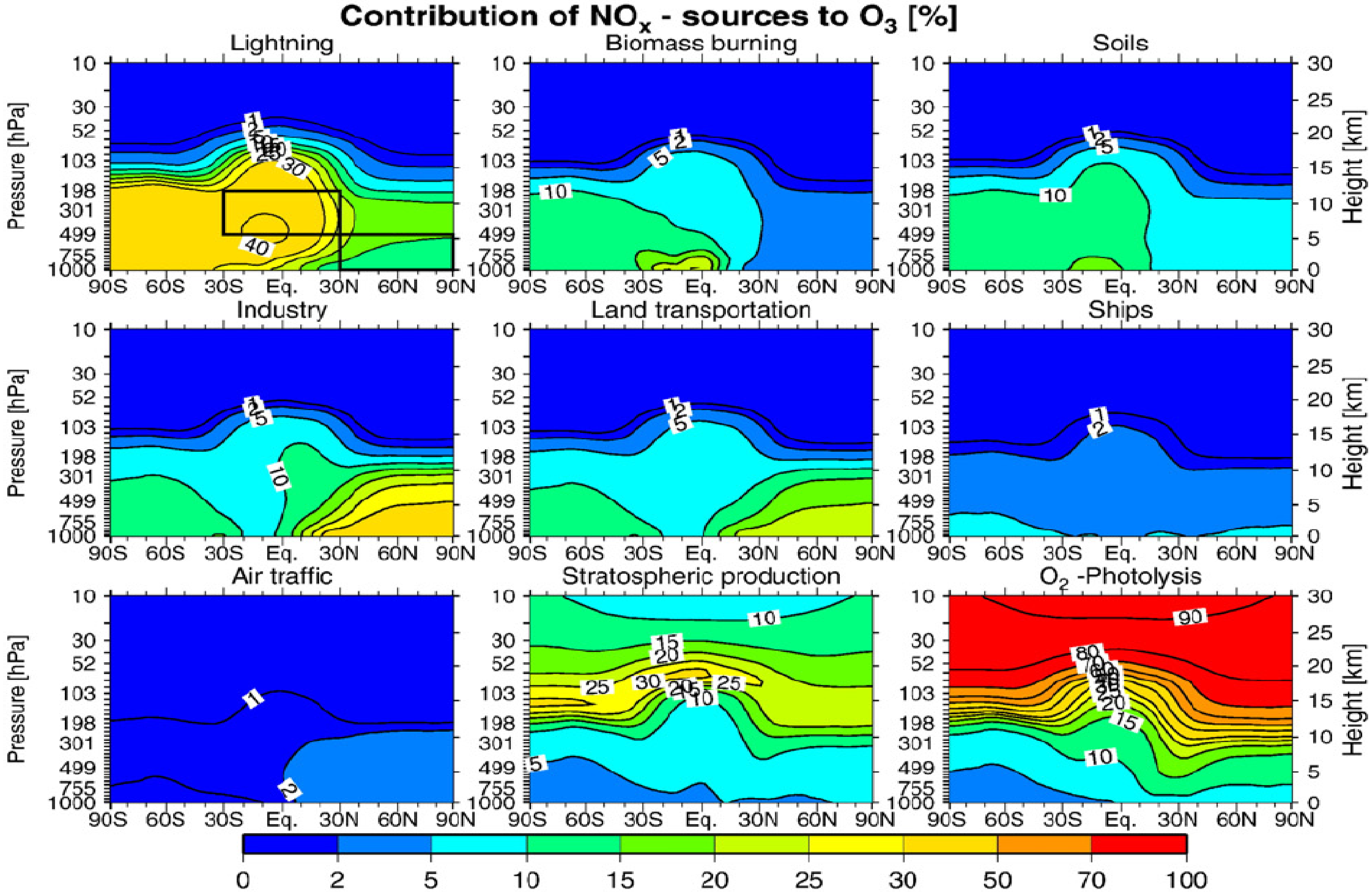
Global chemistry. Dominated by NO_x + CH_4 + sunlight. Timescales are long as are transport distances.

Regional chemistry. Many VOCs are emitted, e.g. over Europe. Each has its own lifetime governed by its rate constant for reaction with OH. The timescales of ozone production takes from hours to days. The transport distance for a wind speed of 5 m s^{-1} and a lifetime of 1 day is ~500 km.

Urban chemistry: high concentrations of NO from transport sources. Ozone is depressed by the reaction:

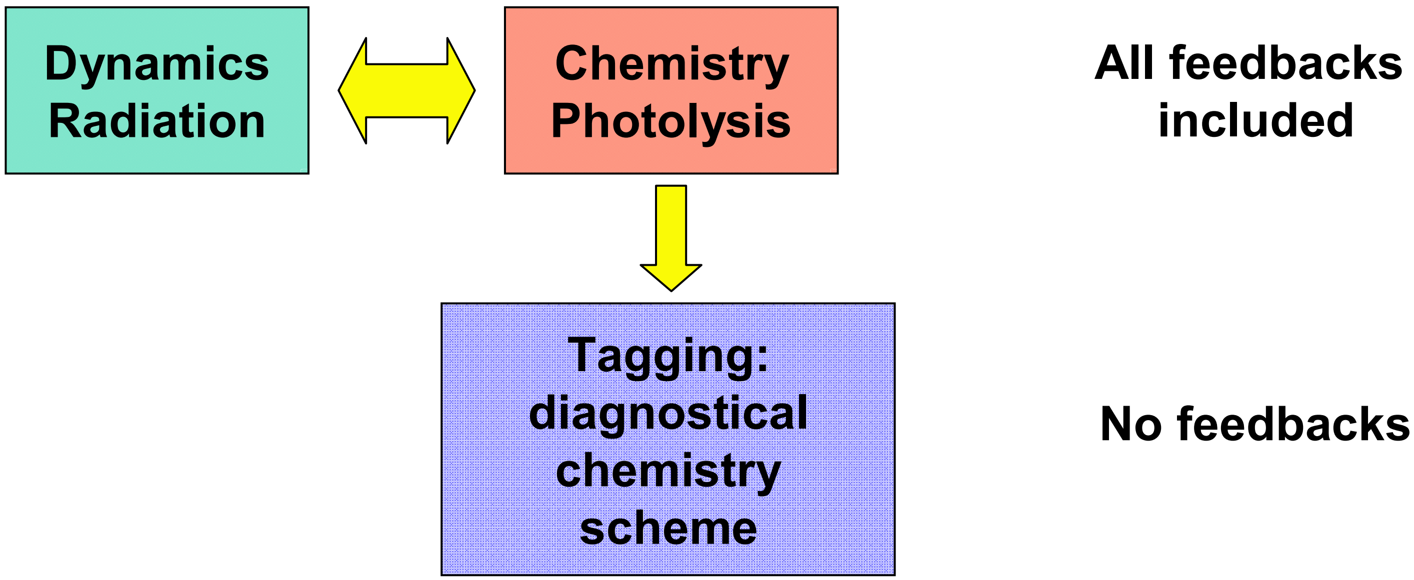
$$NO + O_3 \rightarrow NO_2 + O_2$$

Impact of various NOx sources on ozone

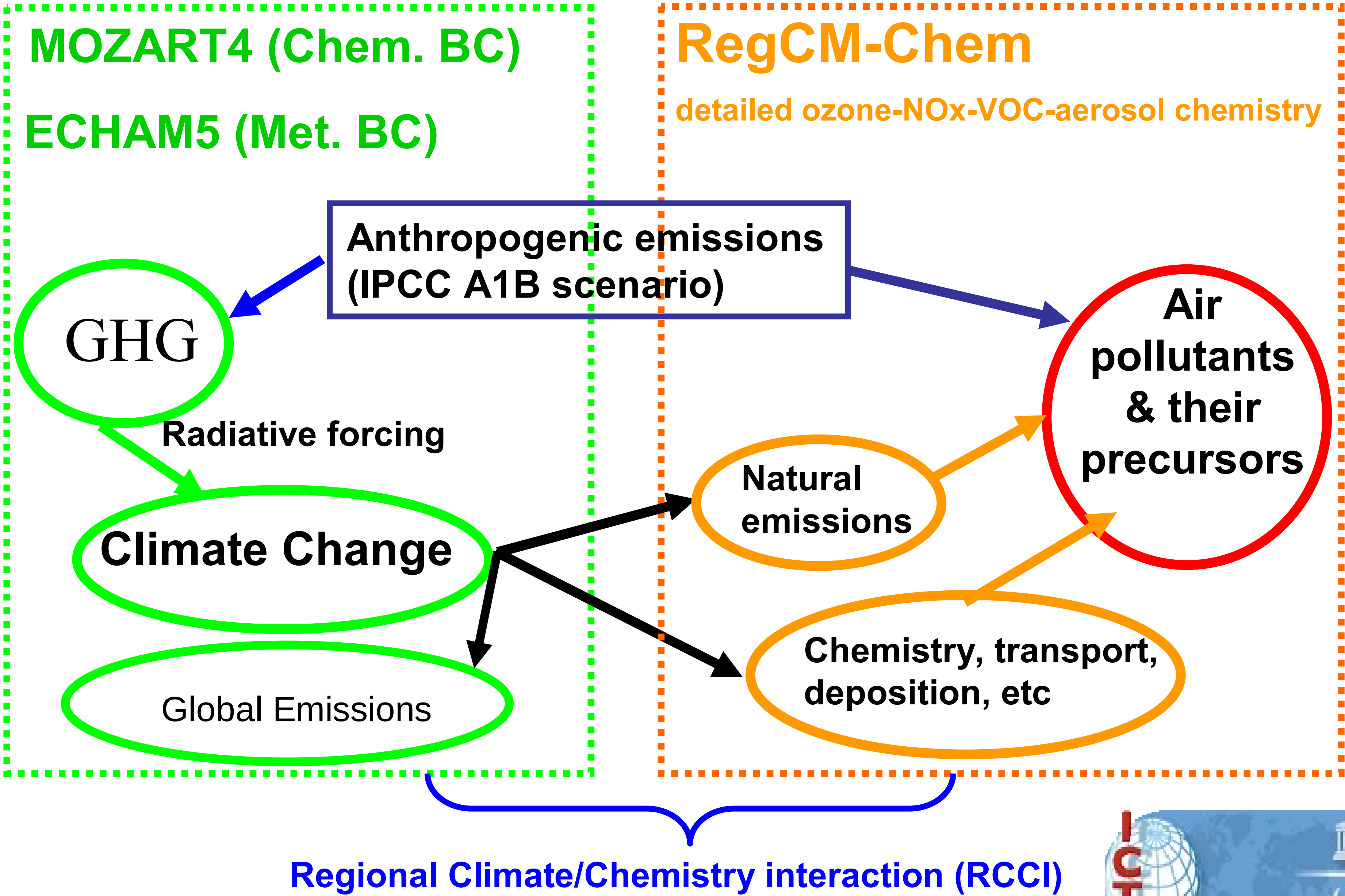


Tagging of chemical tracers

- ➢Understanding of atmospheric composition and changes in the composition
- ➢'Accounting'-System of highly non-linear chemistry



Models and future scenario



Some chemistry questions

What do we want chemistry for?

- Short-lived forcing agents:
  - Aerosols
  - Ozone

How much of the chemistry must be interactive?

What's the lid on the model?

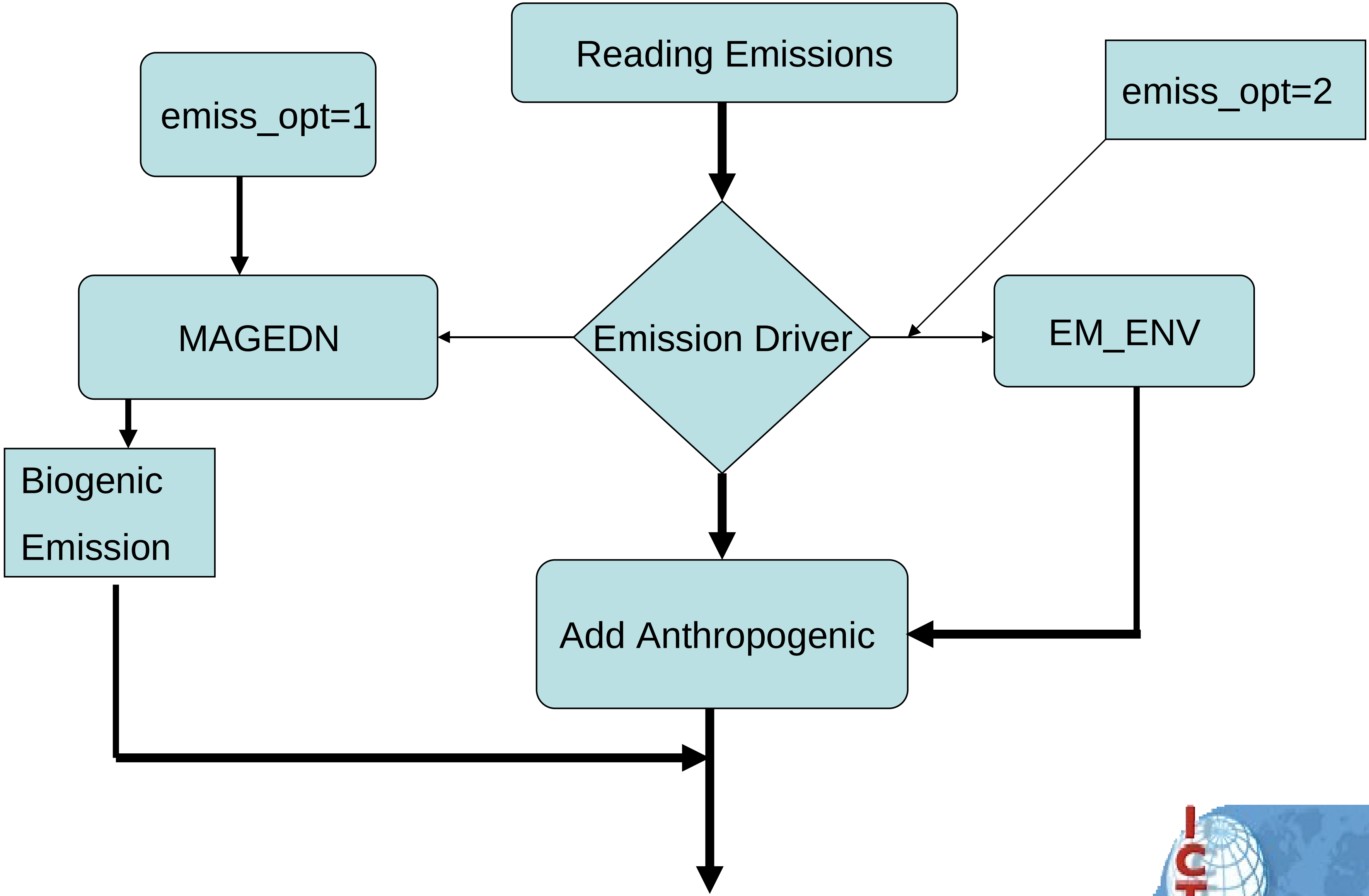
- Tropopause
- Stratopause
- Mesopause
- Higher?

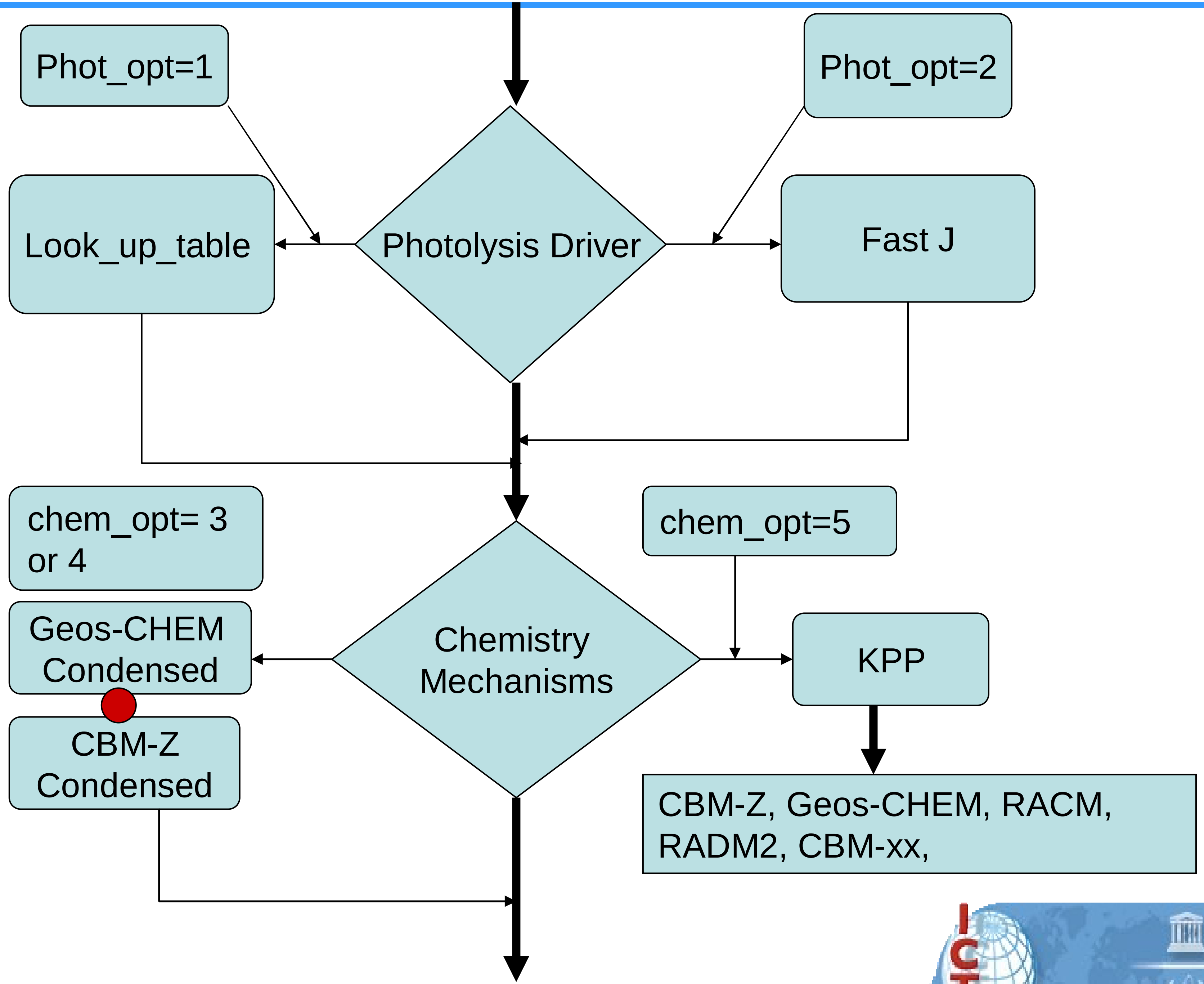
Where do we get the historical emissions data sets for 30-90 chemical species?

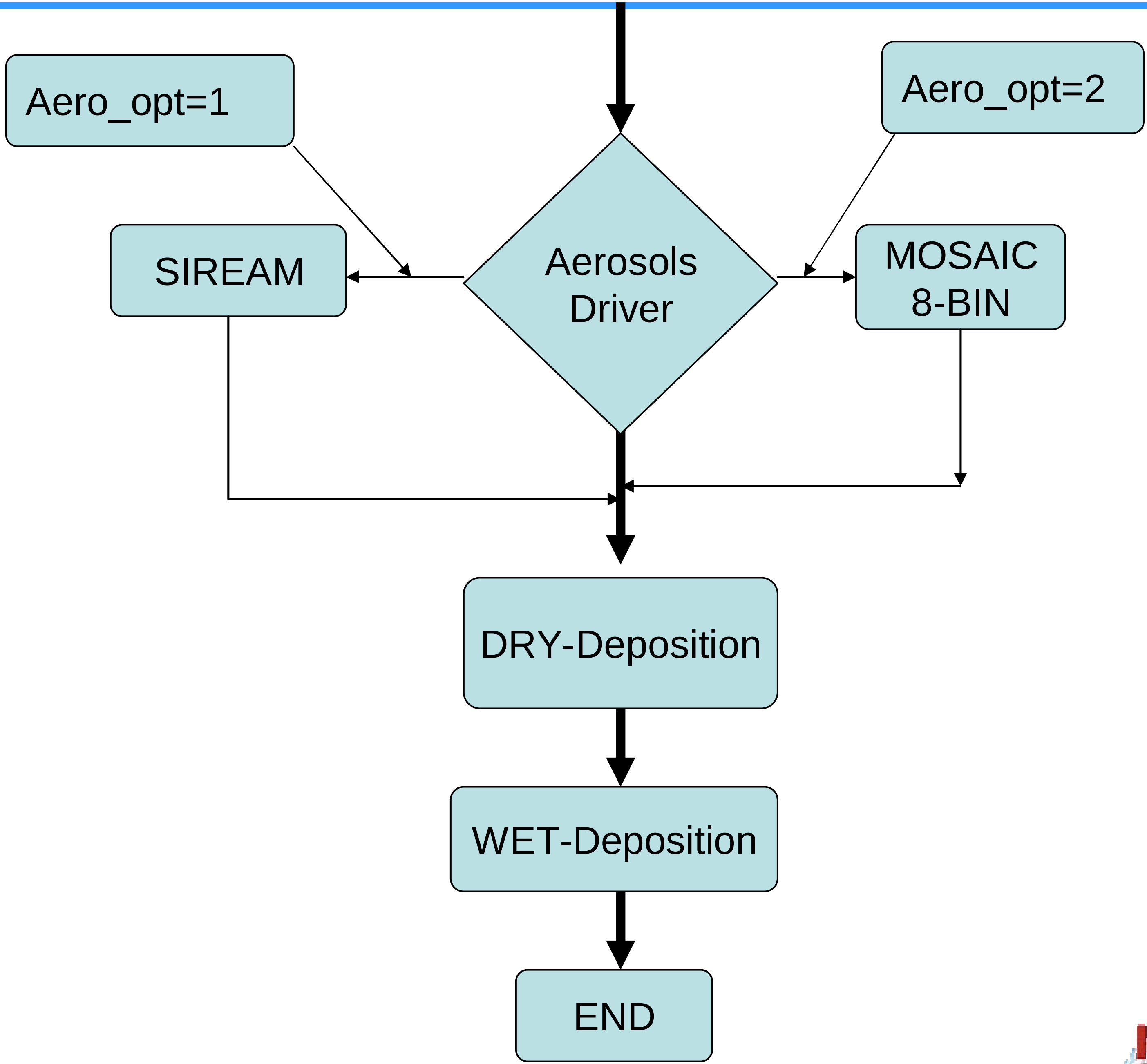
What are your metrics for fidelity?

Coupling tech. info.

Chemistry Flow Chart




Phot_opt=1
Phot_opt=2
Look_up_table
Photolysis Driver
Fast J
chem_opt= 3 or 4
chem_opt=5
Geos-CHEM Condensed
CBM-Z Condensed
Chemistry Mechanisms
KPP
CBM-Z, Geos-CHEM, RACM, RADM2, CBM-xx,


Aero_opt=1
Aero_opt=2
SIREAM
Aerosols
Driver
MOSAIC
8-BIN
DRY-Deposition
WET-Deposition
END

Emissions Inventories

RETRO	Biomass burning and anthropogenic	1960-2000	$0.5^{o}X0.5^{o}$	monthly
POET	Biomass burning, anthropogenic and biogenic	1990-2000	$1^{o}X1^{o}$	annually
EDGAR	Biomass burning, anthropogenic and biogenic	2000	$1^{o}X1^{o}$	annually
GFED v2	Biomass burning	1995-2005	$1^{o}X1^{o}$	annually

Gas-Phase Mechanisms (continue)

Organic species lumping techniques

Most inorganic (inorganic photolysis and inorganic oxidation reactions) in all mechanisms are the same. The basic difference between mechanisms HOW it deal with organic species.

There are two major approach to deal with hundreds of organic species

•**Lumped molecule** (RADM2, RACM, GEOS, GEOS_SILL)

1-surrogate species have similar reactivity range.

2-does not conserve carbon mass.

•**Lumped structure** (CBM-IV, CBM-Z)

1-surrogate species base on carbon bonds single bond species, double bond species

2-relatively fewer categories are needed to represent the organic species.

3-conserve carbon mass

Chemical Mechanisms (continue)

Chemical Mechanism used

1-Updated GEOS-CHEM (SILL), using Sanford Sillman box model code.

2-Updated GEOS-CHEM (GEOS_KPP) using KPP to produce the code.

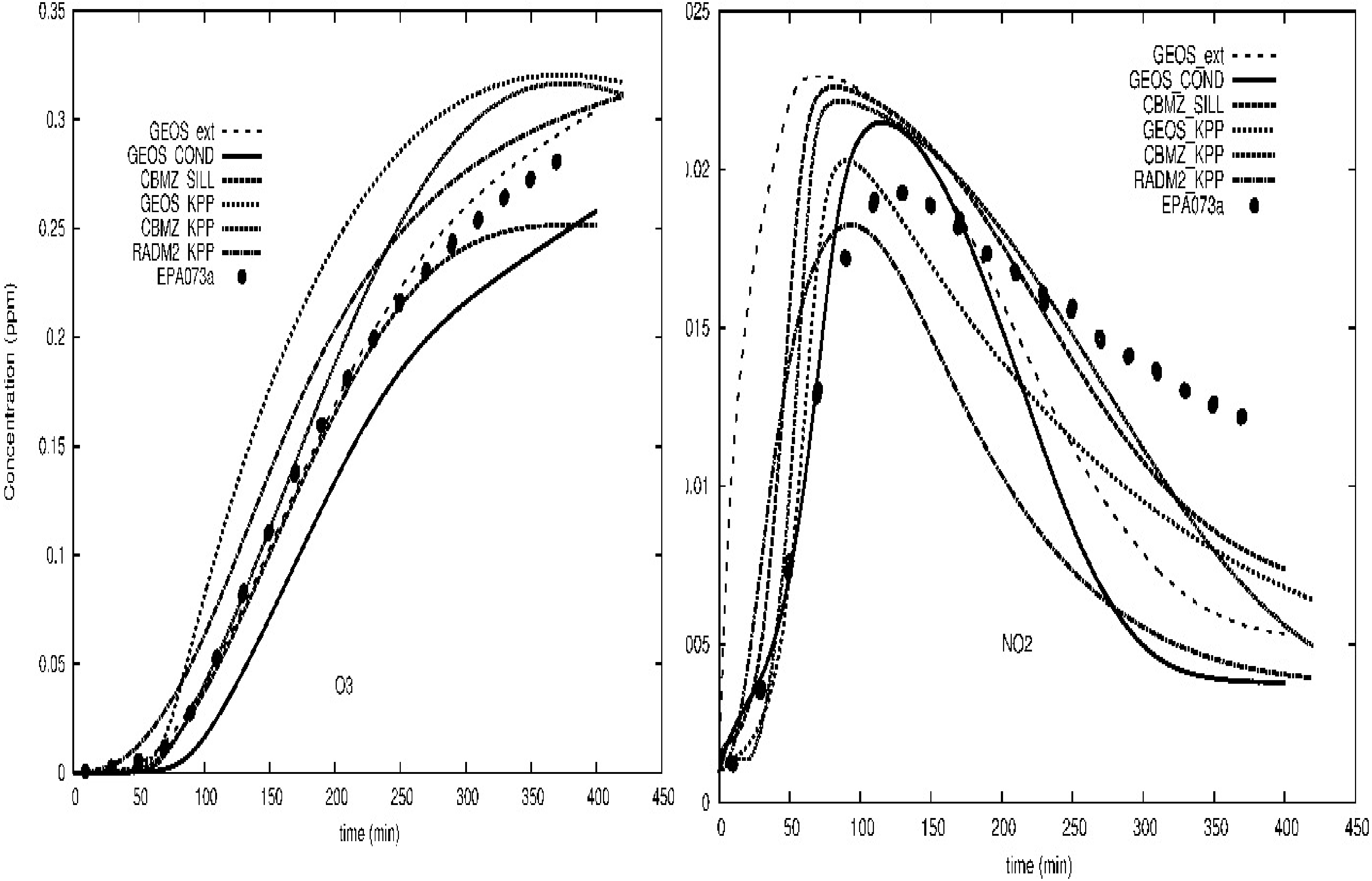
3-CBMZ (CBMZ_KPP) using KPP to produce the code.

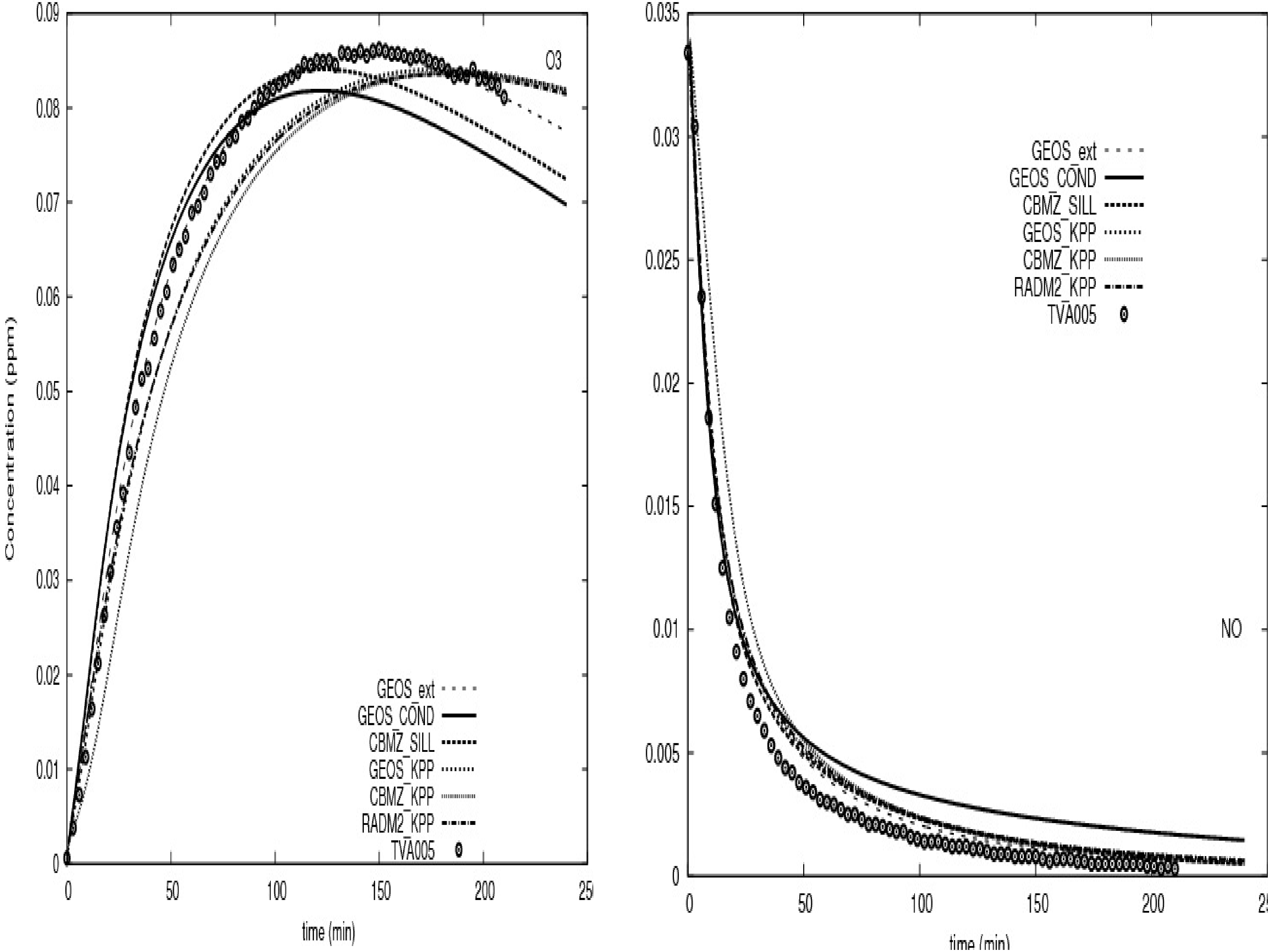
4-RACM (RACM_KPP) using KPP to produce the code.

5- Geos-chem condensed (EBI)

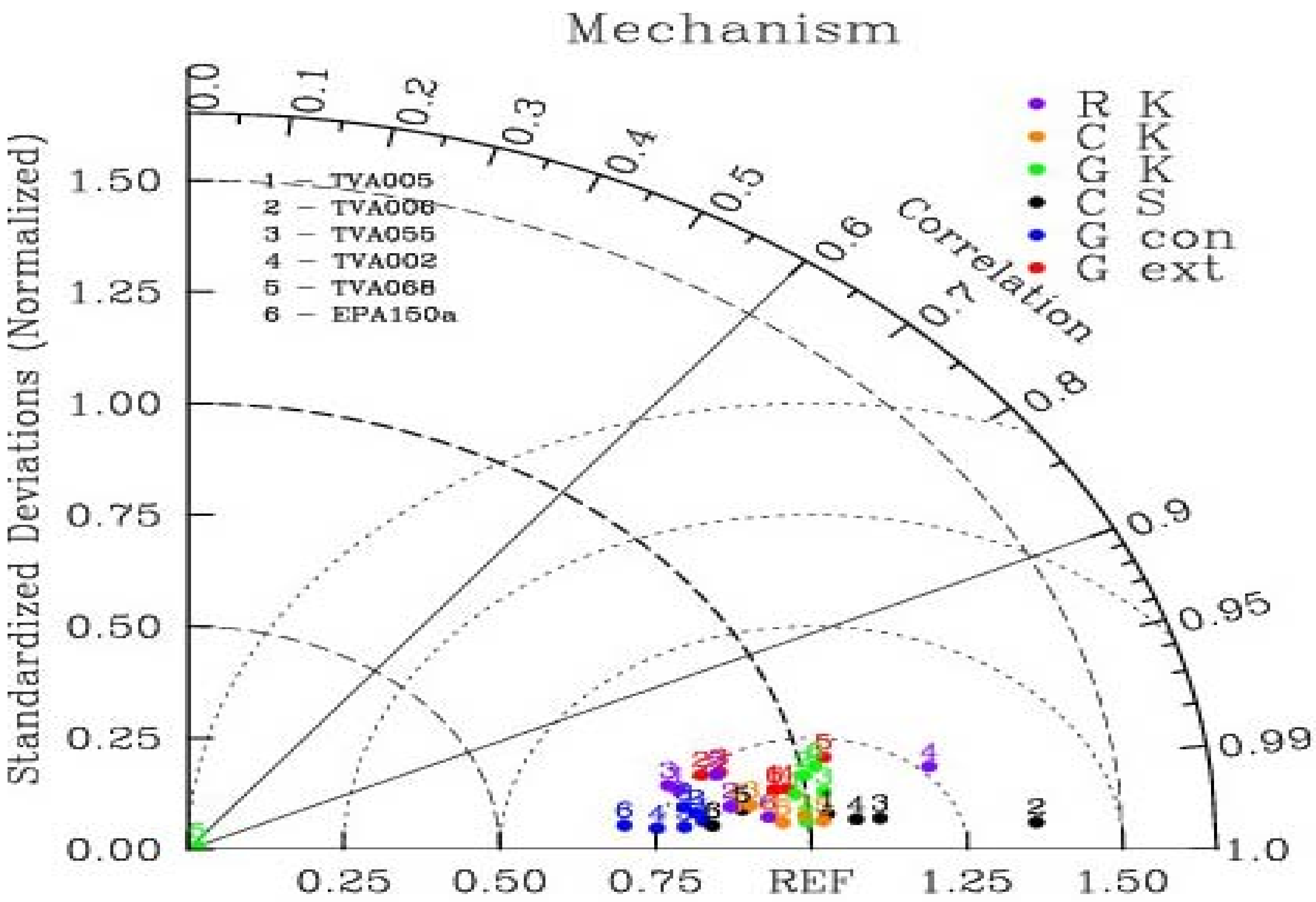
6- CBM-Z condensed

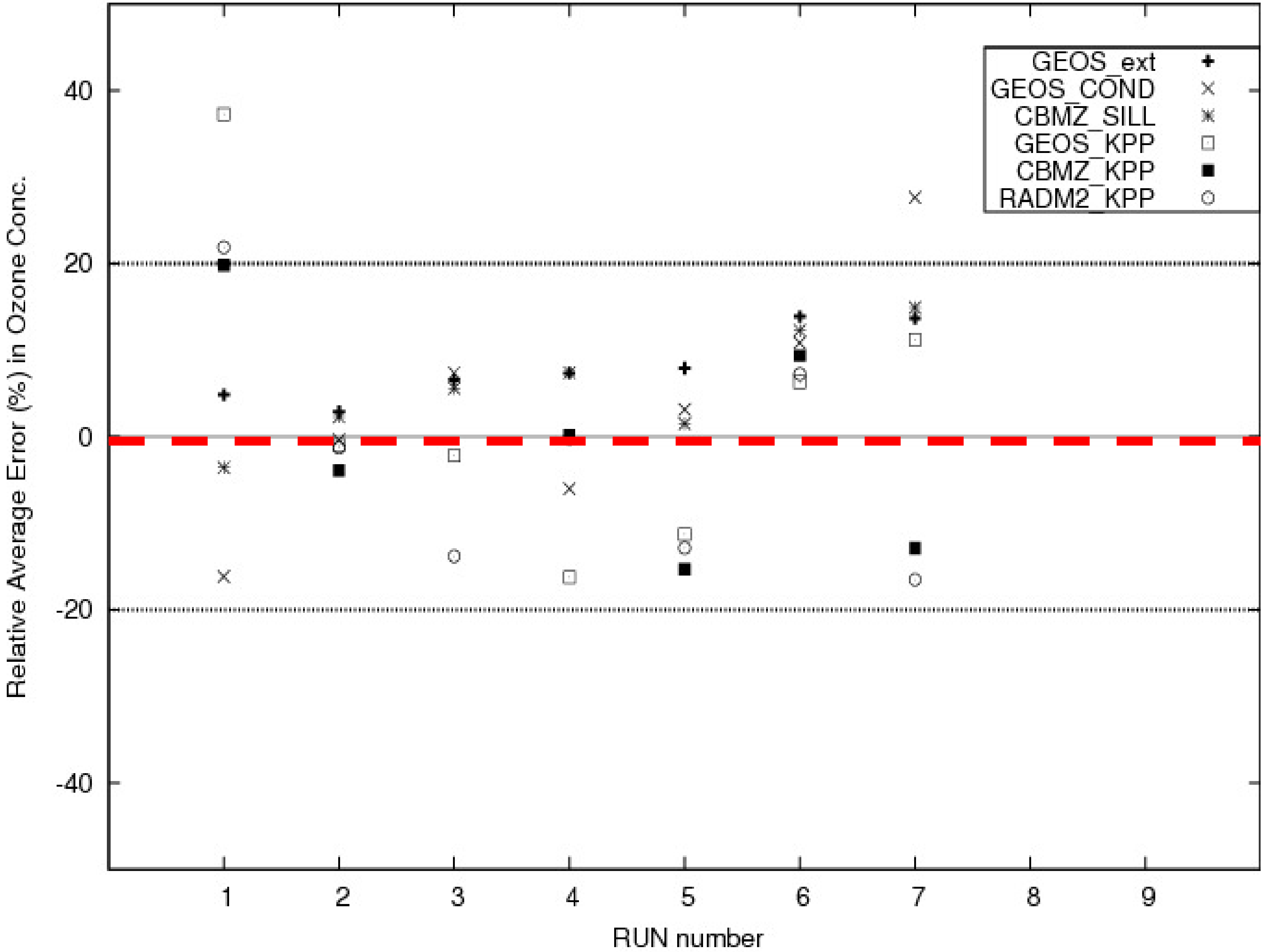
Box-model validation with the gas-chamber data





O3
NO
Concentration (ppm)
time (min)
GEOS_ext
GEOS_COND
CBMZ_SILL
GEOS_KPP
CBMZ_KPP
RADM2_KPP
TVA005


Mechanism
Standardized Deviations (Normalized)
Correlation
1 — TVA005
2 — TVA006
3 — TVA055
4 — TVA002
5 — TVA068
6 — EPA150a
R K
C K
G K
C S
G con
G ext
0.00
0.25
0.50
0.75
1.00
1.25
1.50
REF
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.95
0.99
1.0



GEOS_ext
GEOS_COND
CBMZ_SILL
GEOS_KPP
CBMZ_KPP
RADM2_KPP
40
20
0
-20
-40
1
2
3
4
5
6
7
8
9
RUN number
Relative Average Error (%) in Ozone Conc.

The Kinetic Pre-Processor (KPP) (Sandu, A. and Sander, R. 2006)

- Chemistry Mechanisms includes hundreds of reactions and dozens of chemical species (e.g GEOS_SILL has 533 reactions and 157 species).
- Solving the corresponding huge systems of ODE requires highly efficient numerical integrators, and costly code developments and updates
- Automatic Code generation has become widely used tool to overcome the above problems.
- KPP needs only three files (user defined) one for the set of mechanism equations, one for definitions of species and the last one for initialization and inline code.
- KPP will process such files and produce a complete package for simulation of such mechanisms.
- KPP used to produces the chemical mechanisms for the gas-phase (RADM2, CBM-Z and RACM).

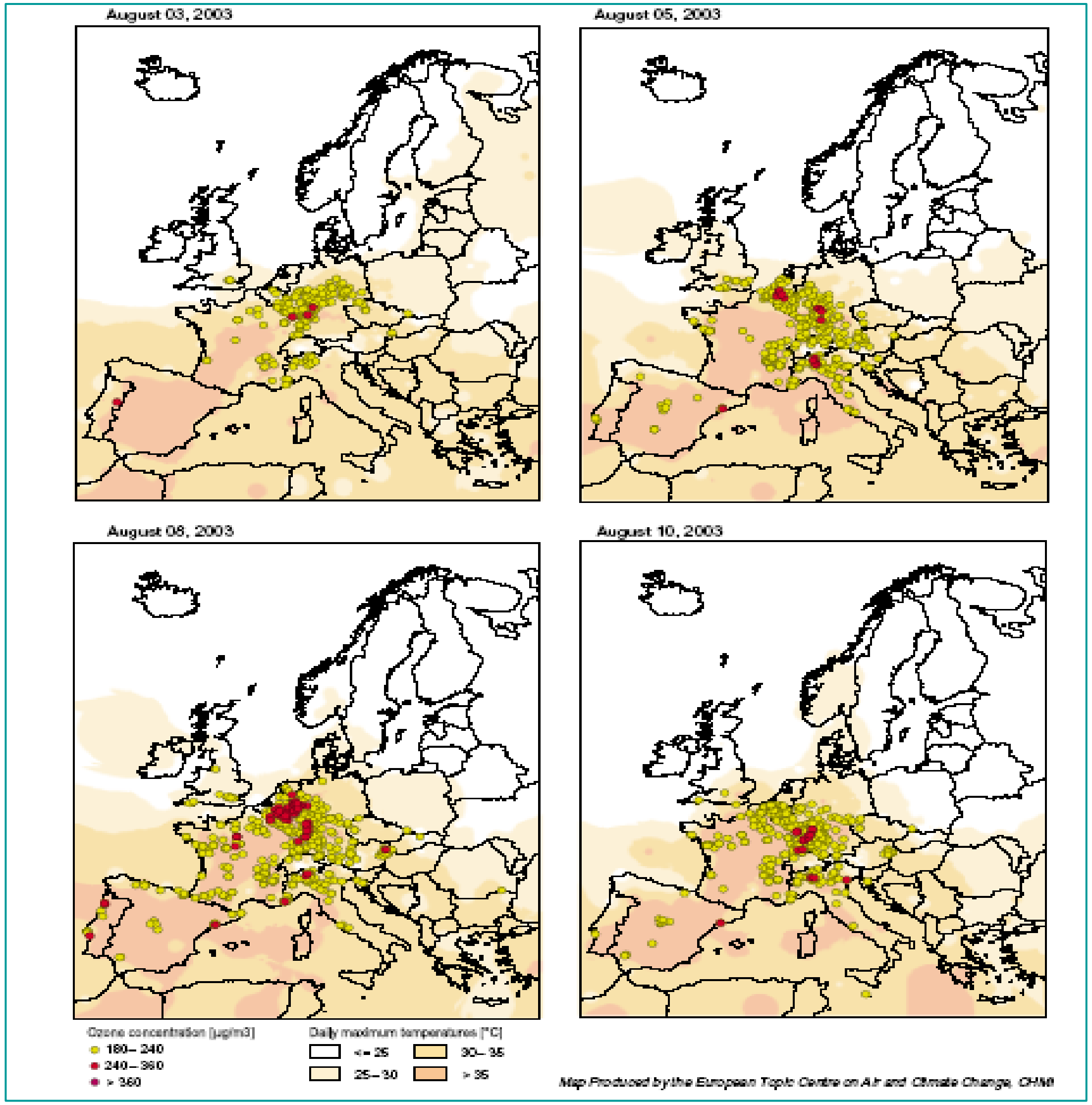
August 2003 Case study

In August 2003, Europe has been suffered from a heat wave last 15 days, this heat wave is accompanied by a high level of ozone. We chose this period as a case study to evaluate the model.

We use EMEP stations network for ozone to validate the outputs.

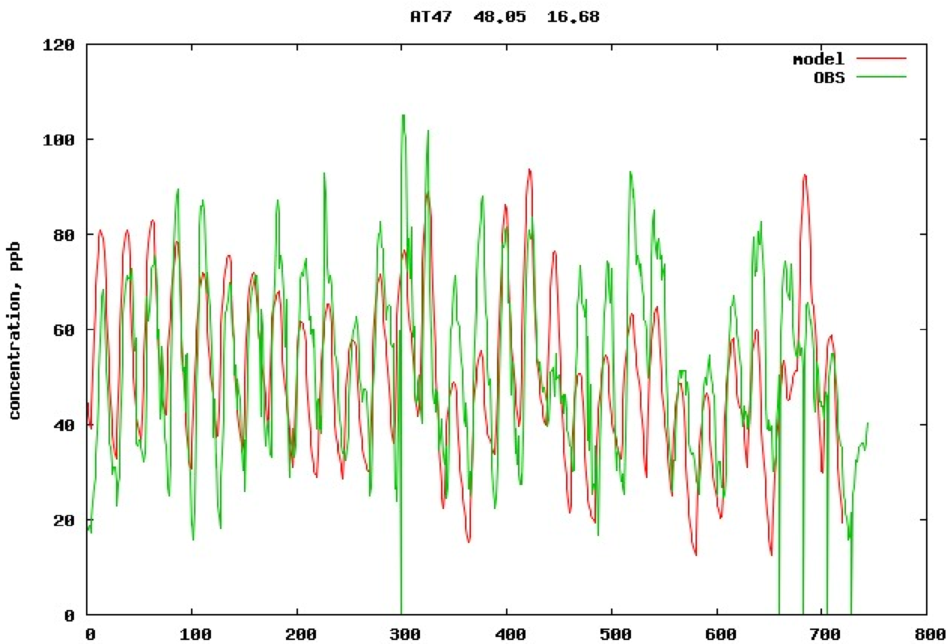
Next slides will represent Ozone spatial distribution, Ozone vertical profiles, and time series of different chemical mechanisms in comparison with observations.

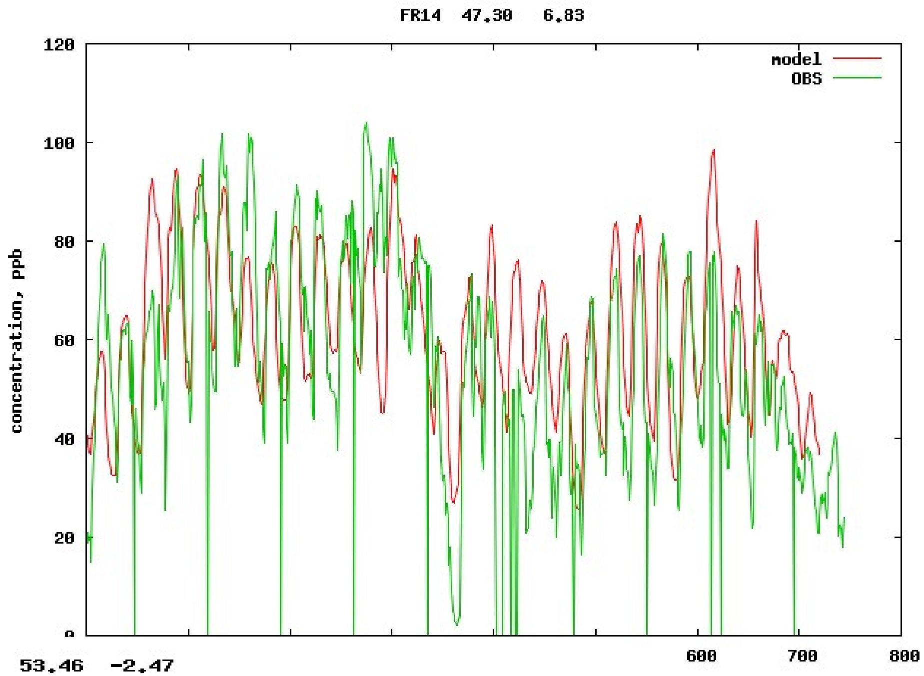
Heat wave in Europe, August 2003

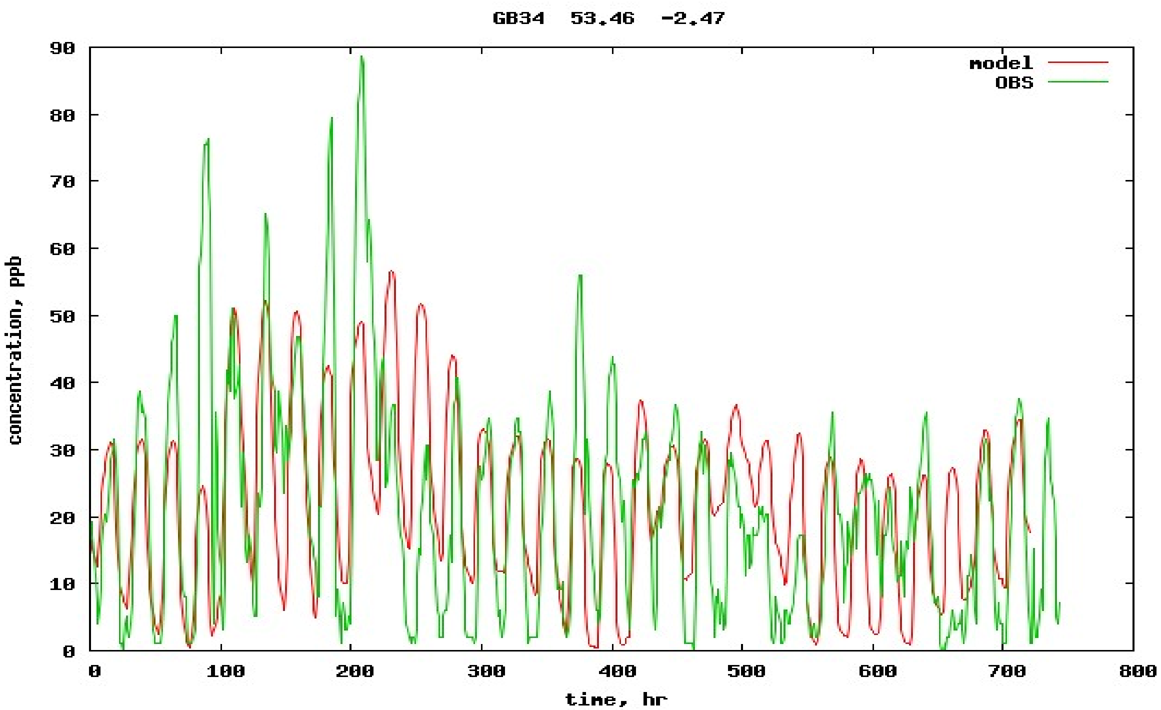


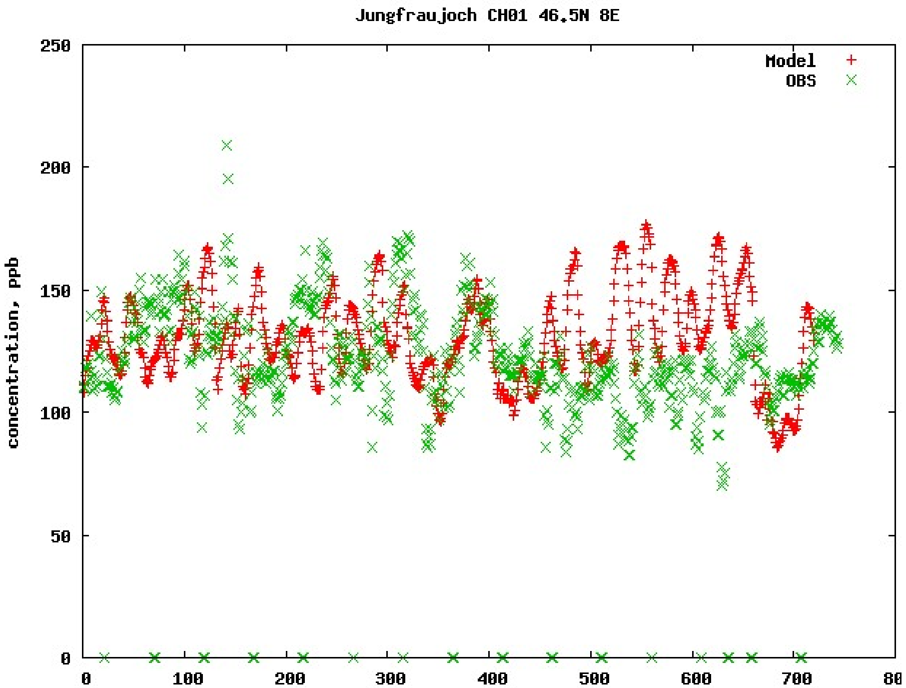
- Monitoring stations in Europe reporting high band concentrations of ozone
- >15 000 ‘excess deaths’ in France; 2000 in UK, ~30% from air pollution.
- Temperatures exceeded 35^{0}C in SE England.
- How frequent will such summers be in the future?

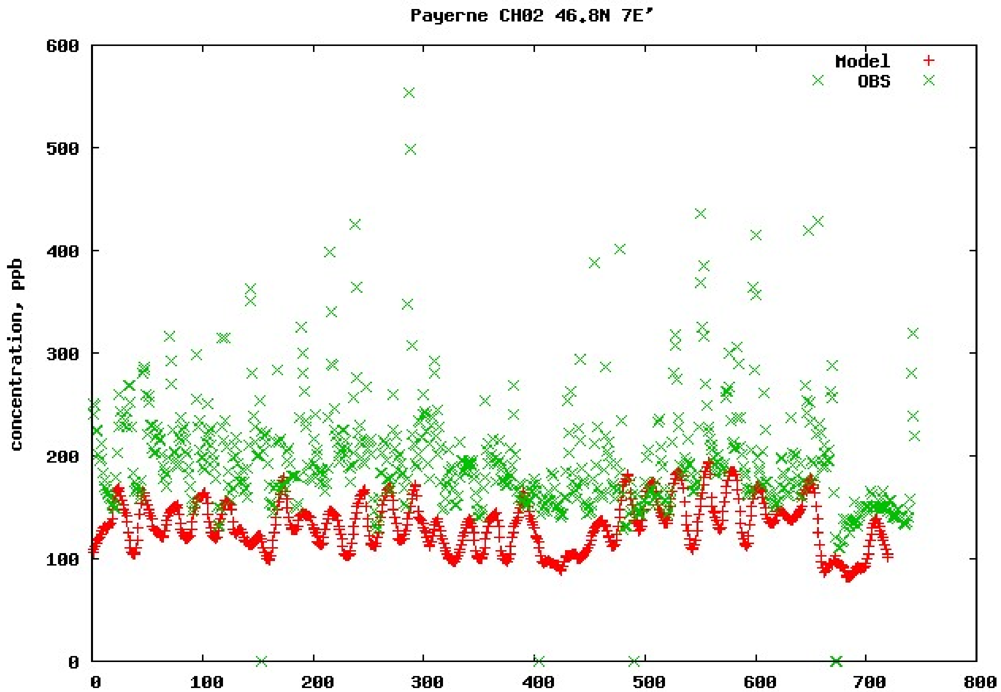
	KPP_CBMZ (by KPP)	KPP_GEOS (by KPP)	Updated-GEOS by sanford sillman)	KPP_RACM (by KPP)
NO. of Species	58	175	175	75
No. of Reaction	134	533	533	237
Solvers	Rosenbrock	Rosenbrock	Radical balance solver	Rosenbrock
Lumping Technique	Lumped structure	Lumped molecule	Lumped molecule	Lumped molecule
No. of Transported species	19	19	19	19

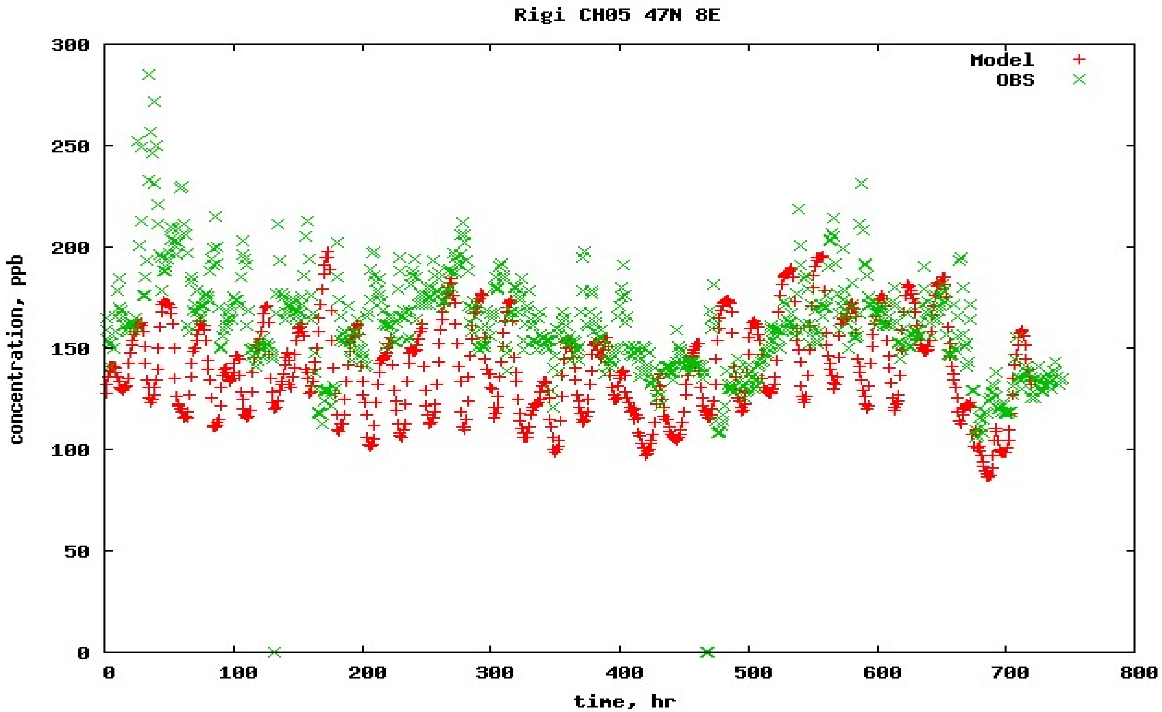

AT47 48.05 16.68
model
OBS
concentration, ppb
120
100
80
60
40
20
0
0
100
200
300
400
500
600
700
800

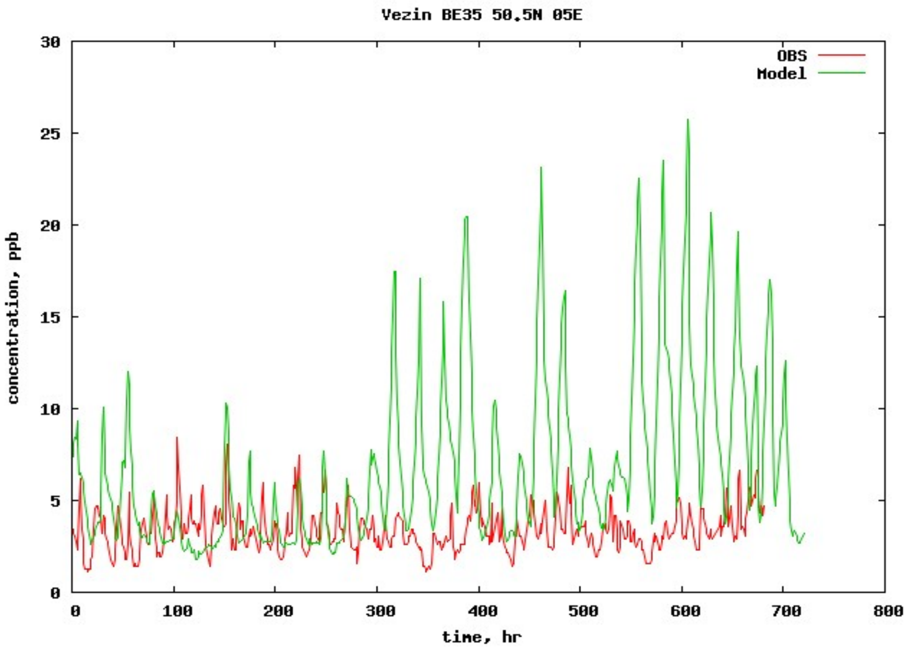

FR14 47.30 6.83
model
OBS
concentration, ppb
120
100
80
60
40
20
600
700
800

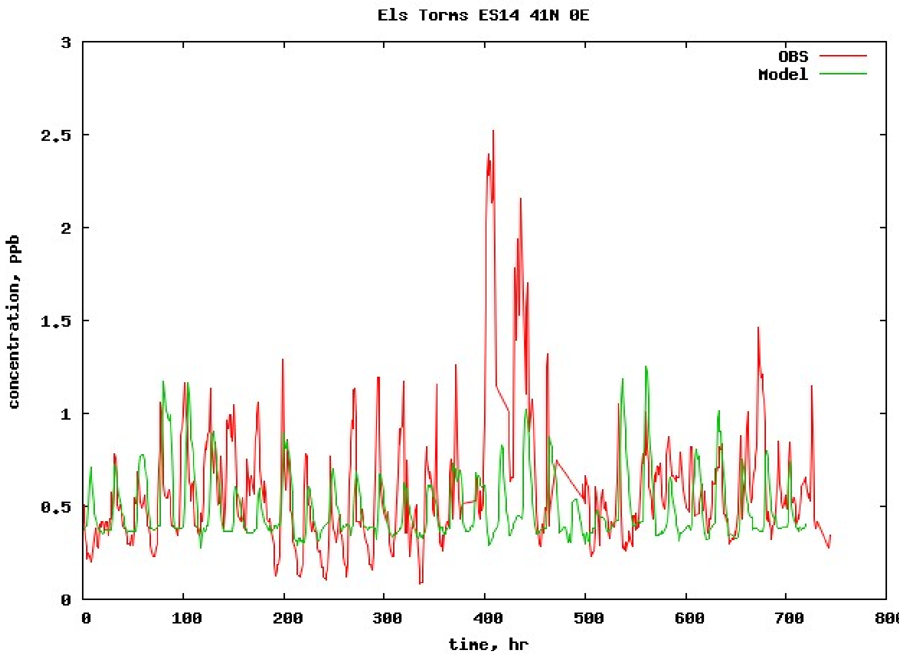

GB34 53.46 -2.47
model
OBS
concentration, ppb
90
80
70
60
50
40
30
20
10
0
0
100
200
300
400
500
600
700
800
time, hr

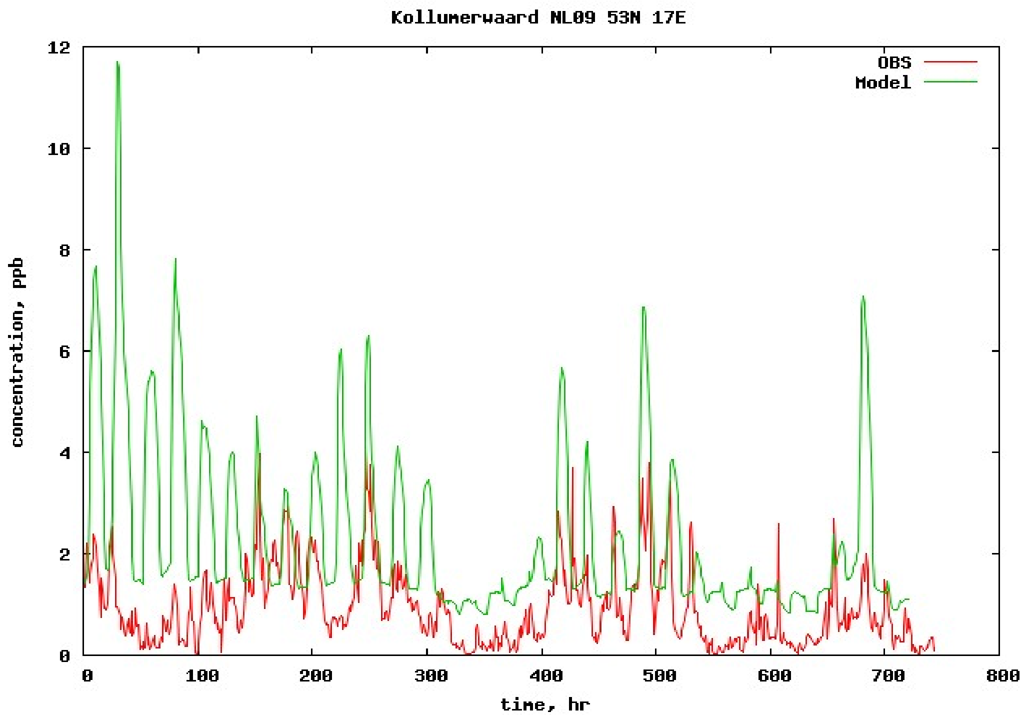

Jungfraujoch CH01 46.5N 8E
concentration, ppb
Model
OBS
0
50
100
150
200
250
0
100
200
300
400
500
600
700
80


Payerne CH02 46.8N 7E'
concentration, ppb
Model
OBS
0
100
200
300
400
500
600
0
100
200
300
400
500
600
700
800

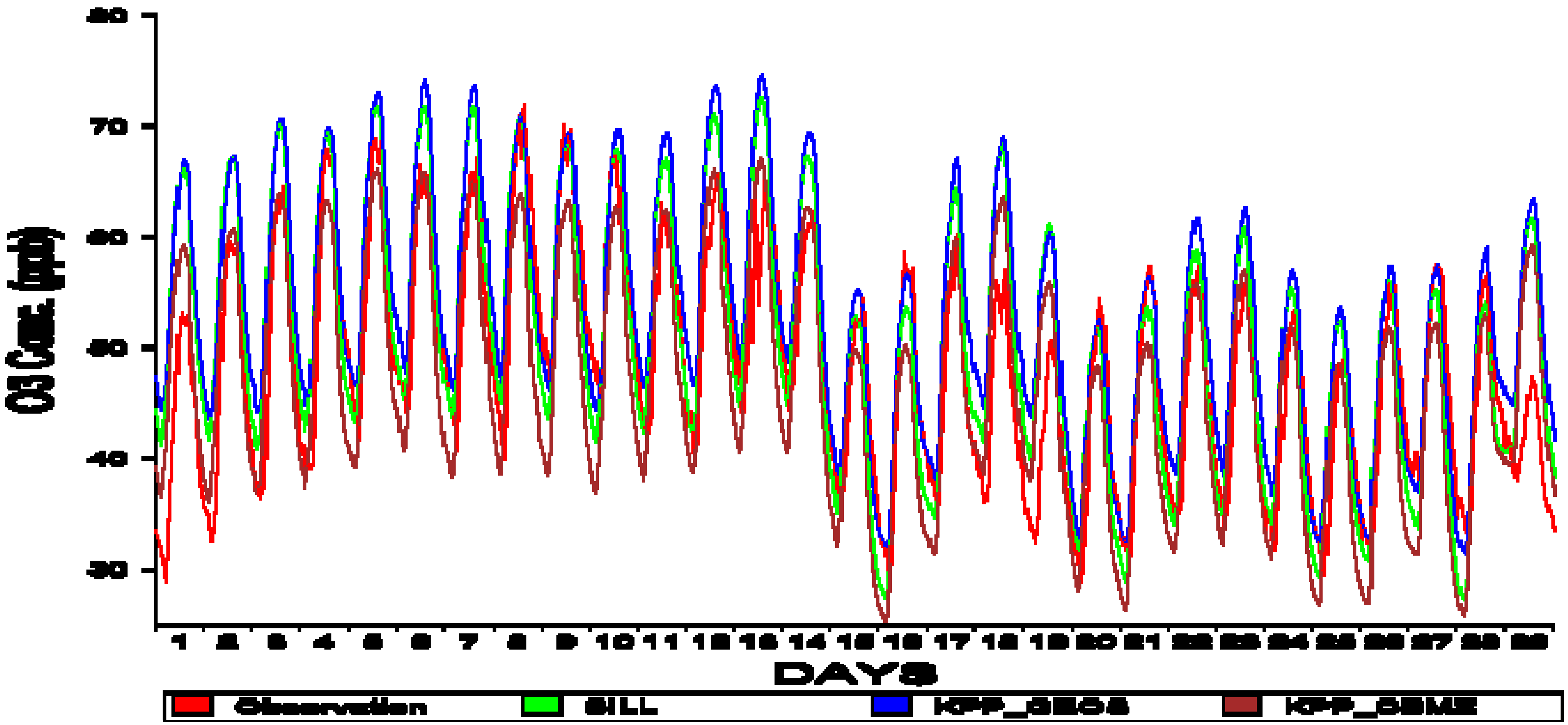

Rigi CH05 47N 8E
concentration, ppb
time, hr
Model
OBS
0
50
100
150
200
250
300
0
100
200
300
400
500
600
700
800


Vezin BE35 50.5N 05E
OBS
Model
concentration, ppb
time, hr

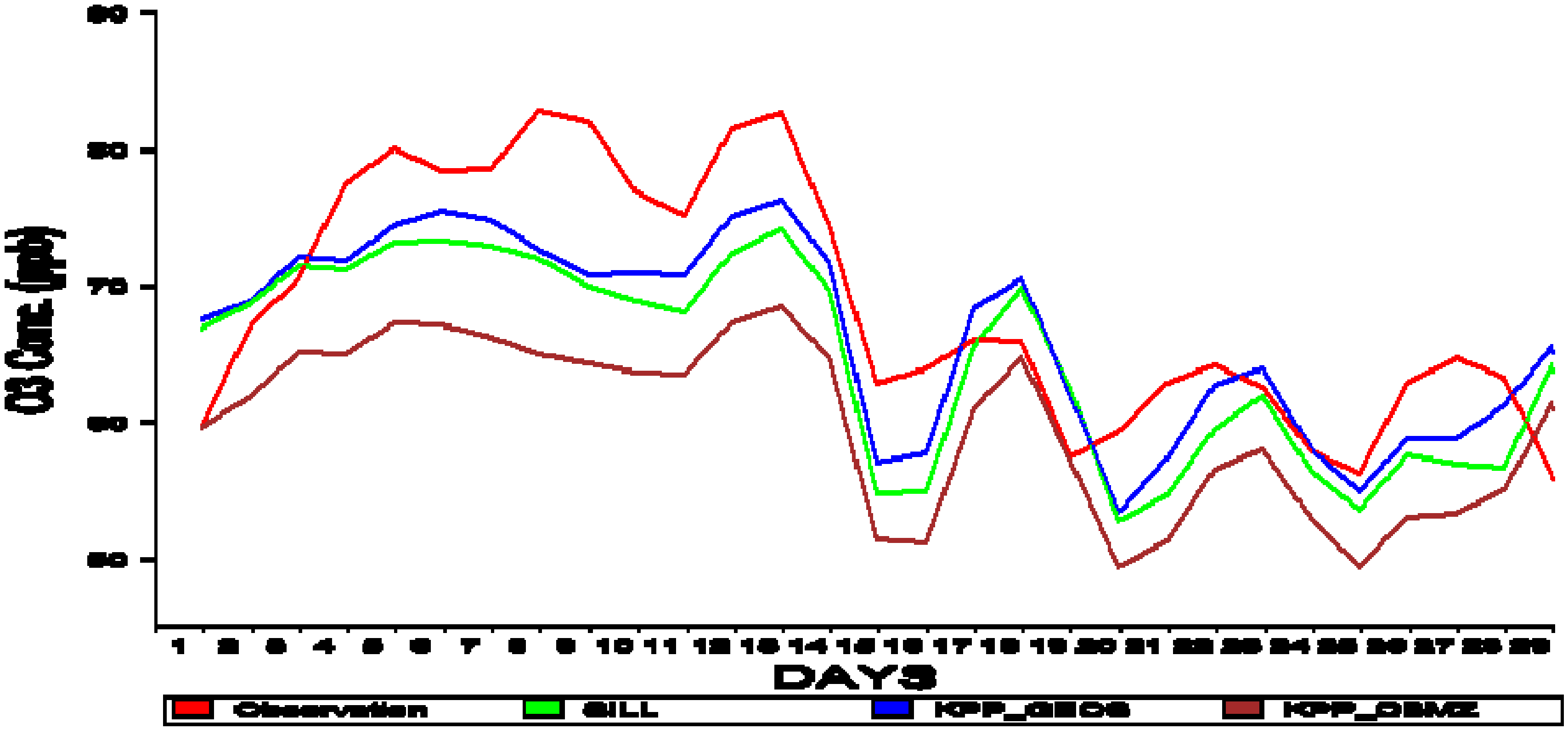

Els Torms ES14 41N 0E
OBS
Model
concentration, ppb
time, hr

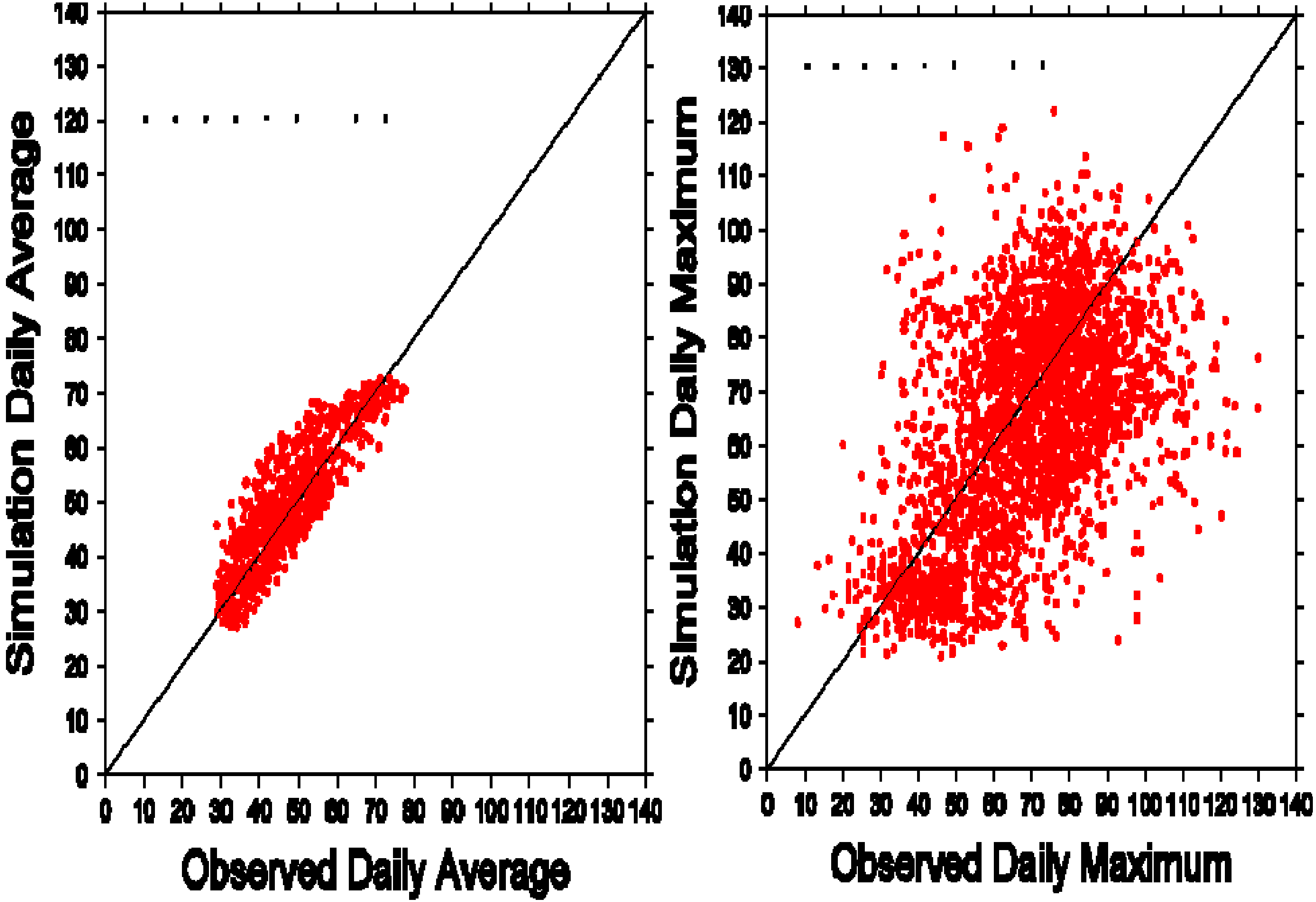

Kollumerwaard NL09 53N 17E
OBS
Model
concentration, ppb
time, hr

Daily Average for 88 stations

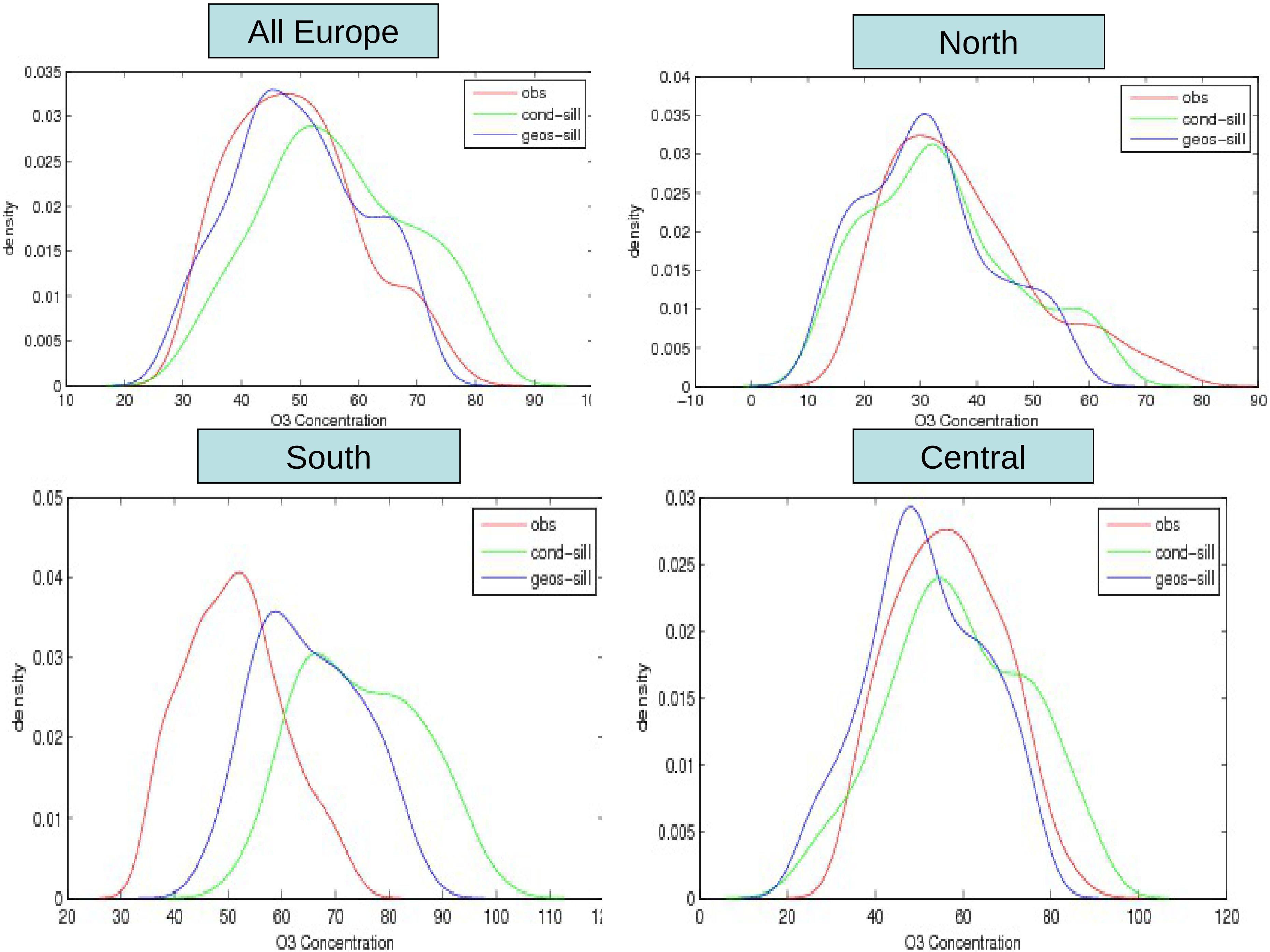


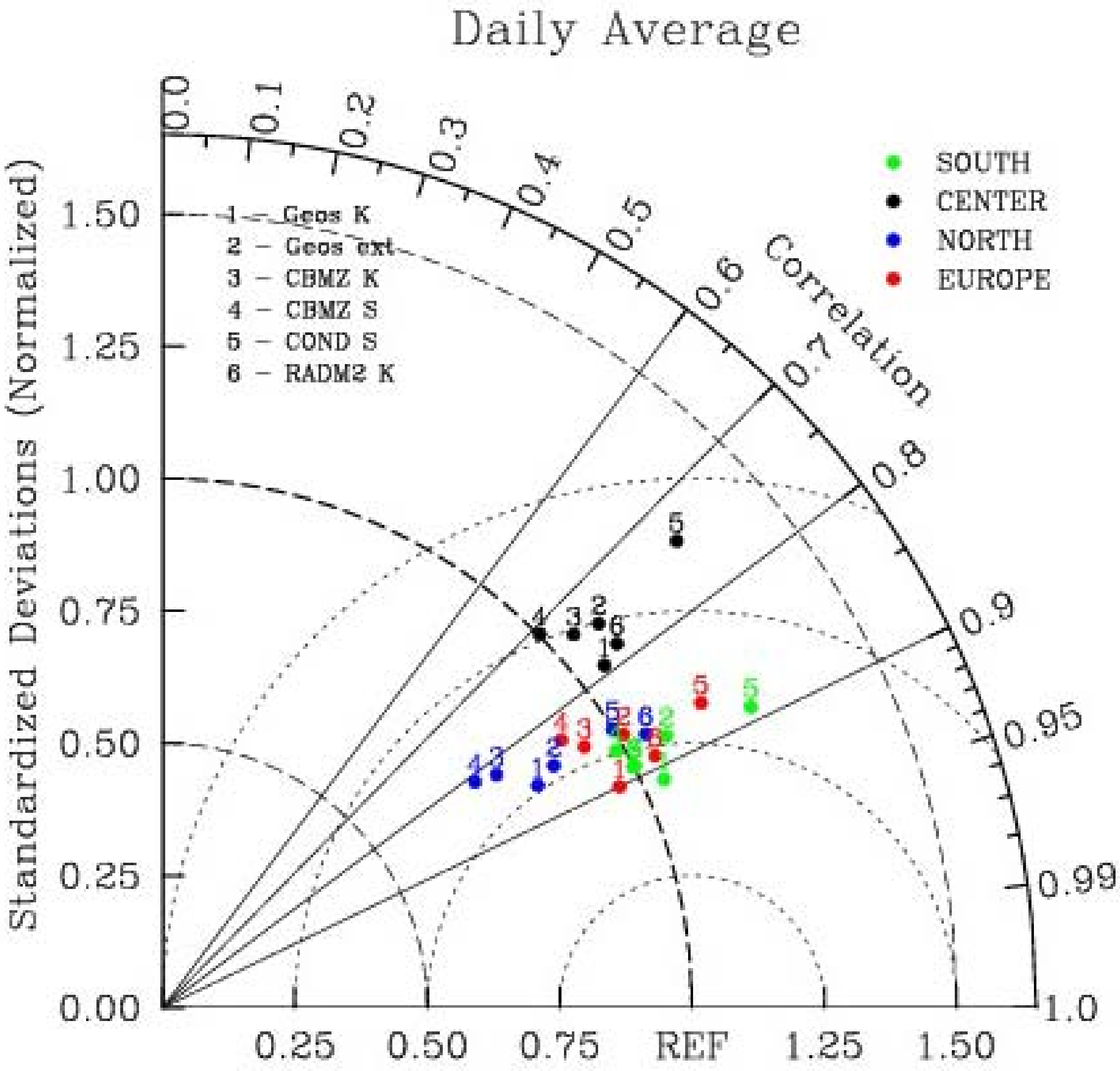
Daily Maximum averaged over 88 stations



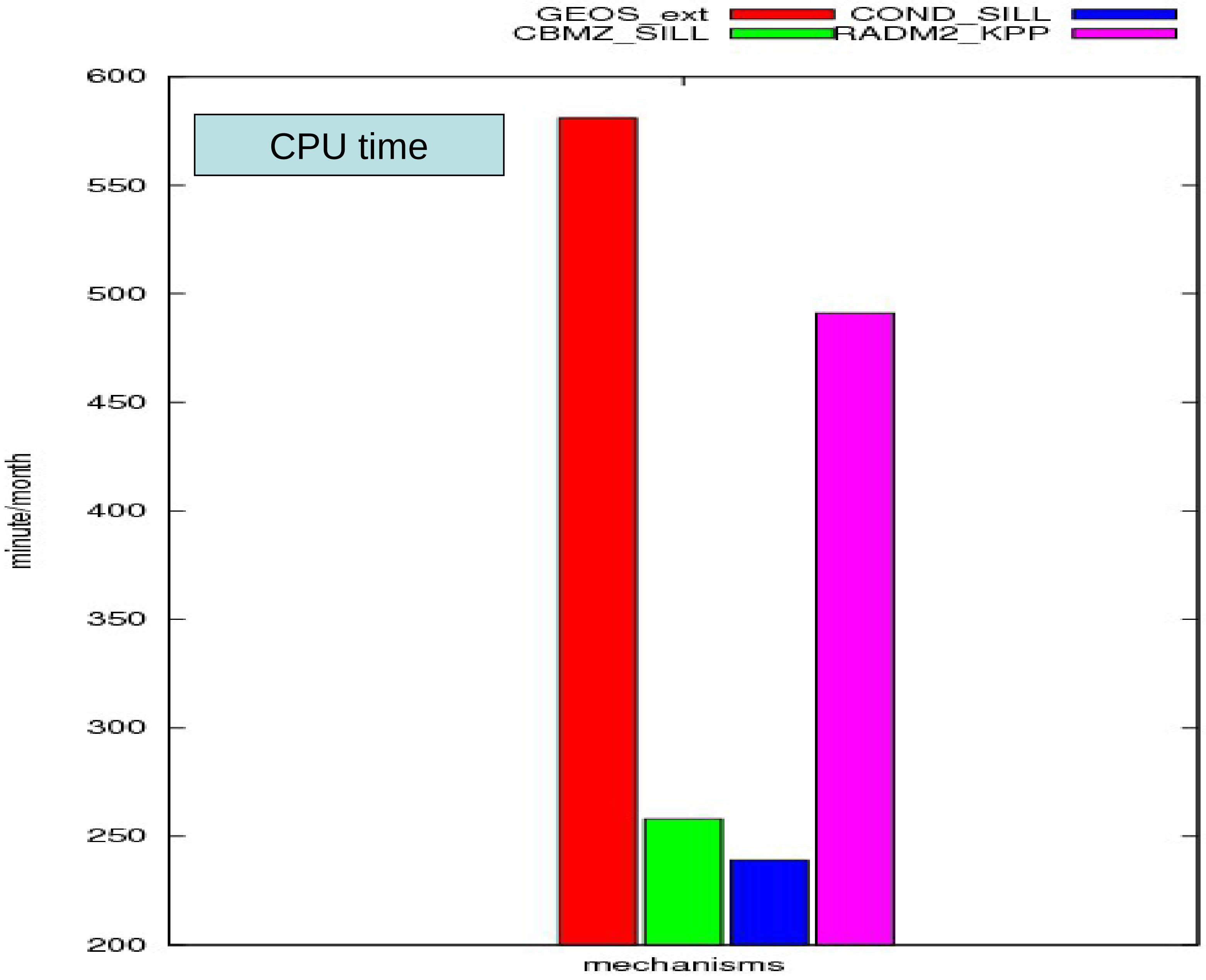


Simulation Daily Average
Observed Daily Average
Simulation Daily Maximum
Observed Daily Maximum
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140


All Europe
obs
cond-sill
geos-sill
density
O3 Concentration
North
obs
cond-sill
geos-sill
density
O3 Concentration
South
obs
cond-sill
geos-sill
density
O3 Concentration
Central
obs
cond-sill
geos-sill
density
O3 Concentration

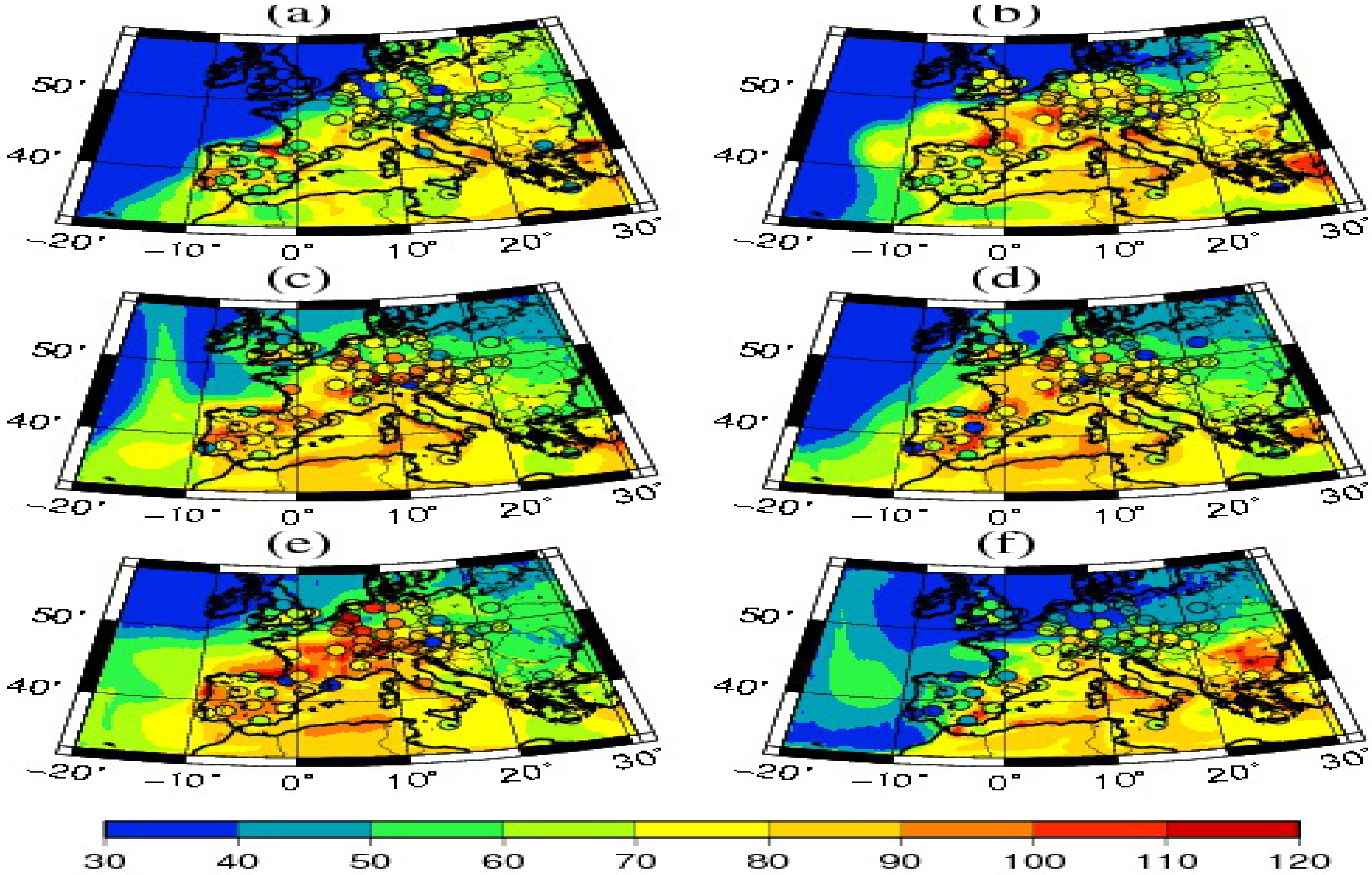


Daily Average
Standardized Deviations (Normalized)
Correlation
1 – Geos K
2 – Geos ext
3 – CBMZ K
4 – CBMZ S
5 – COND S
6 – RADM2 K
SOUTH
CENTER
NORTH
EUROPE
0.00
0.25
0.50
0.75
1.00
1.25
1.50
REF
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.95
0.99
1.0

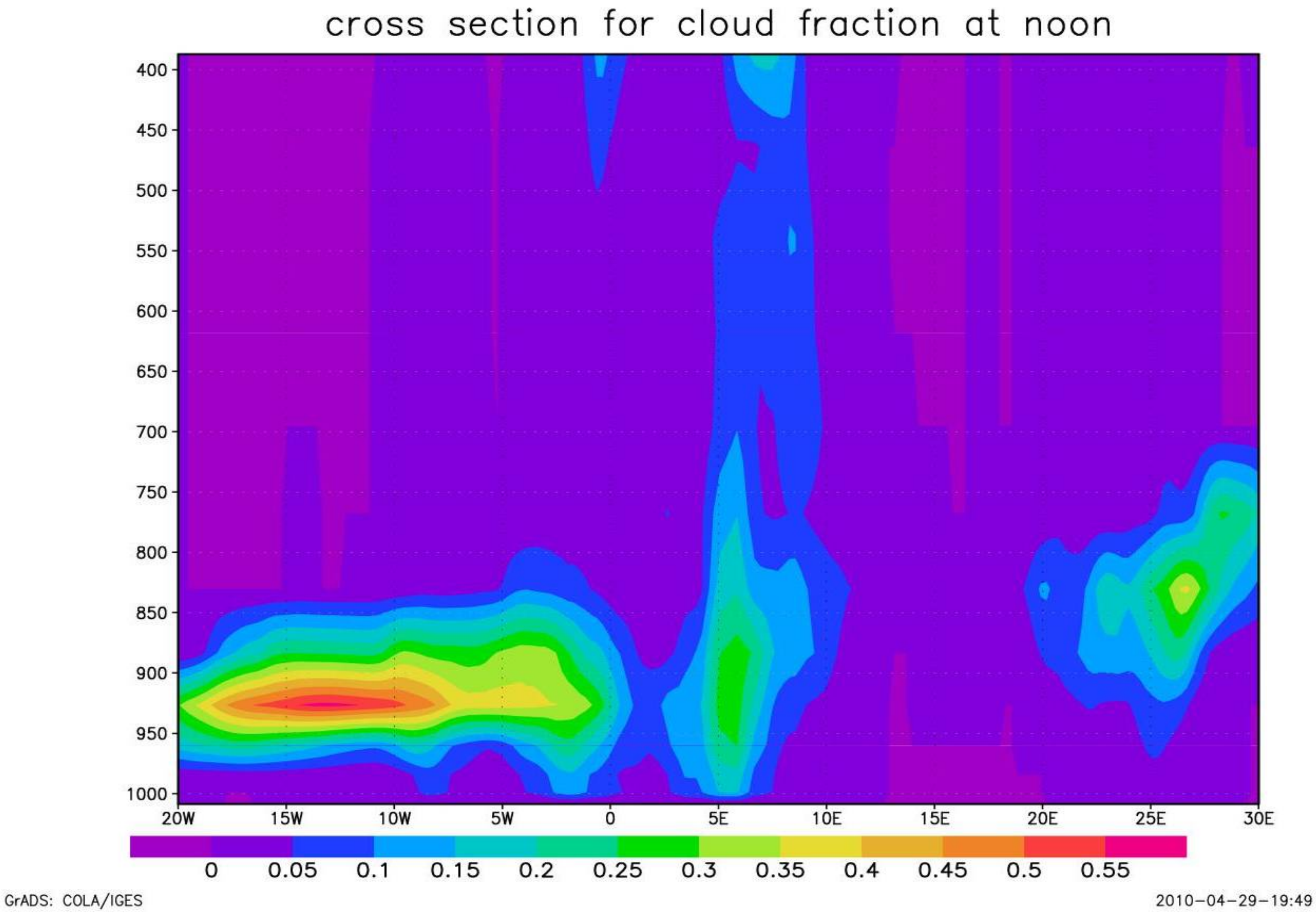


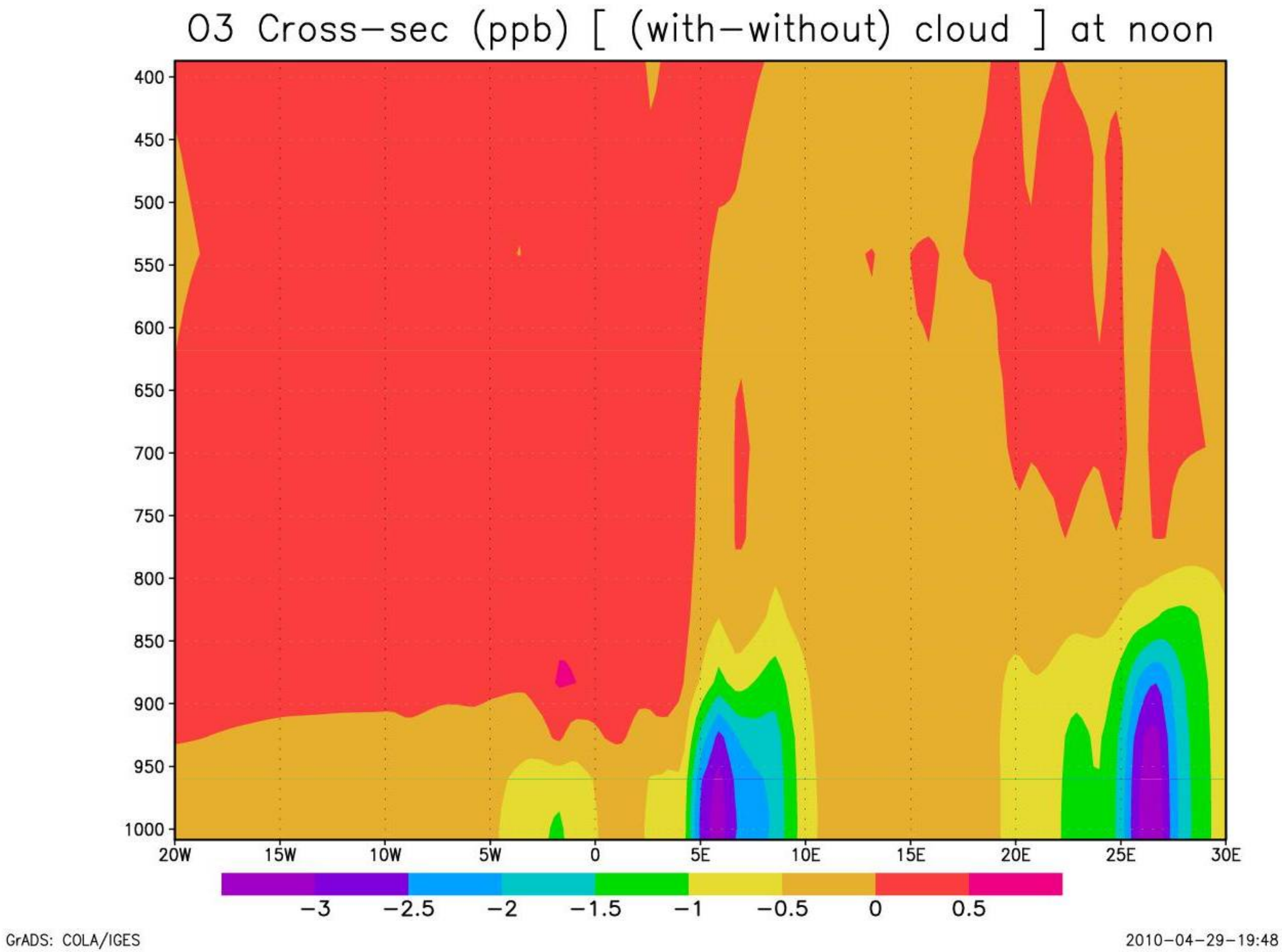
GEOS_ext
COND_SILL
CBMZ_SILL
RADM2_KPP
CPU time
minute/month
600
550
500
450
400
350
300
250
200
mechanisms

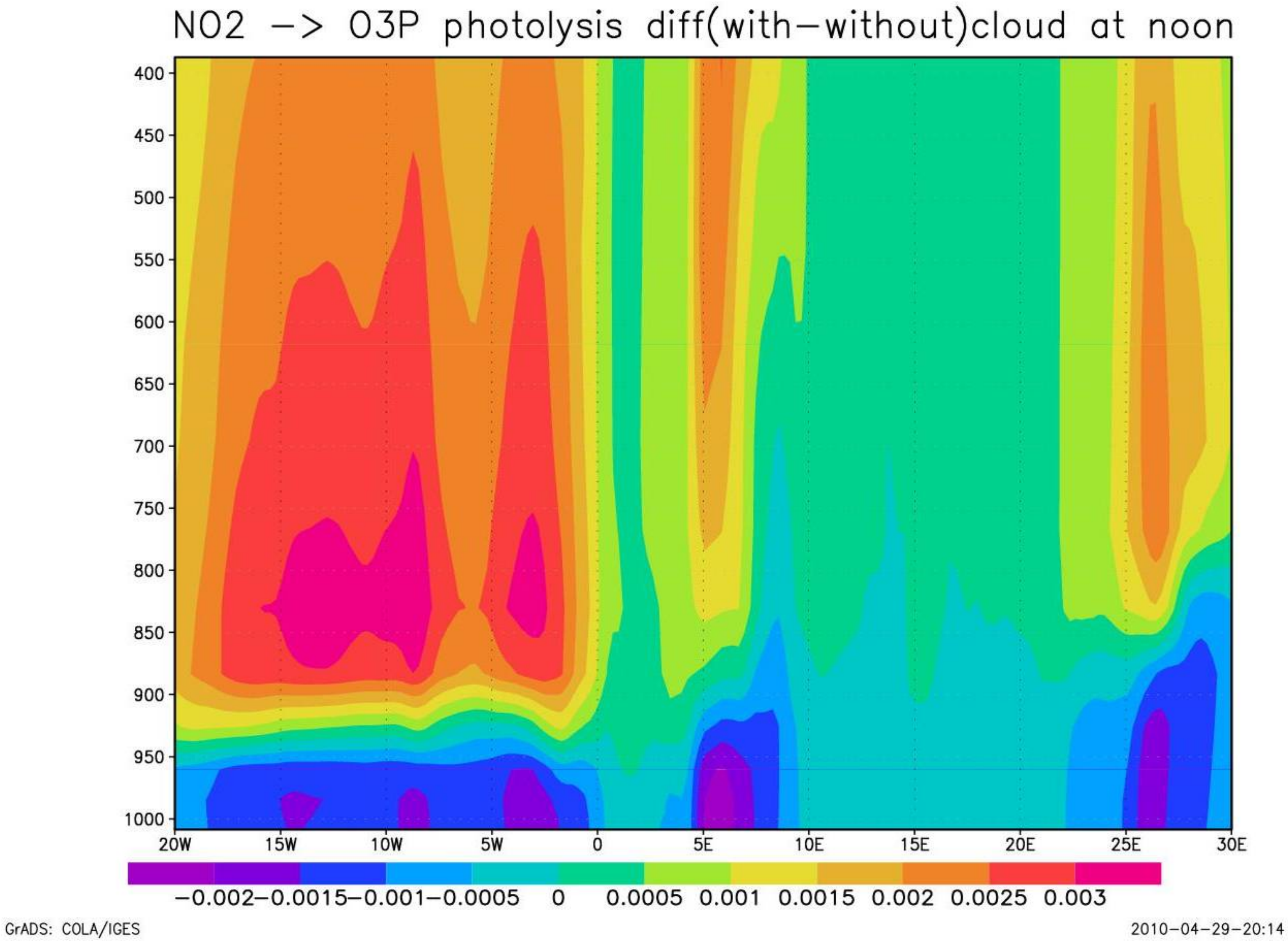
Model vs. Observation stations

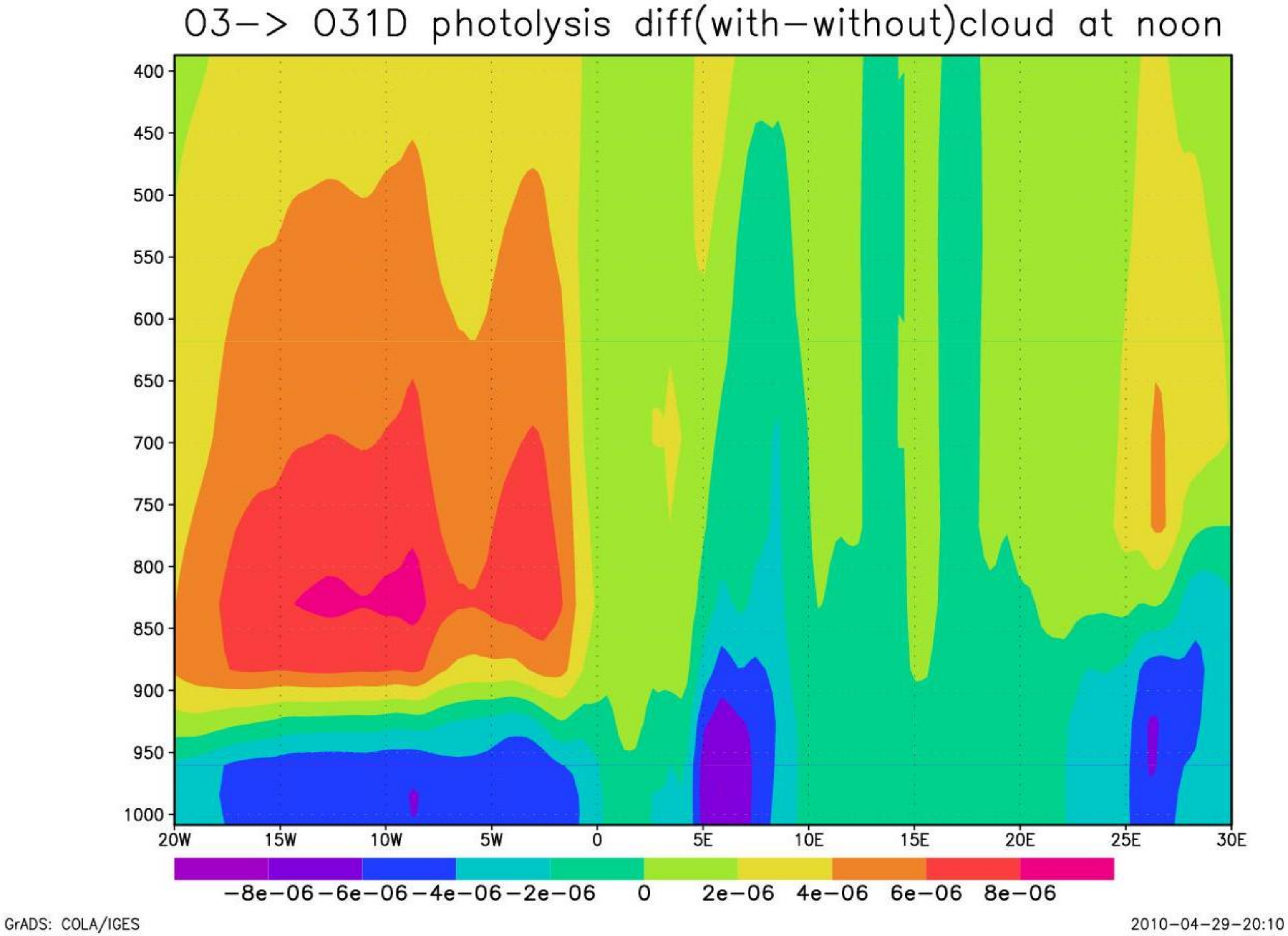


Effects of clouds on ozone and photolysis


cross section for cloud fraction at noon
400
450
500
550
600
650
700
750
800
850
900
950
1000
20W
15W
10W
5W
0
5E
10E
15E
20E
25E
30E
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
GrADS: COLA/IGES
2010-04-29-19:49


O3 Cross-sec (ppb) [(with-without) cloud] at noon
400
450
500
550
600
650
700
750
800
850
900
950
1000
20W
15W
10W
5W
0
5E
10E
15E
20E
25E
30E
-3
-2.5
-2
-1.5
-1
-0.5
0
0.5
GrADS: COLA/IGES
2010-04-29-19:48


NO2 -> O3P photolysis diff(with-without)cloud at noon
400
450
500
550
600
650
700
750
800
850
900
950
1000
20W
15W
10W
5W
0
5E
10E
15E
20E
25E
30E
-0.002 -0.0015 -0.001 -0.0005 0 0.0005 0.001 0.0015 0.002 0.0025 0.003
GrADS: COLA/IGES
2010-04-29-20:14


O3-> O31D photolysis diff(with-without)cloud at noon
400
450
500
550
600
650
700
750
800
850
900
950
1000
20W
15W
10W
5W
0
5E
10E
15E
20E
25E
30E
-8e-06 -6e-06 -4e-06 -2e-06 0 2e-06 4e-06 6e-06 8e-06
GrADS: COLA/IGES
2010-04-29-20:10

Why DMS in Regional Model (RegCM) ?

- **This Study…**

- Based on *regional scale*, this study presents a first attempt to investigate the link between **DMS** emissions/oxidation to the atmosphere and sulfur budget in *Regional Climate Model (RegCM V3)*. Very few RCMs deals with DMS.

- **Why is DMS Important?**

- *Dimethylsulphide (DMS)* is the most abundant volatile sulphur compound at the sea surface.
- It is derived from the precursor dimethylsulphoniopropionate (DMSP) which is directly synthesized by many algae. DMSP production by phytoplankton is highly species specific.
- Once in the marine environment, DMSP is readily broken down into DMS and acrylate. This breakdown process is the product of the microbial ecology of the surface waters.
- Research suggests that most (90%) of the oceanic biogenic flux to the atmosphere occurs via emission of gaseous DMS.

The influence of DMS on Climate

"Life on Earth itself generates a stabilizing system to keep the global climate favourable for life itself. "
Gaia, a new look on life, 1979, J. Lovelock

The CLAW hypothesis (Charlson et al., 1987) coupled the production of DMS by the plankton community to climate forcing .The hypothesis described how an increase in global phytoplankton production can be expected due to higher CO2 levels and the increase of the oceans surface temperature caused by the enhanced greenhouse effect. The increase in phytoplankton production would then lead to possibly higher DMS production.

Recent global estimates of ***DMS flux from the oceans range from 8 to 51 Tg S y-1***
This is *50%* of total natural S-emissions (presently nearly equivalent to anthropogenic emissions, 76 Tg S a-1).

Uncertainties are due to:

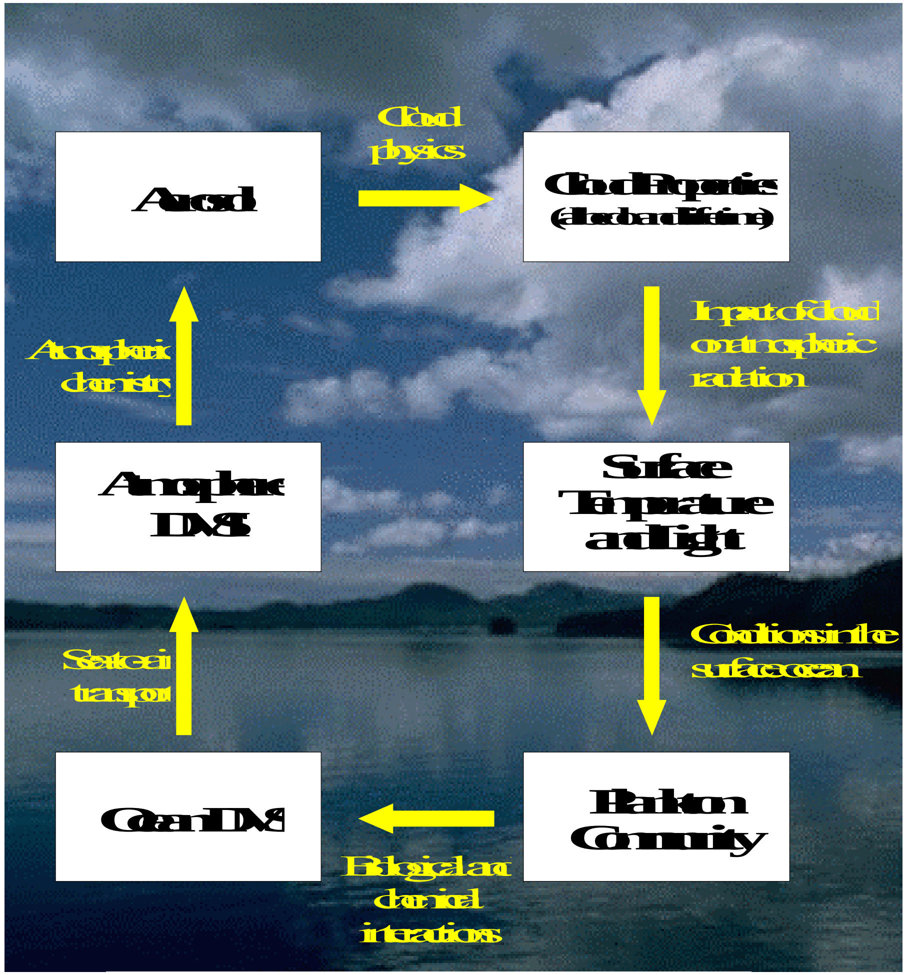
- Wind velocity close to the surface (U10)
- Differences in the transfer velocities in sea-to-air calculations
- DMS seawater measurements (paucity of data in winter months and at high latitudes)

The CLAW Hypothesis

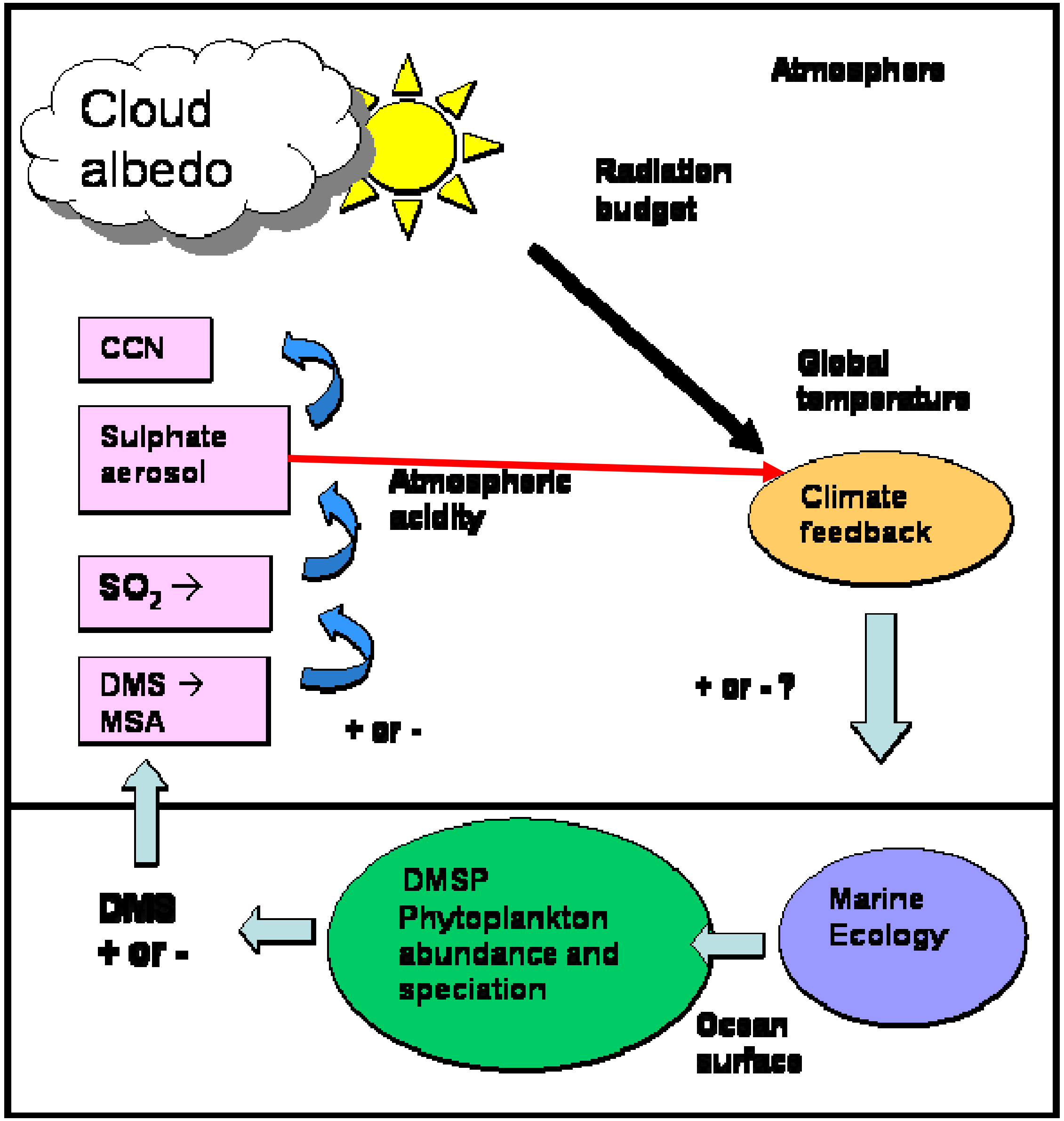
(Charlson, Lovelock, Andreae and Warren, 1987)

- DMS from the ocean affects cloud properties and can feedback to the plankton community

- This acts to regulate climate by increasing cloud albedo when sea-surface temperatures rise.

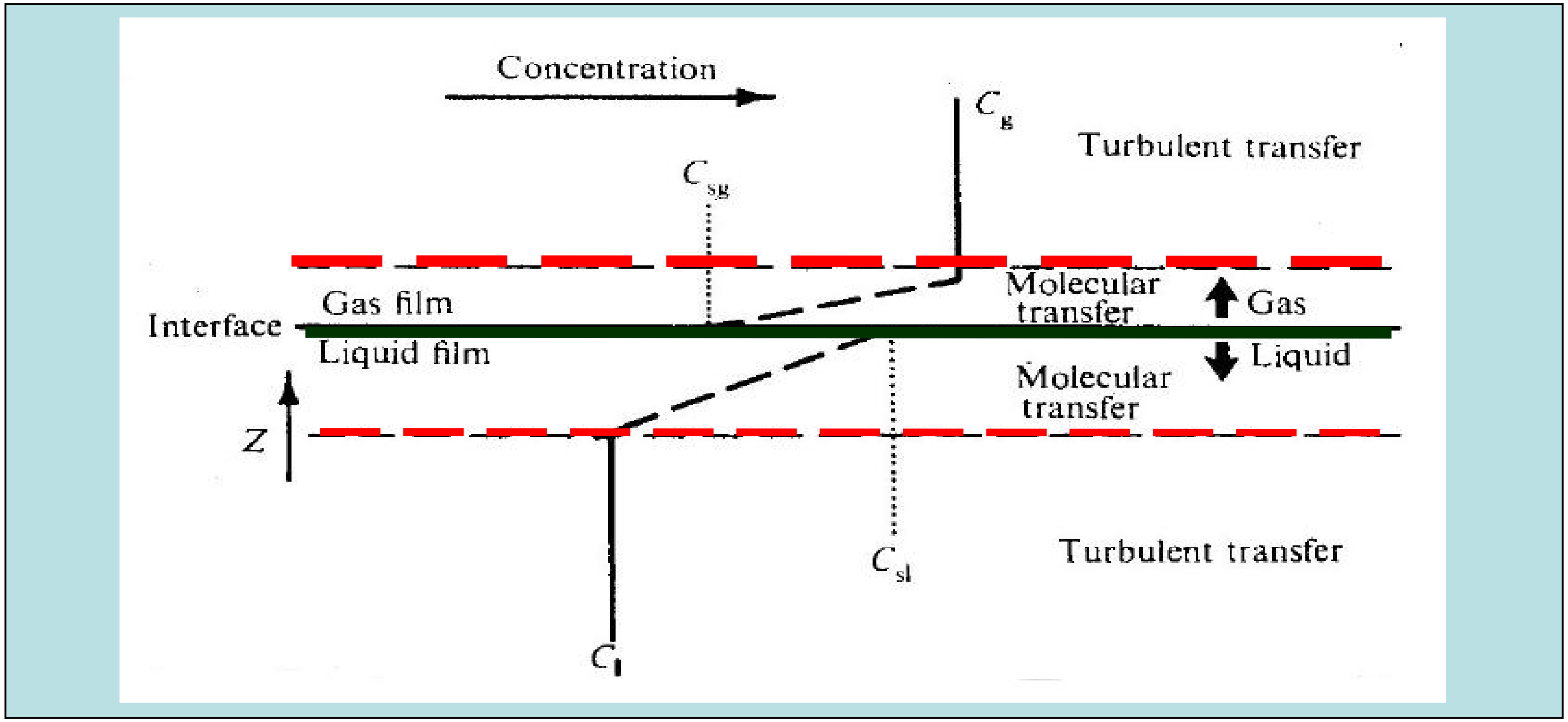


Backdrop photo from the NOAA Central Library Photo Collection

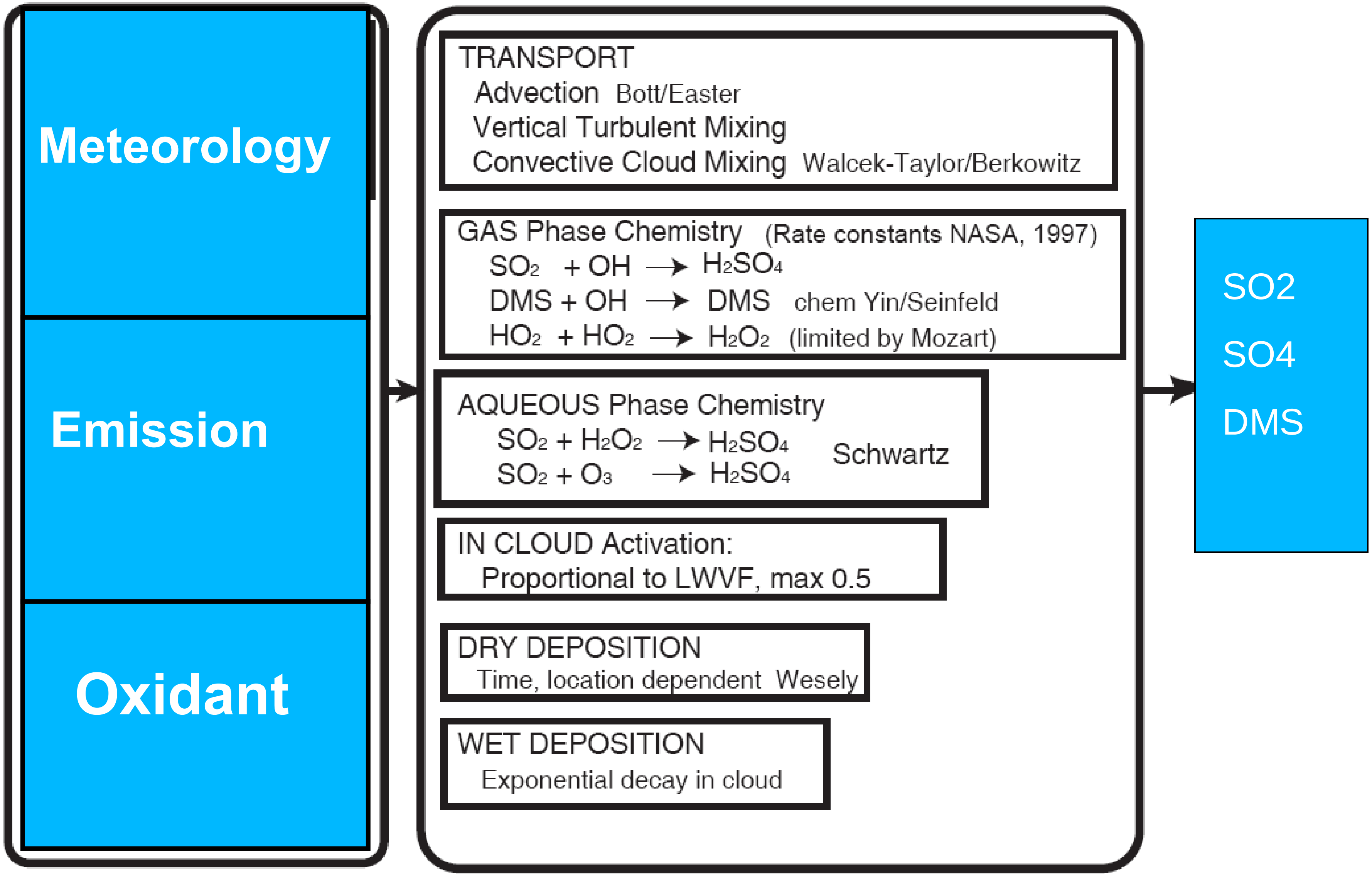


The possible climatic feedback loop as it is suggested by the CLAW hypothesis. The signs indicate that it is not known whether there is a negative or a positive feedback effect between the parameters involved. The plankton climate connection, emissions from plankton influence the climate via cloud properties (adapted from Charlson et al., 1987).

Air-Sea gas exchange



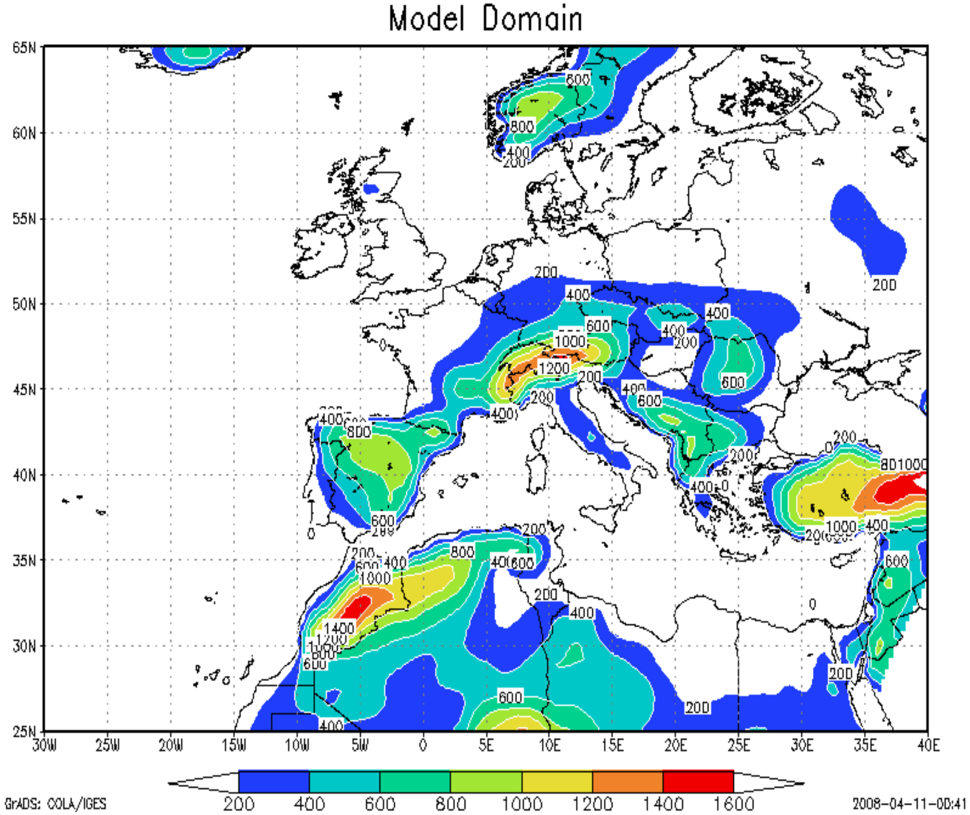
DMS Cycle in RegCM



RegCM Simulation

from

1 January 2000 to 31 December 2006

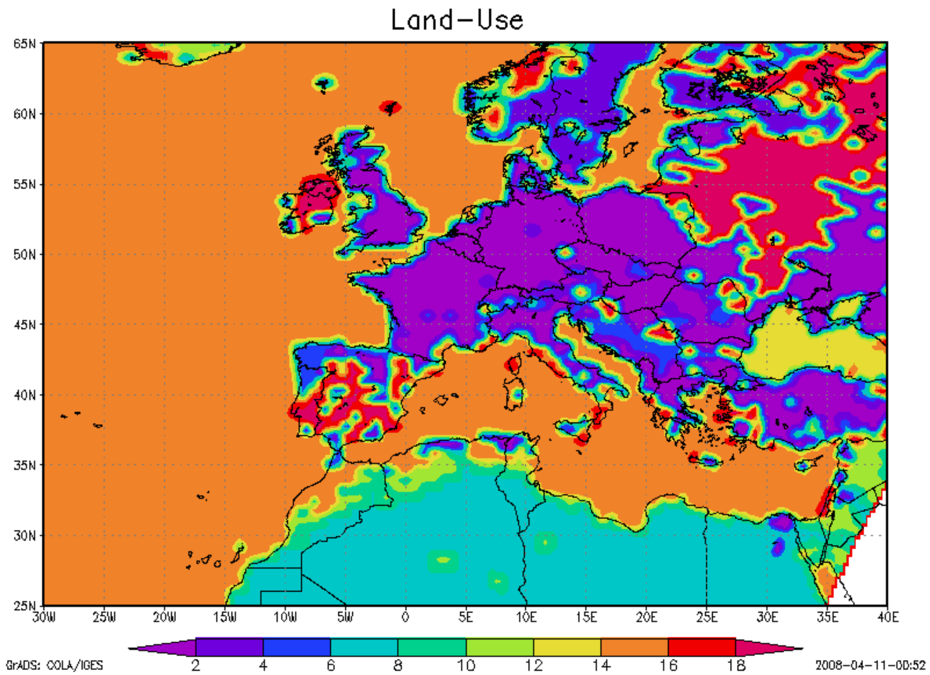


- RegCM3 (Regional Climate Model Ver.3)
- Resolution
  : 60 km

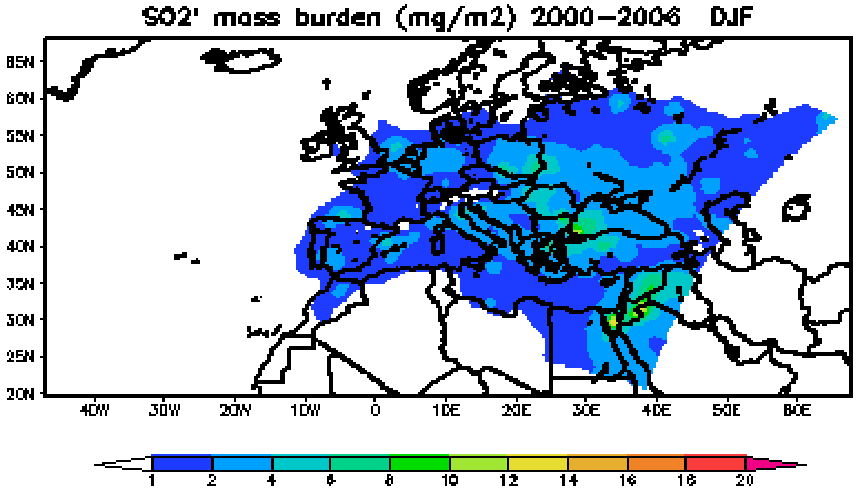
Initial & Boundary Condition

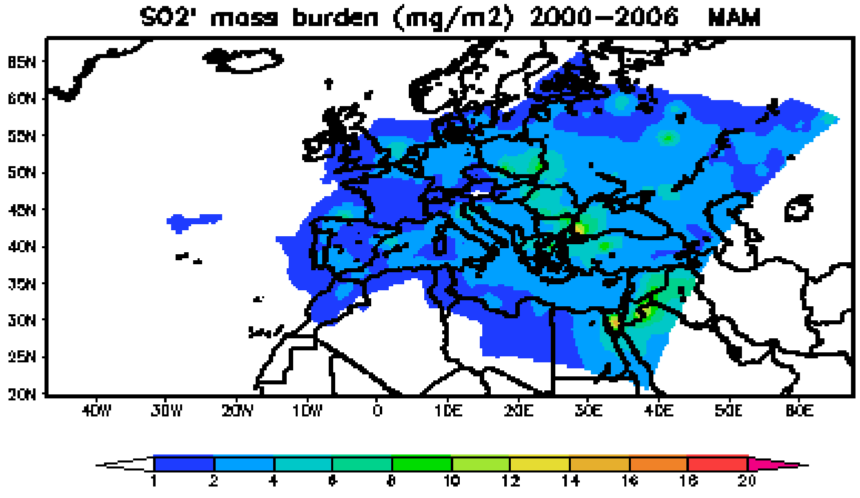
: NCEP reanalysis

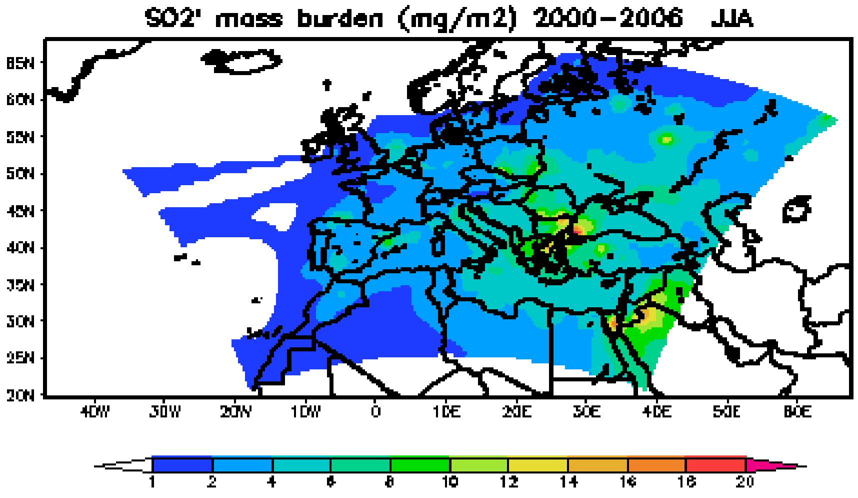
- Physics parameterization
  : Cumulus – Grell (1993)
  : Radiation – CCM3 (Kiehl et al. 1996)
  : PBL – Holtslag et al. (1990)
  : Dust module – Zakey et al. (2006)

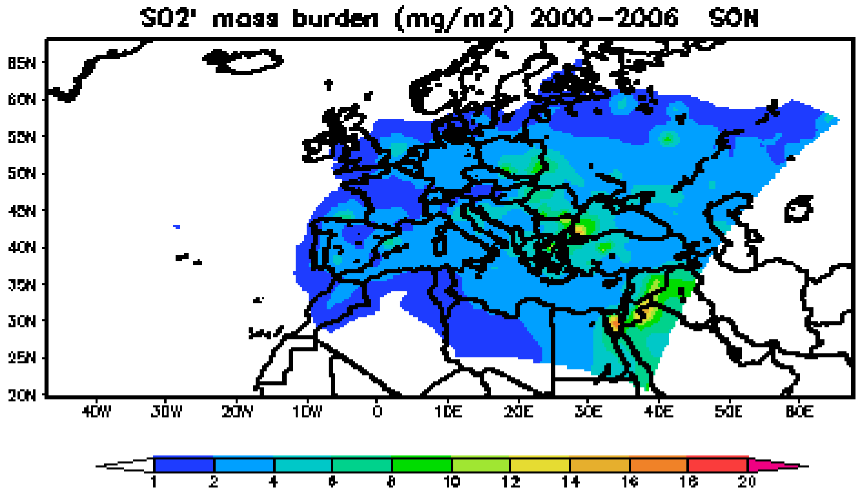


Sulfur Dioxide mass load (burden)   mg/m2

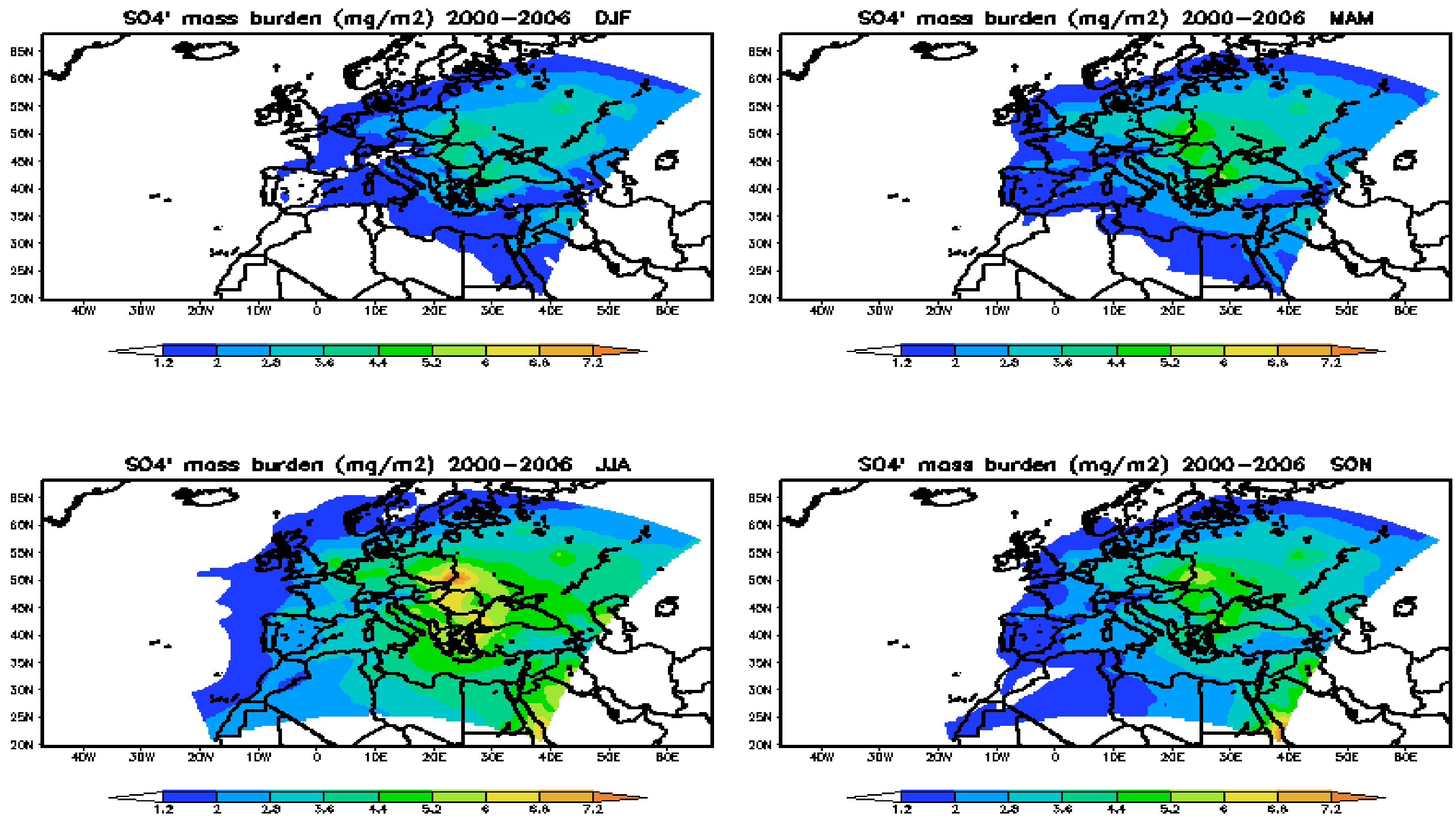






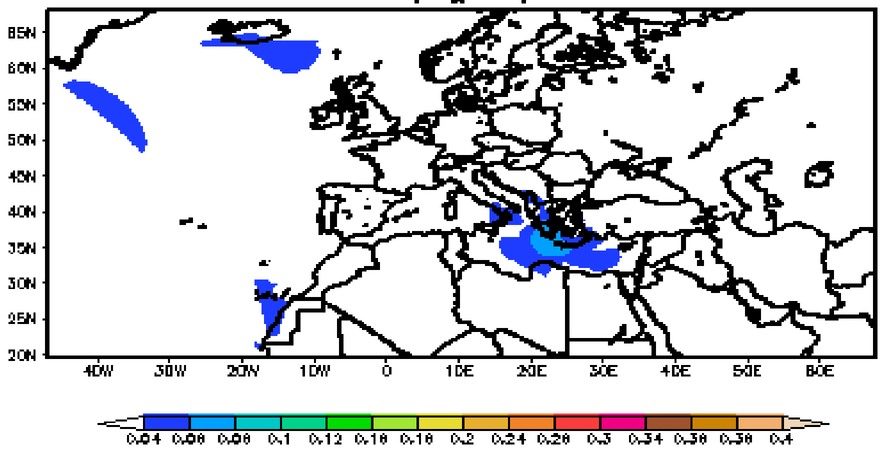


Sulfate mass load (burden) mg/m2

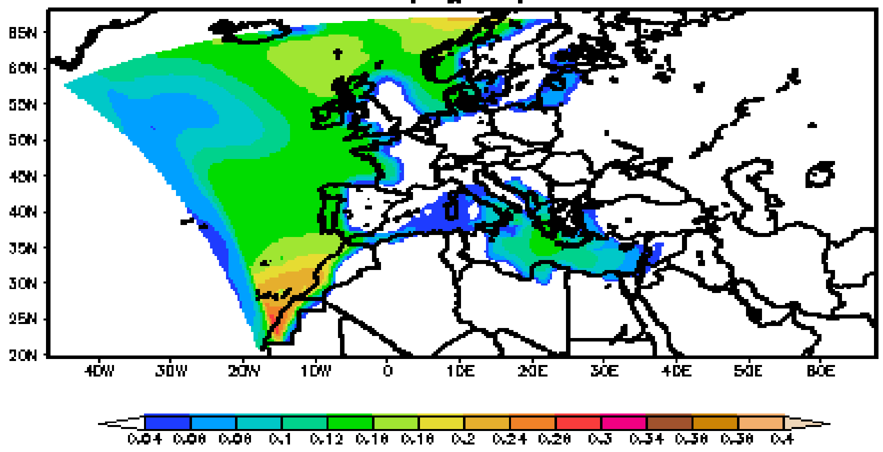


DMS mass load (burden) mg/m2

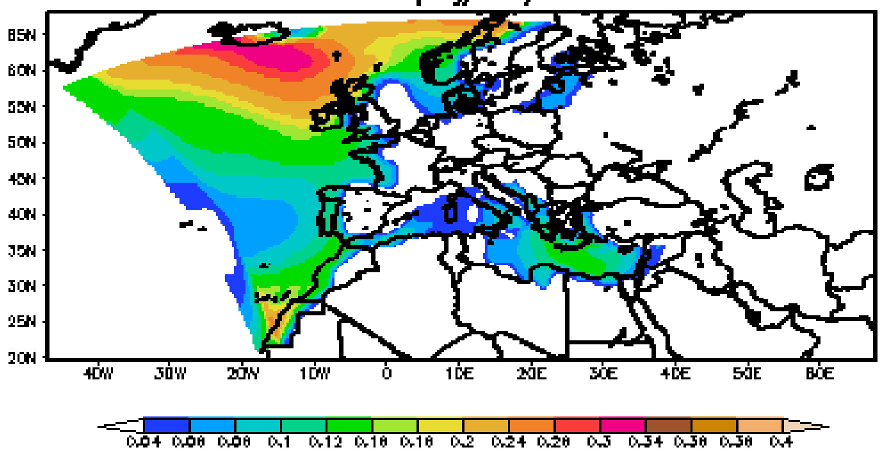
DMS' mass burden (mg/m2) 2000–2006 DJF



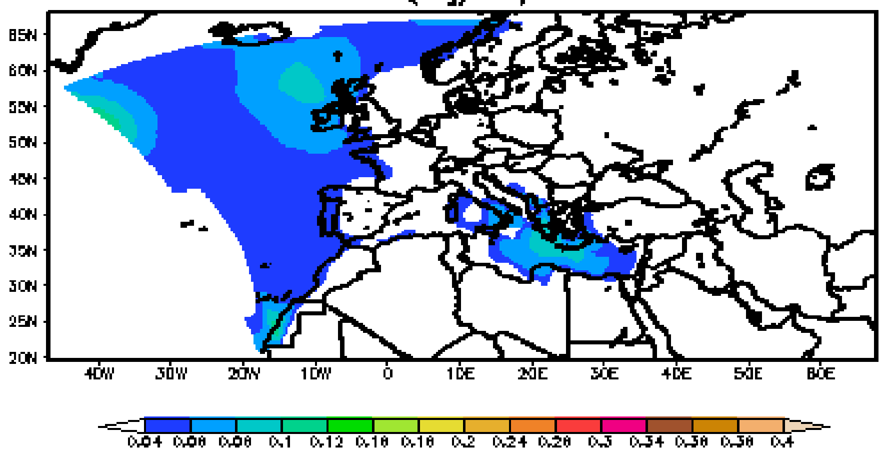
DMS' mass burden (mg/m2) 2000–2006 MAM

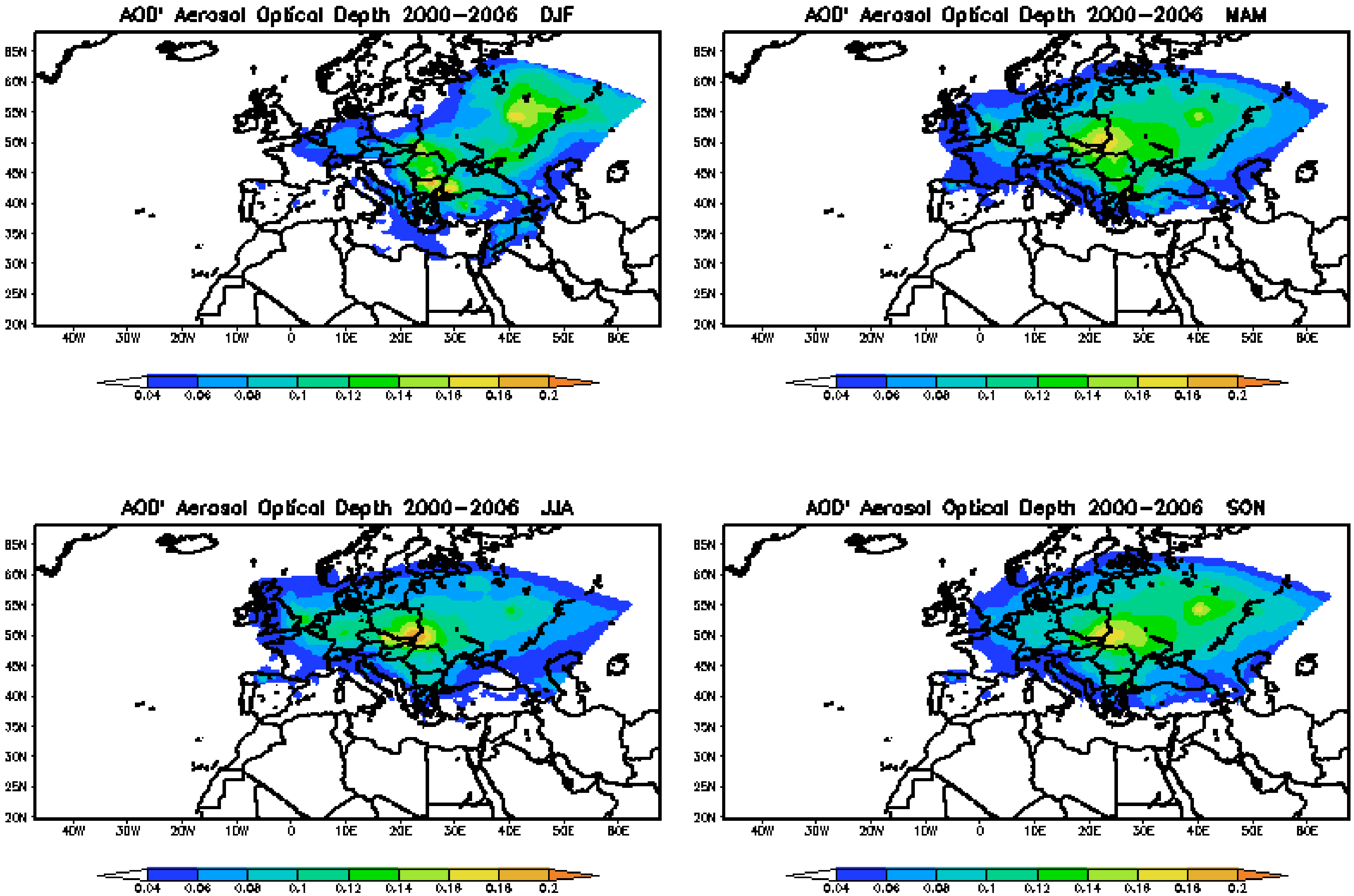


DMS' mass burden (mg/m2) 2000–2006 JJA



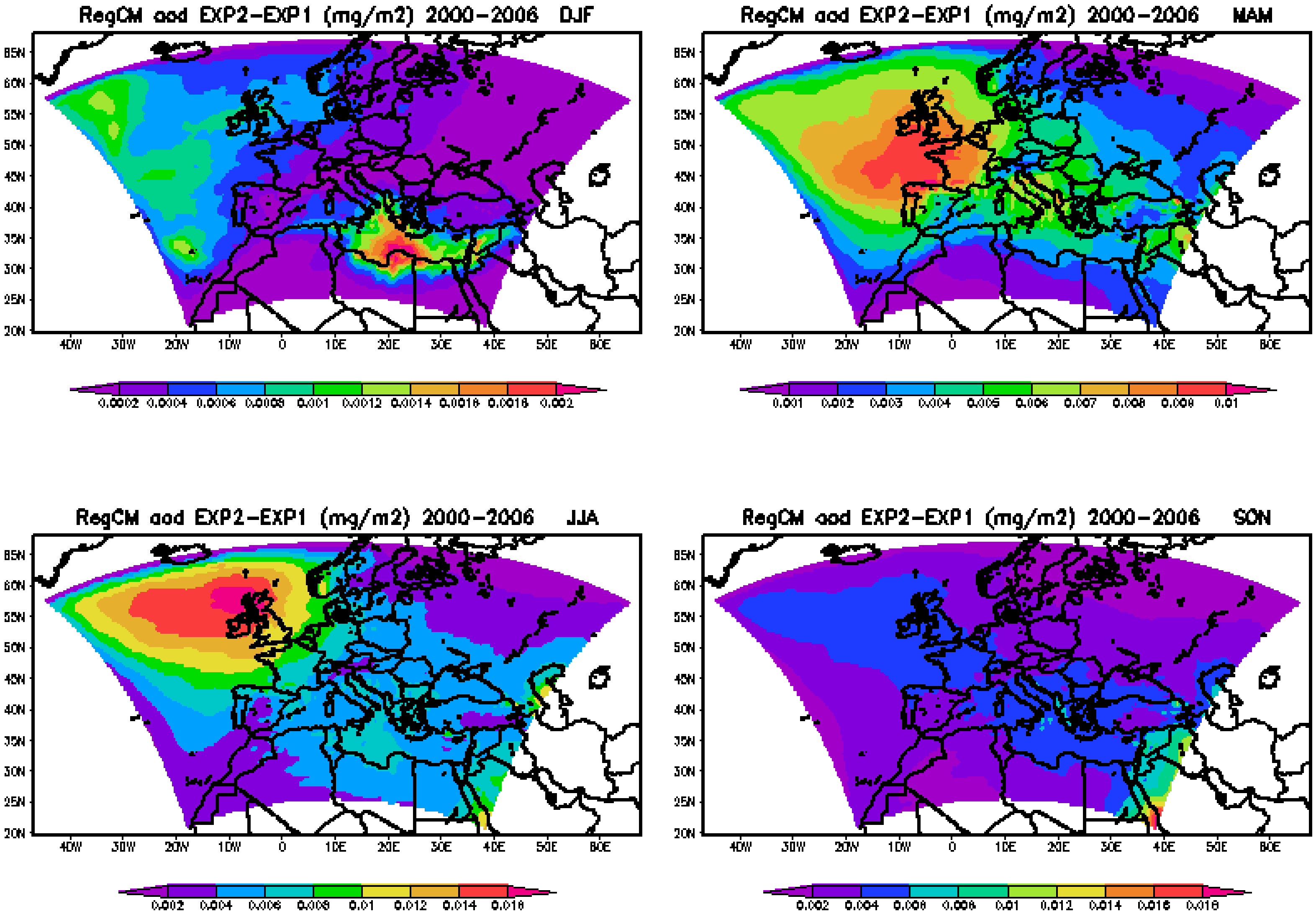
DMS' mass burden (mg/m2) 2000–2006 SON





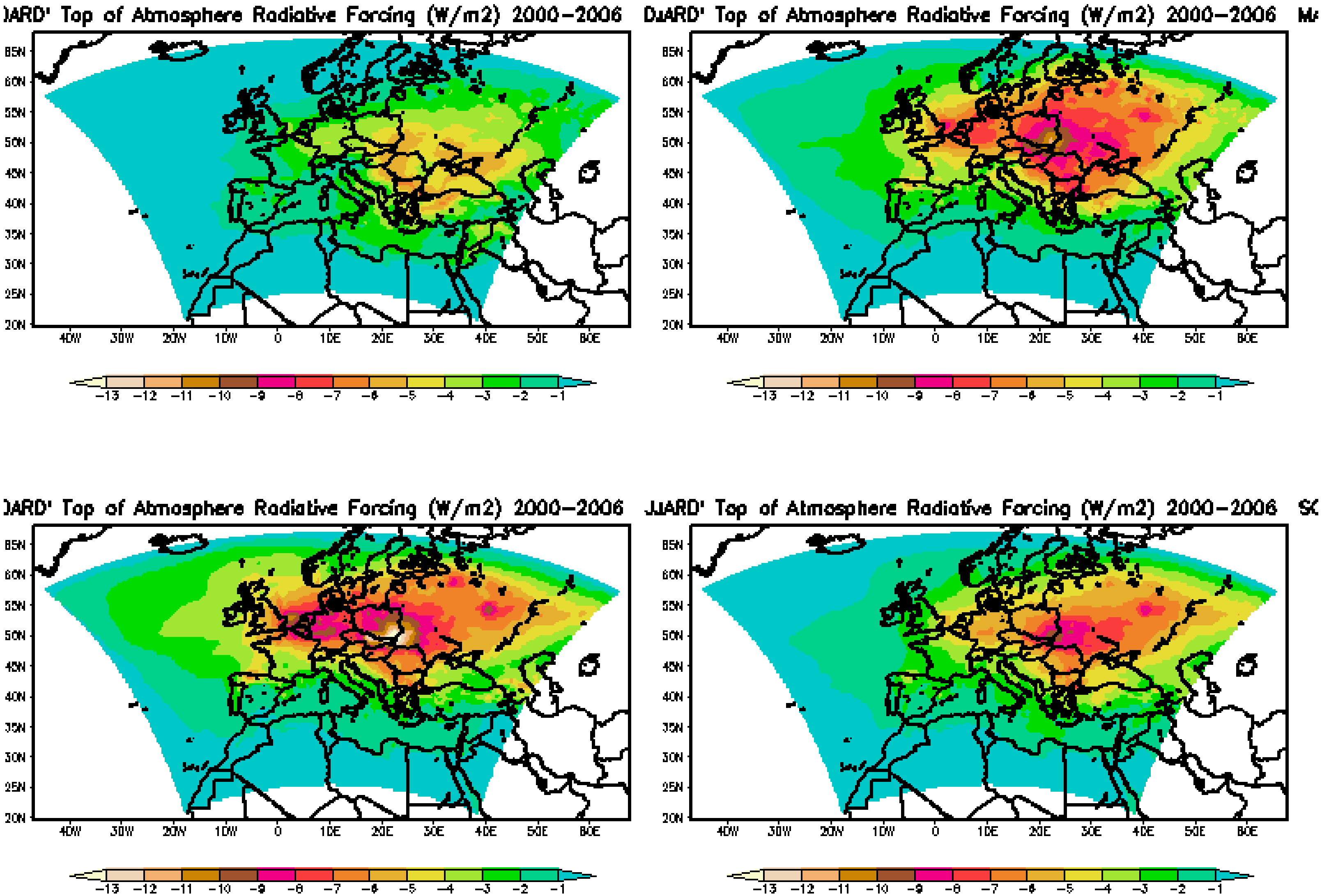
AOD' Aerosol Optical Depth 2000–2006 DJF
AOD' Aerosol Optical Depth 2000–2006 MAM
AOD' Aerosol Optical Depth 2000–2006 JJA
AOD' Aerosol Optical Depth 2000–2006 SON
65N 60N 55N 50N 45N 40N 35N 30N 25N 20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
0.04 0.06 0.08 0.1 0.12 0.14 0.16 0.18 0.2

DMS Contribution to Sulfate aerosols

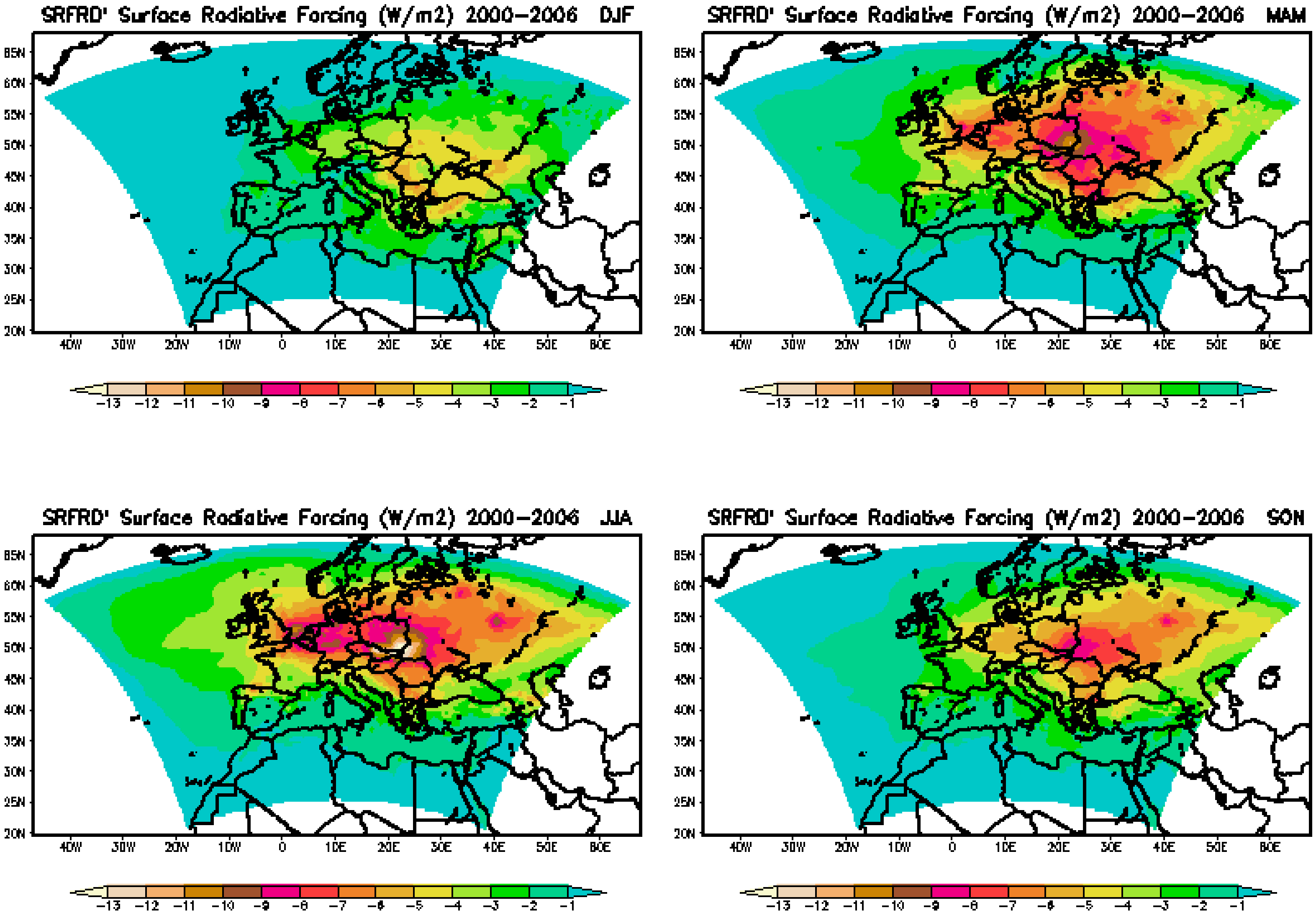

RegCM aod EXP2-EXP1 (mg/m2) 2000-2006 DJF
0.0002 0.0004 0.0006 0.0008 0.001 0.0012 0.0014 0.0016 0.0018 0.002
RegCM aod EXP2-EXP1 (mg/m2) 2000-2006 MAM
0.001 0.002 0.003 0.004 0.005 0.006 0.007 0.008 0.009 0.01
RegCM aod EXP2-EXP1 (mg/m2) 2000-2006 JJA
0.002 0.004 0.006 0.008 0.01 0.012 0.014 0.016
RegCM aod EXP2-EXP1 (mg/m2) 2000-2006 SON
0.002 0.004 0.006 0.008 0.01 0.012 0.014 0.016 0.018

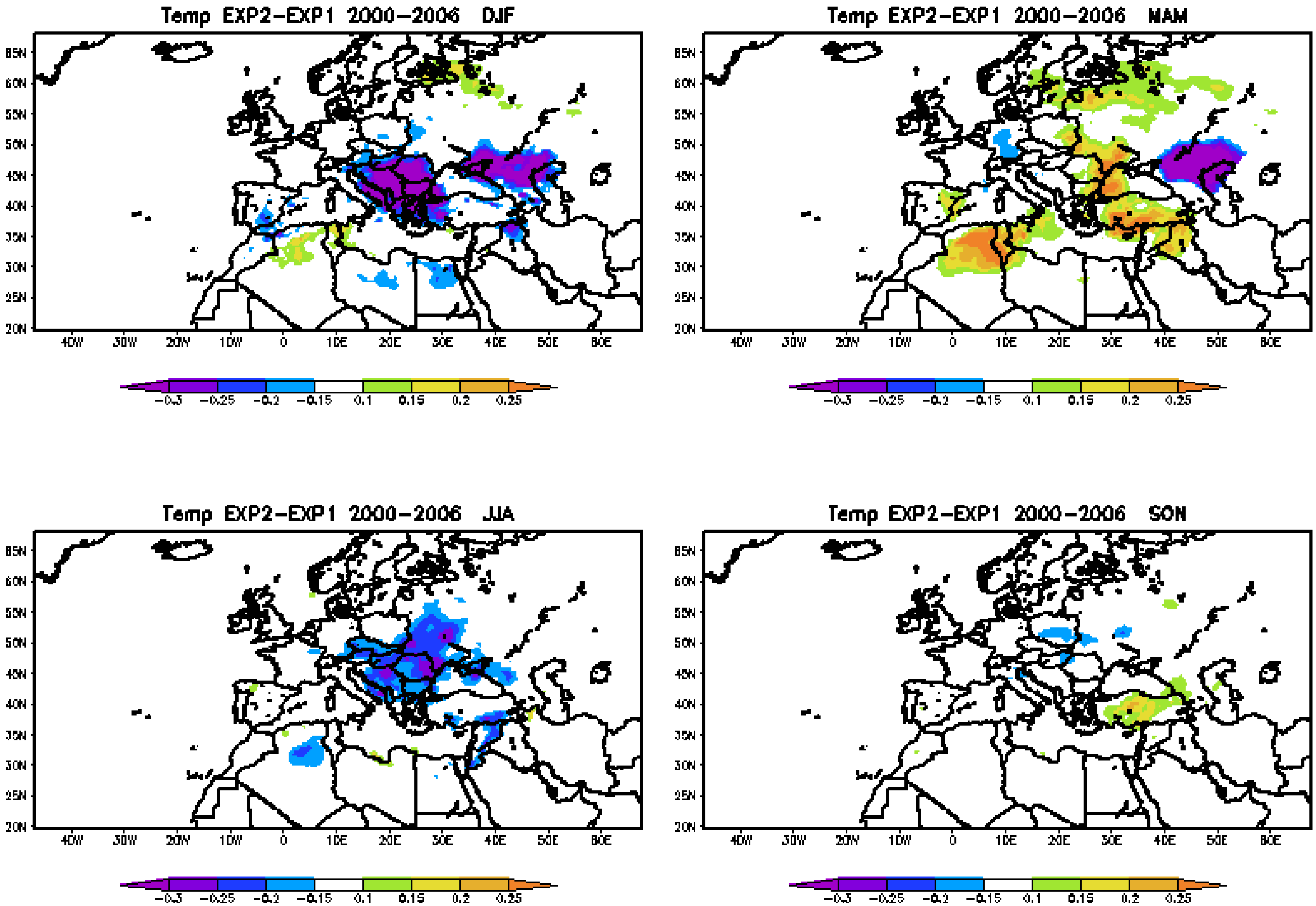
Climate feedback

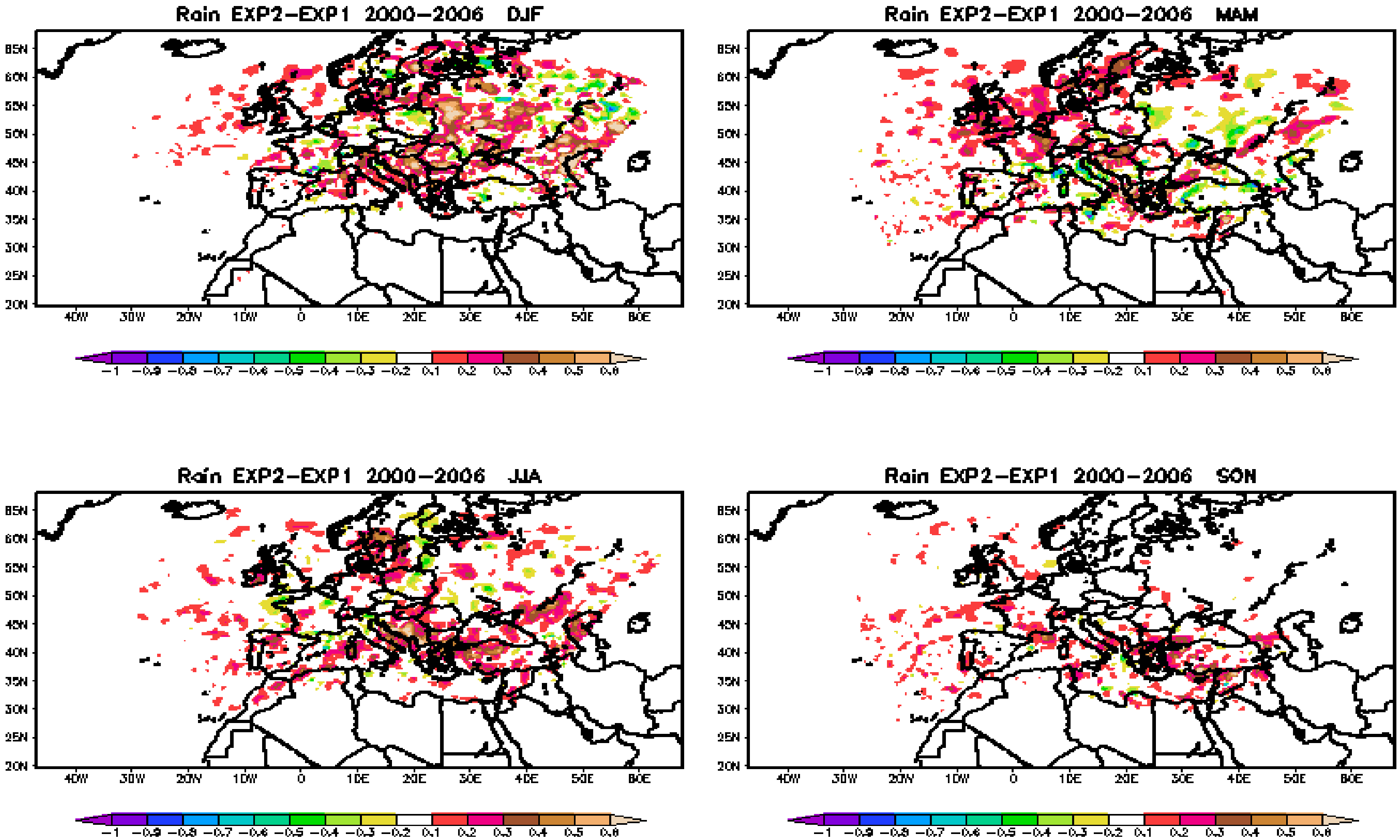
Top-Atmosphere Radiative Forcing W/m2

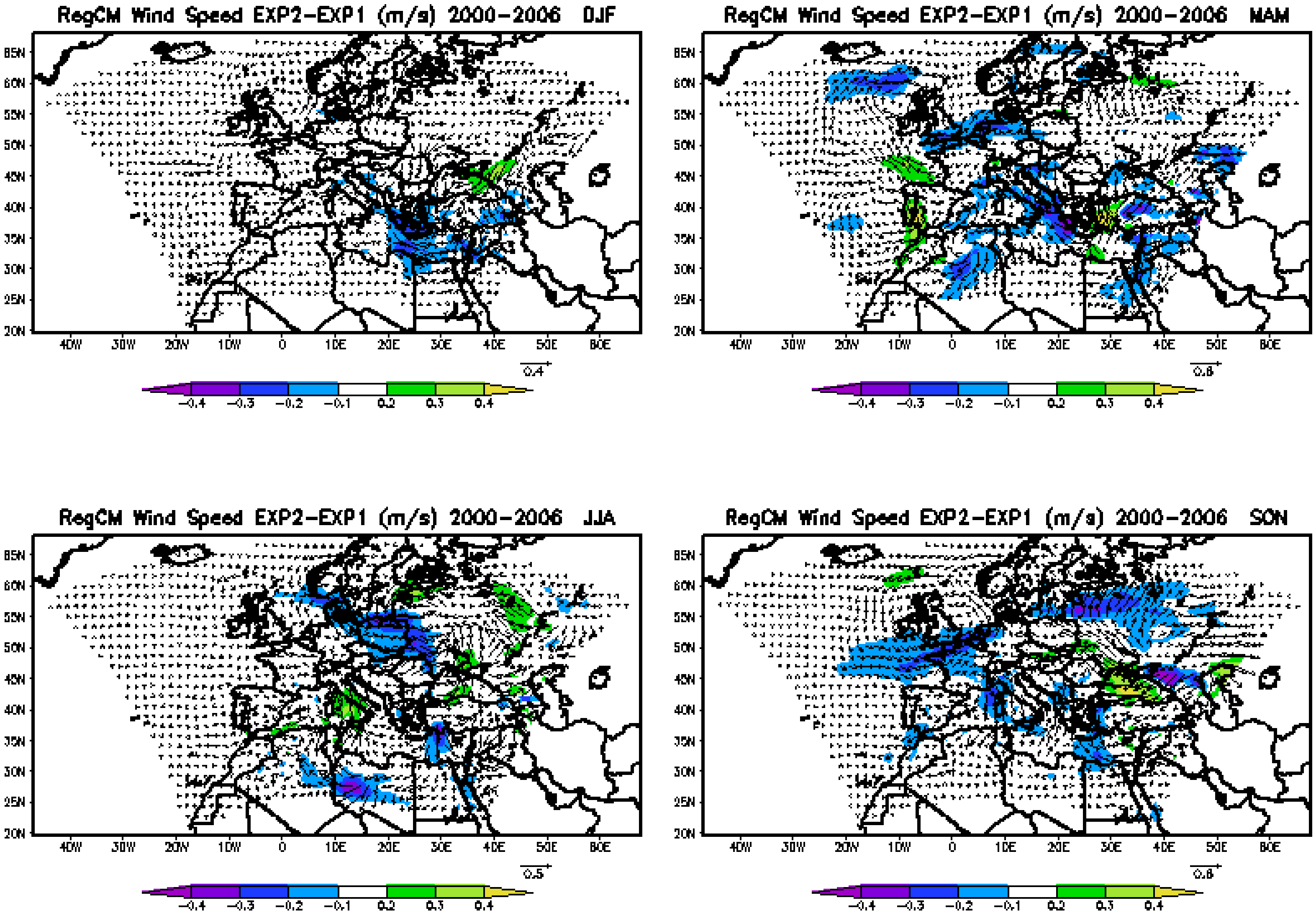


Surface Radiative Forcing W/m2




Temp EXP2-EXP1 2000-2006 DJF
65N
60N
55N
50N
45N
40N
35N
30N
25N
20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
-0.3 -0.25 -0.2 -0.15 0.1 0.15 0.2 0.25
Temp EXP2-EXP1 2000-2006 MAM
65N
60N
55N
50N
45N
40N
35N
30N
25N
20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
-0.3 -0.25 -0.2 -0.15 0.1 0.15 0.2 0.25
Temp EXP2-EXP1 2000-2006 JJA
65N
60N
55N
50N
45N
40N
35N
30N
25N
20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
-0.3 -0.25 -0.2 -0.15 0.1 0.15 0.2 0.25
Temp EXP2-EXP1 2000-2006 SON
65N
60N
55N
50N
45N
40N
35N
30N
25N
20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
-0.3 -0.25 -0.2 -0.15 0.1 0.15 0.2 0.25


Rain EXP2-EXP1 2000-2006 DJF
Rain EXP2-EXP1 2000-2006 MAM
Rain EXP2-EXP1 2000-2006 JJA
Rain EXP2-EXP1 2000-2006 SON
65N
60N
55N
50N
45N
40N
35N
30N
25N
20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
-1 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 0.1 0.2 0.3 0.4 0.5 0.6


RegCM Wind Speed EXP2-EXP1 (m/s) 2000-2006 DJF
RegCM Wind Speed EXP2-EXP1 (m/s) 2000-2006 MAM
RegCM Wind Speed EXP2-EXP1 (m/s) 2000-2006 JJA
RegCM Wind Speed EXP2-EXP1 (m/s) 2000-2006 SON
85N 60N 55N 50N 45N 40N 35N 30N 25N 20N
40W 30W 20W 10W 0 10E 20E 30E 40E 50E 60E
0.4
0.8
0.5
0.8
−0.4 −0.3 −0.2 −0.1 0.2 0.3 0.4


• Thank you for your attention