The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2148-23

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

31 May - 11 June, 2010

RegCM-CHEM tutorial

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ESP-ICTP
Trieste
ITALY

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Cairo
EGYPT

RegCM-CHEM tutorial

A. Shalaby[(a)], A. Zakey[(b)]

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

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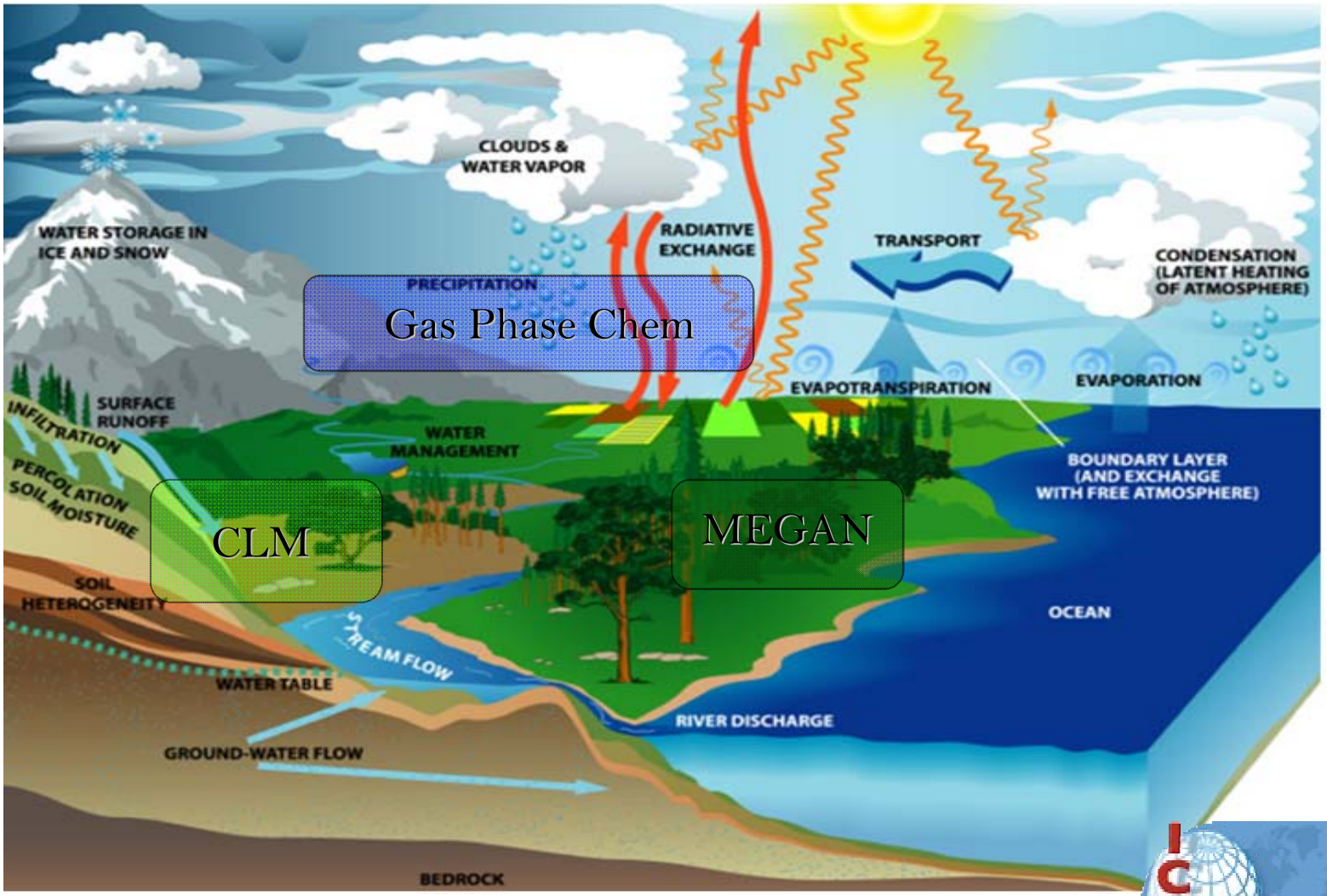
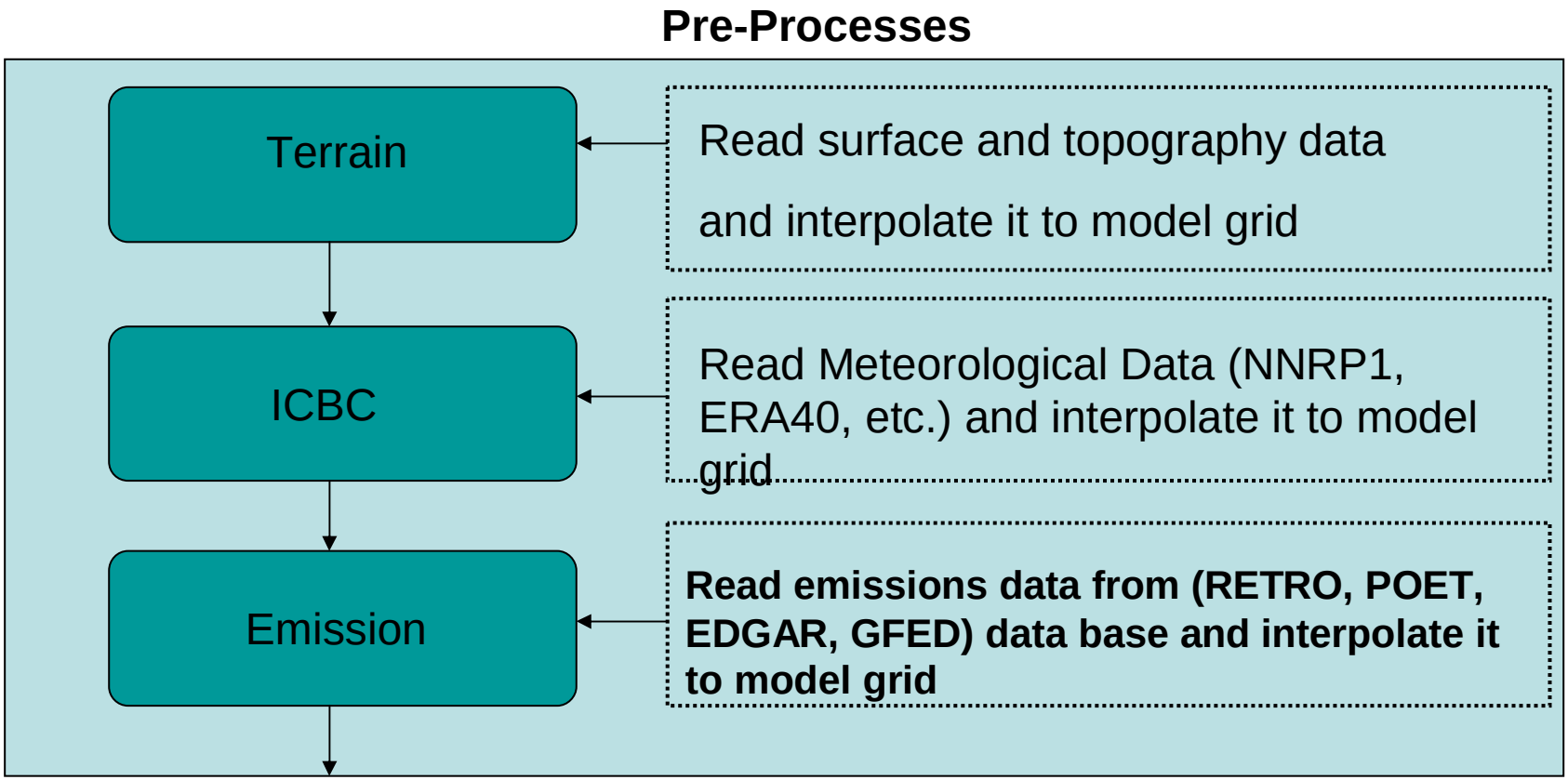
(a) ICTP and Egyptian Meteorological Authority, Cairo, Egypt

(b) ICTP

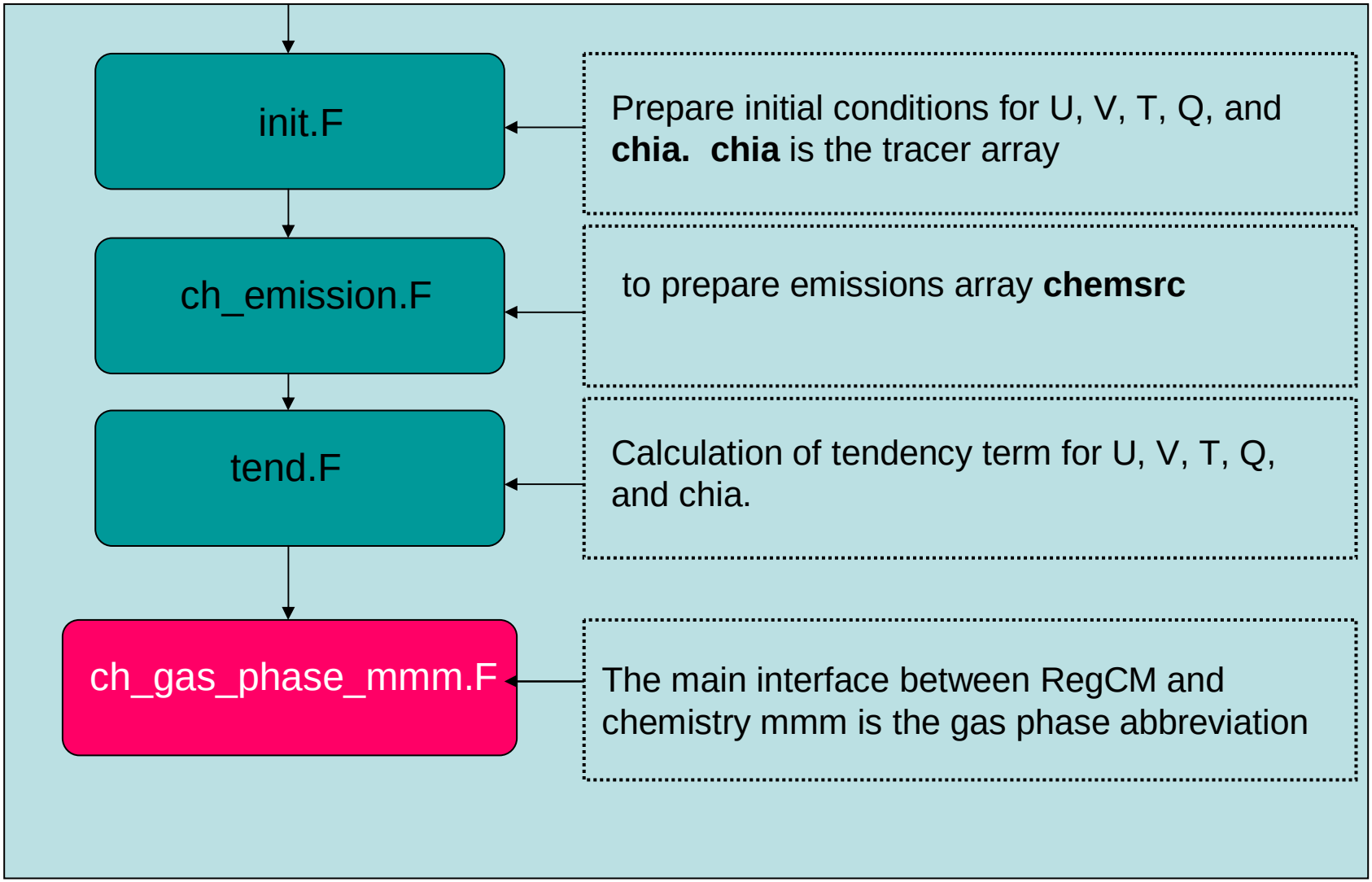
Why Chemistry?



RegCM-CHEM Flow Charts



Main (regcm.F)


init.F
Prepare initial conditions for U, V, T, Q, and **chia.** **chia** is the tracer array
ch_emission.F
to prepare emissions array **chemsrc**
tend.F
Calculation of tendency term for U, V, T, Q, and chia.
ch_gas_phase_mmm.F
The main interface between RegCM and chemistry mmm is the gas phase abbreviation

Emissions Inventories

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

List of species

Species	POET	RETRO	EDGAR	GFED
CO	•	•	•	•
NOx	•	•	•	•
CH4(methane)	•	• (burning only)	•	•
C_2H_6(ethane)	•	•		
C_2H_4(ethene)	•	•		
C_3H_8(propane)	•	•		
C_3H_6(propene)	•	•		
Butane and higher	•	•		
Toluene	•	•		
CH_3OH(methanol)	•	•		
C_2H_5OH(ethanol)	•	•		
C_3H_7OH(propanol)	•	•		

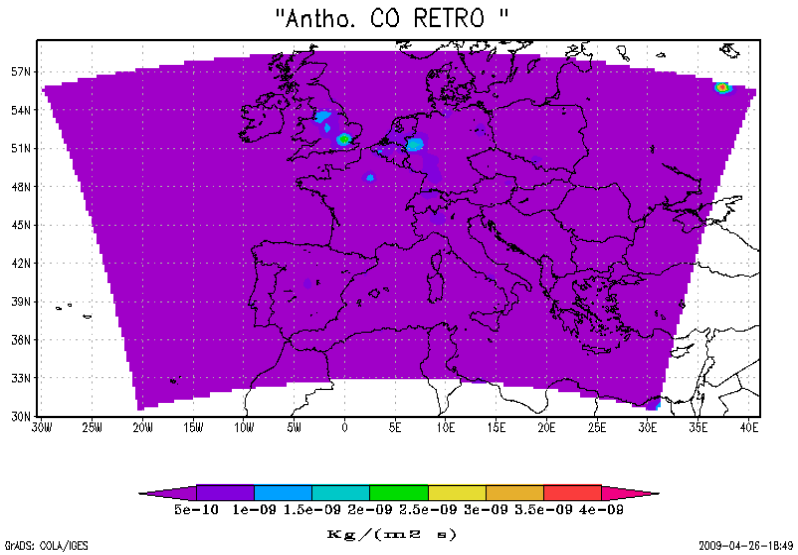
CH_2OH(formaldehyde)	•	• (burning only)		
CH_3CHO(acetaldehyde)	•	• (burning only)		
CH3COCH3 (acetone)	•	•		
CH3COCH2CH3 (Mek)	•			
C2H2 (ethyne)		•		
C6H6 (benzene)		•		
Xylene		•		
Isoprene (C4Hx)	•(biogenic)	• (burning only)		
Monoterpenes	•(biogenic)	• (burning only)		
H2 (hydrogen)	•	• (burning only)		
N_2O	•	• (burning only)	•	•
NH_3(ammonia)	•	• (burning only)		
Organic Carbon ('OC')	•	• (burning only)		•

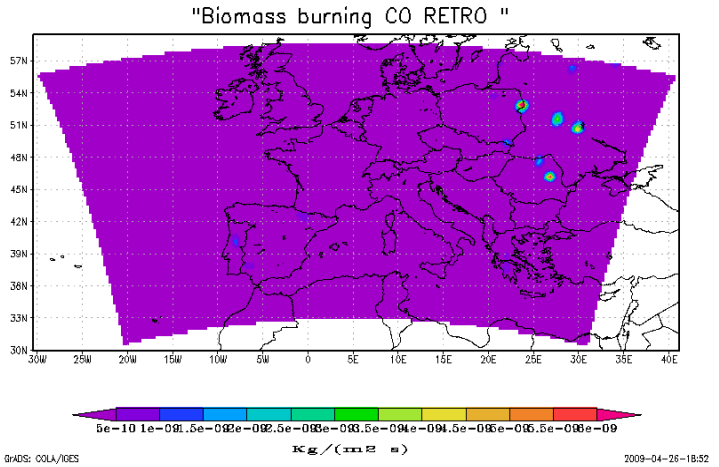
Black Carbon ('BC')				•
Total Carbon ('TC')				
SO2			•	
('PM2.5')				•
NMVOC				•
CO_2		•(burning only)	•	•
C				•
DMS			•	

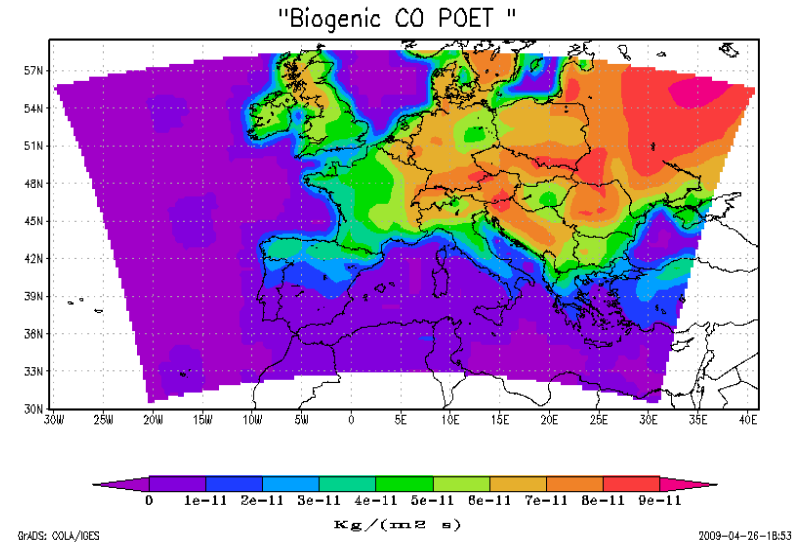
Emissions Pre-Process

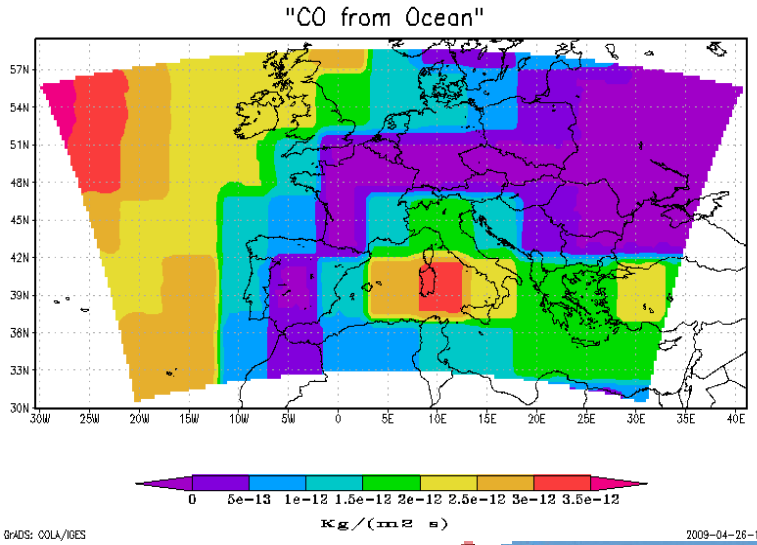
- All emissions are in NetCDF format, and been read directly and interpolated to model grid
- User can choose among several emission inventories
- User can switch between anthropogenic and biogenic emissions
- The availability to add more emission inventories
- The output is AERO.dat AERO.ctl, AERO.dat is multi month file.

Emission maps

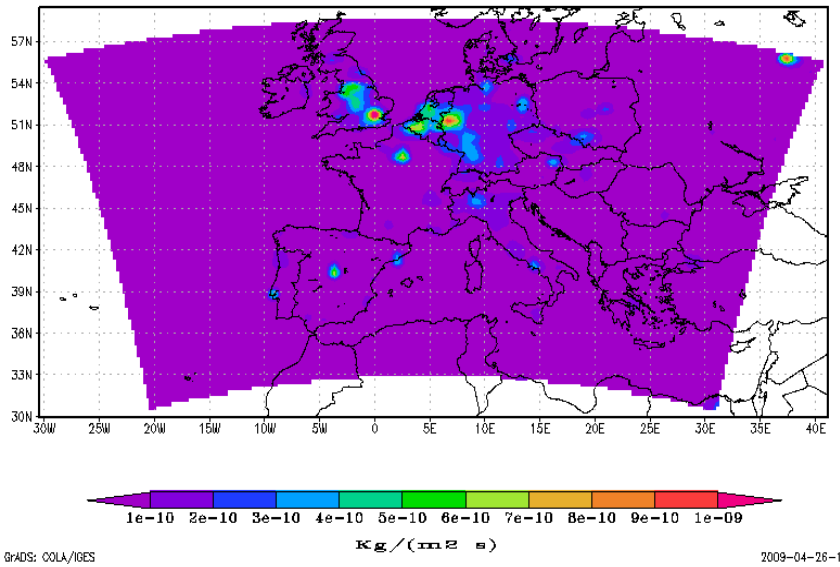




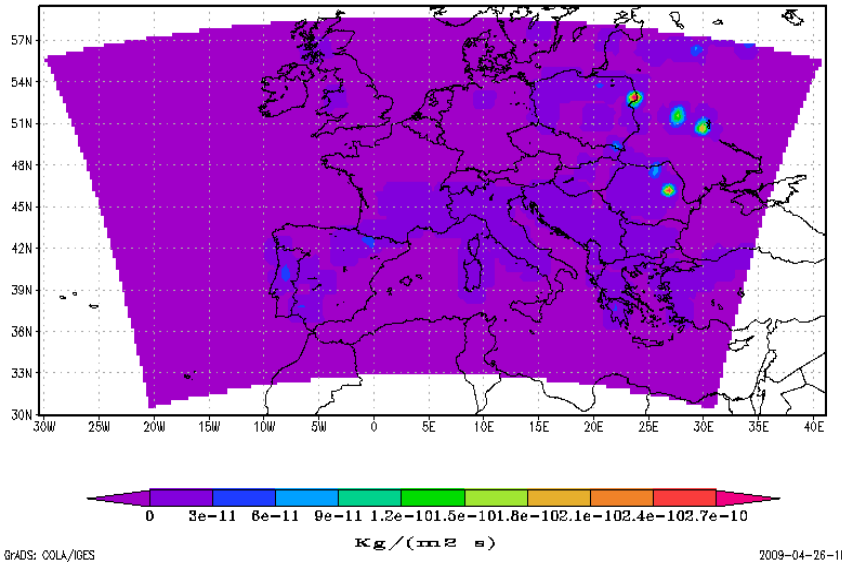




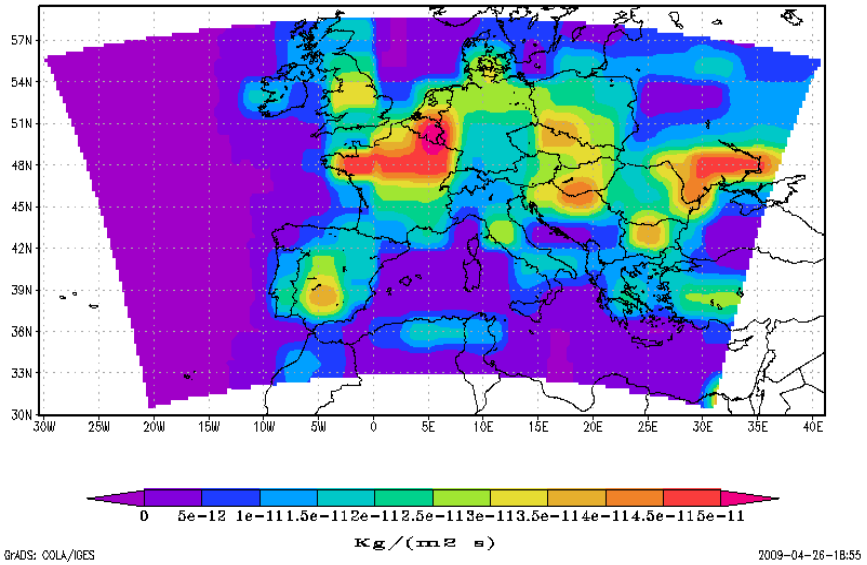
"Antho. NOx RETRO "



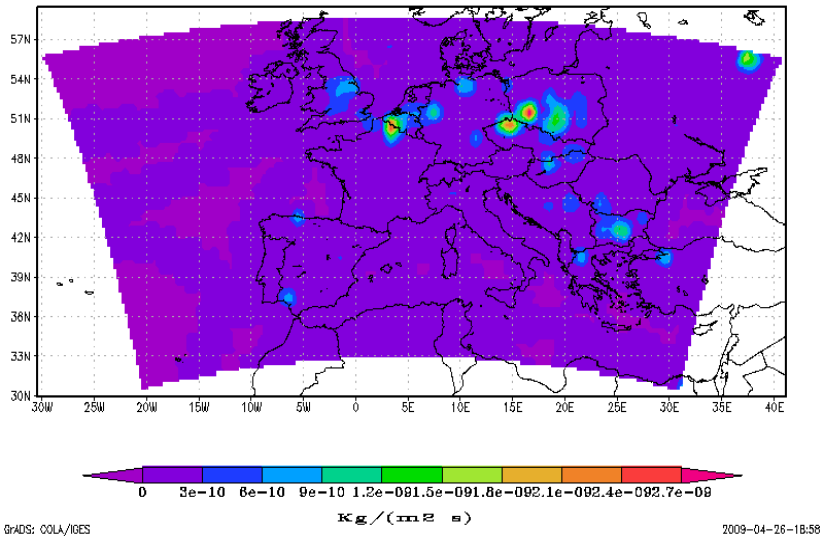
"Biomass Burning NOx RETRO "



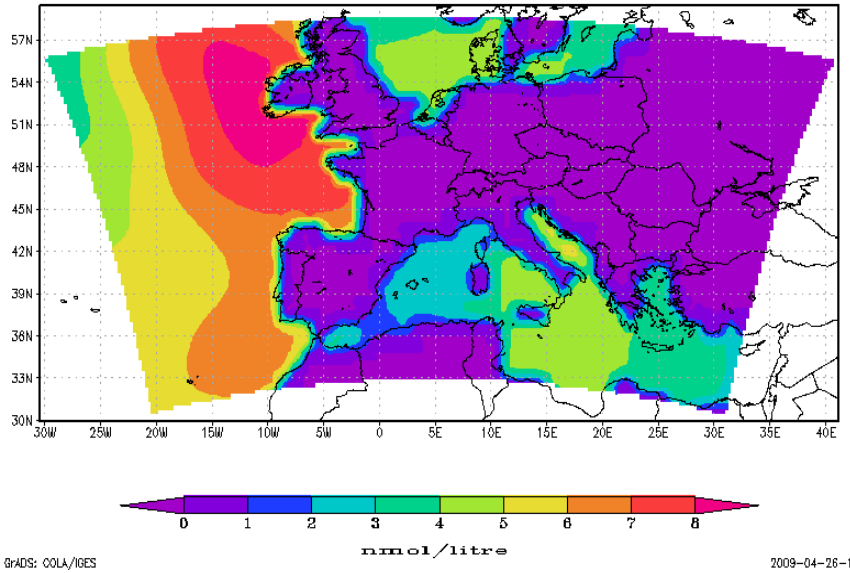
"Biogenic NOx POET "



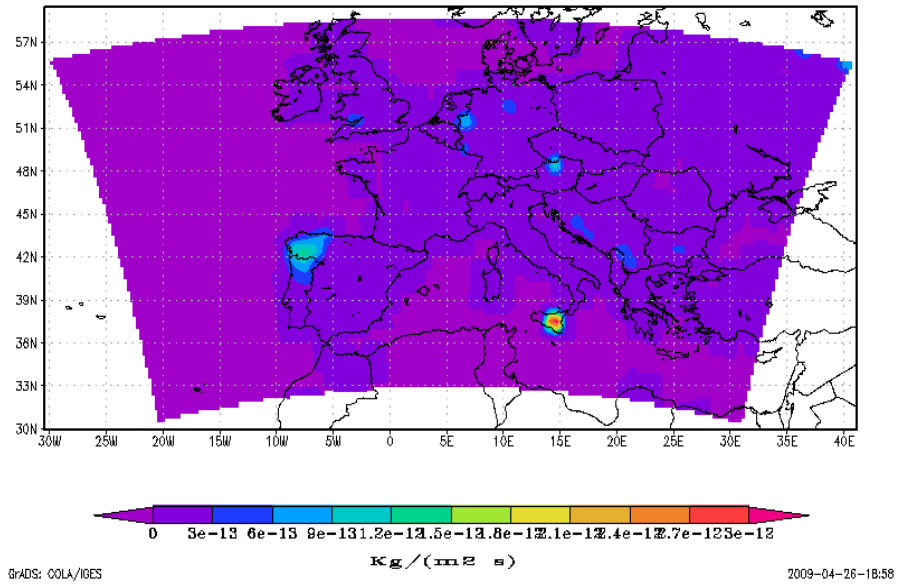
"Anthro. SO2 EDGAR "

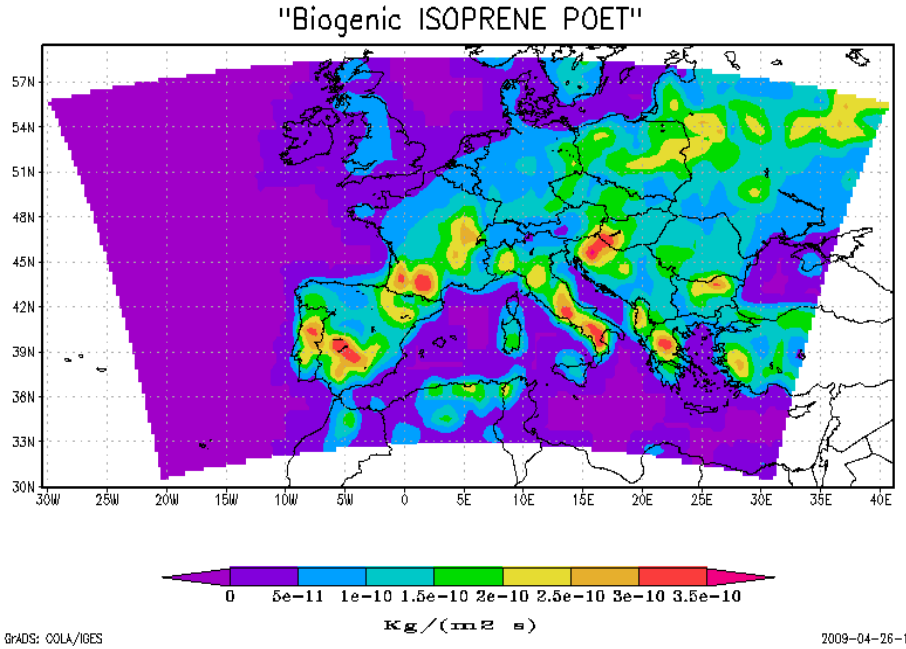


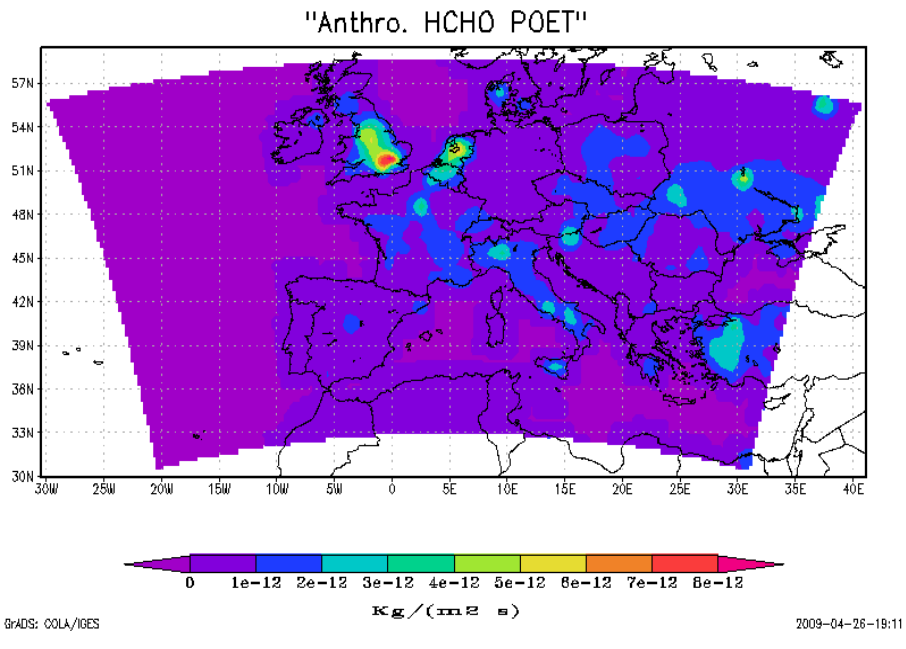
"DMS EMISSION"



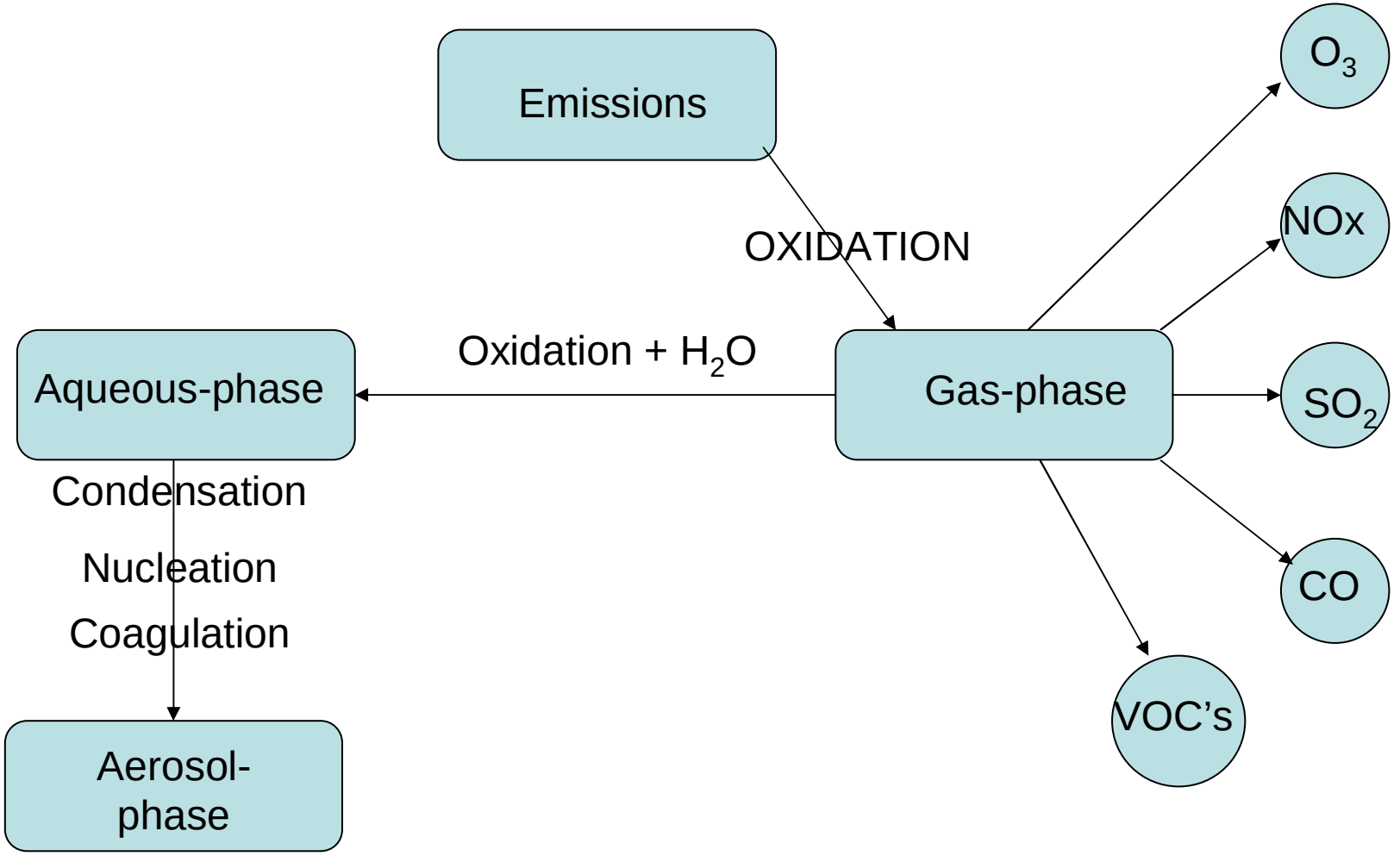
"Biomass burning SO2 EDGAR "




"Biogenic ISOPRENE POET"
57N
54N
51N
48N
45N
42N
39N
36N
33N
30N
30W 25W 20W 15W 10W 5W 0 5E 10E 15E 20E 25E 30E 35E 40E
0 5e-11 1e-10 1.5e-10 2e-10 2.5e-10 3e-10 3.5e-10
Kg/(m2 s)
GrADS: COLA/IGES
2009-04-26-19:12


"Anthro. HCHO POET"
57N
54N
51N
48N
45N
42N
39N
36N
33N
30N
30W 25W 20W 15W 10W 5W 0 5E 10E 15E 20E 25E 30E 35E 40E
0 1e-12 2e-12 3e-12 4e-12 5e-12 6e-12 7e-12 8e-12
Kg/(m2 s)
GrADS: COLA/IGES
2009-04-26-19:11

Chemistry inside the Atmosphere



Gas-Phase Mechanisms

Gas-Phase Mechanism is “a set of photolysis, inorganic, and organic reactions of a group of (inorganic and organic gas phase species)”

Example for photolysis reaction to produce ozone.

$NO + O_3 = NO_2 + O_2$ (1)

$NO_2 + hv = NO + O$ (2)

$O + O_2 + M = O_3 + M$ (3)

Each reaction is represent by a certain ordinary differential equation

$D[NO_2]/Dt = k_2[NO][O_3] – j[NO_2]$

$D[X]/Dt = \Sigma Pc - \Sigma Lc$ →

There are many ways to solve such system of ODE like

Euler

Backward-Forward

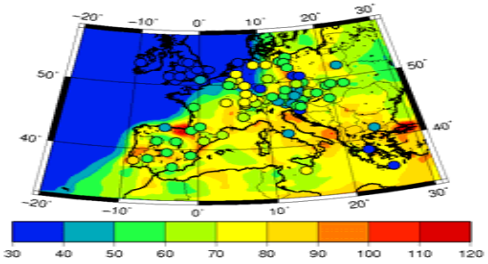
Gear’s method

Rosenbrock

LSODE

Model vs. Observation station

RegCM/OBS 2003/08/01



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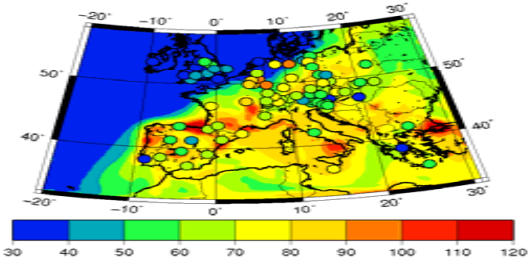

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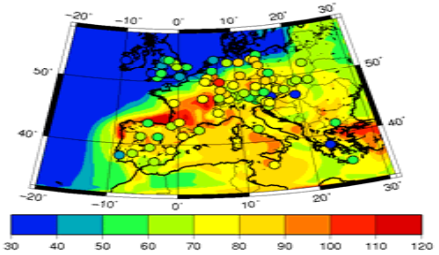
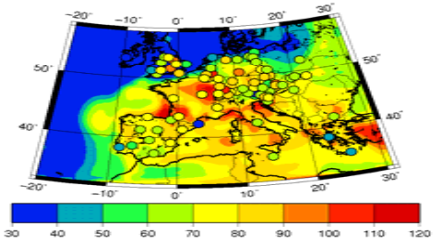
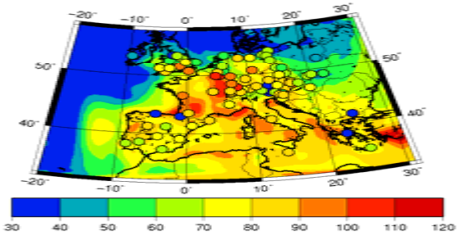


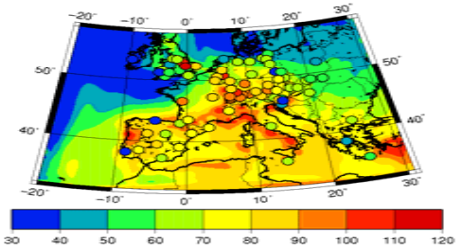
RegCM/OBS 2003/08/04



RegCM/OBS 2003/08/05

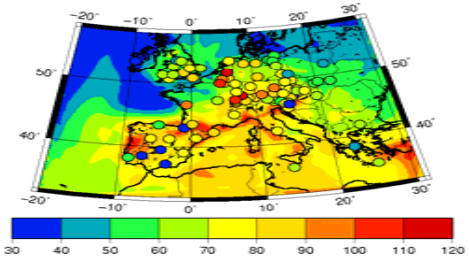


RegCM/OBS 2003/08/06

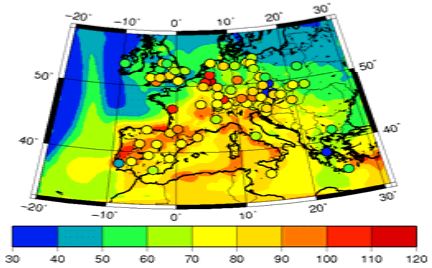


Model vs. Observation stations (cont.)

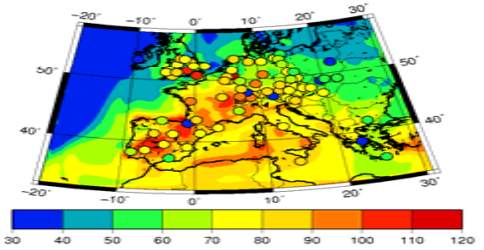
RegCM/OBS 2003/08/07



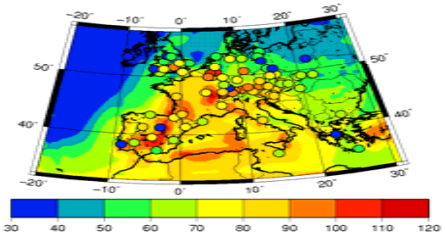
RegCM/OBS 2003/08/08



RegCM/OBS 2003/08/09



RegCM/OBS 2003/08/10



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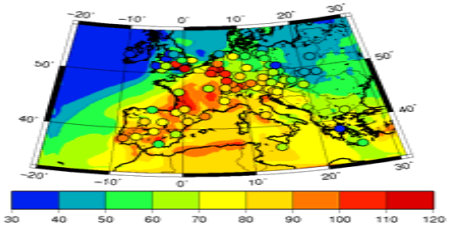

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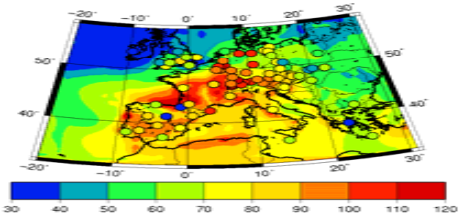
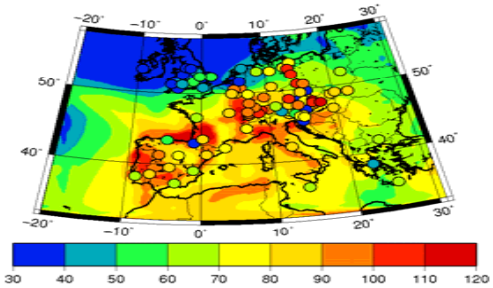


Model vs. Observation stations (cont.)

RegCM/OBS 2003/08/13



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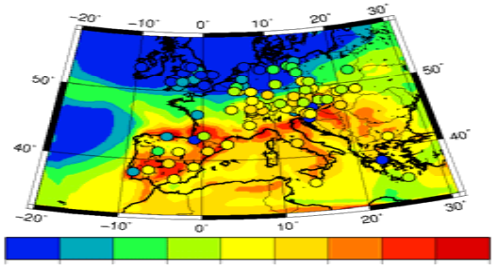

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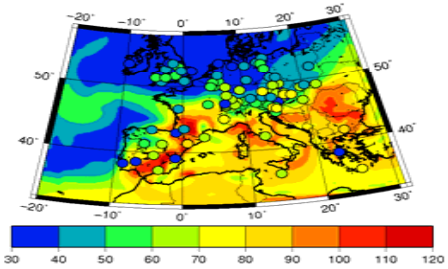

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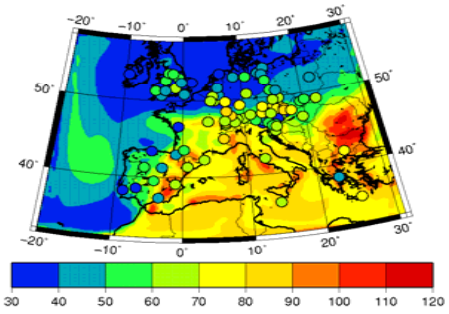
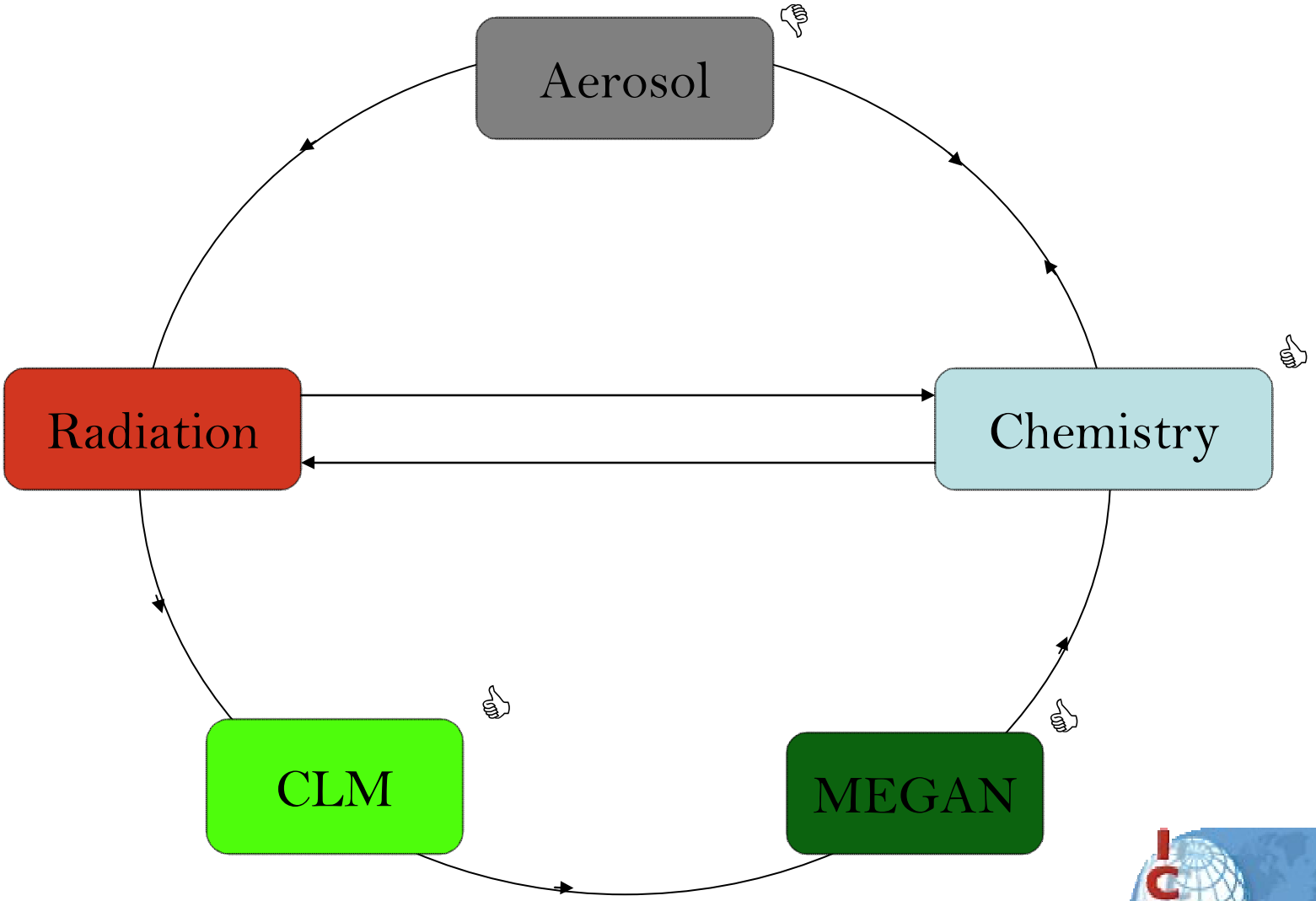


Land-Atmosphere-Chemistry



Thanks for Your Attention