Climate Chemistry simulation using RegCM4.5

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ICTP-Earth System Physics

7th ICTP workshop on the Theory and Use of Regional Climate Models

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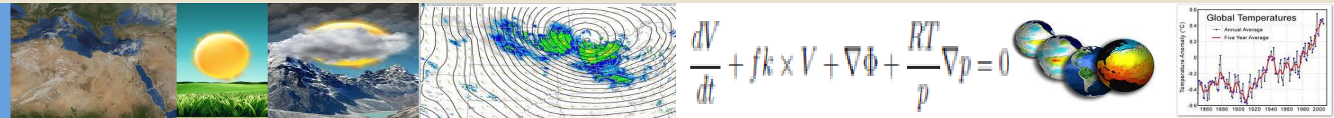
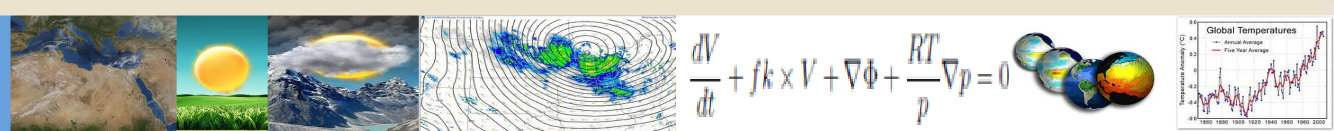


Objective

To show the current capabilities of RegCM4.5 to simulate the atmospheric chemistry of gases and aerosol and their feedbacks

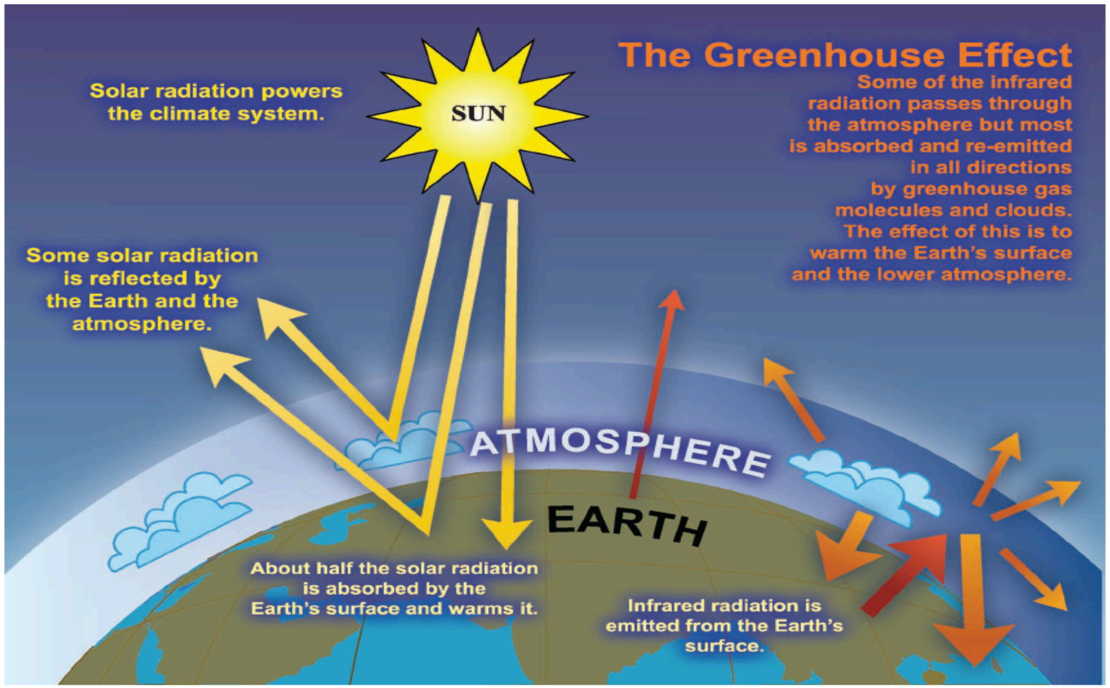
Outline

-Climate system (atmospheric chemistry perspective)
-Regional climate chemistry model
-Ozone modeling
-Aerosol modeling

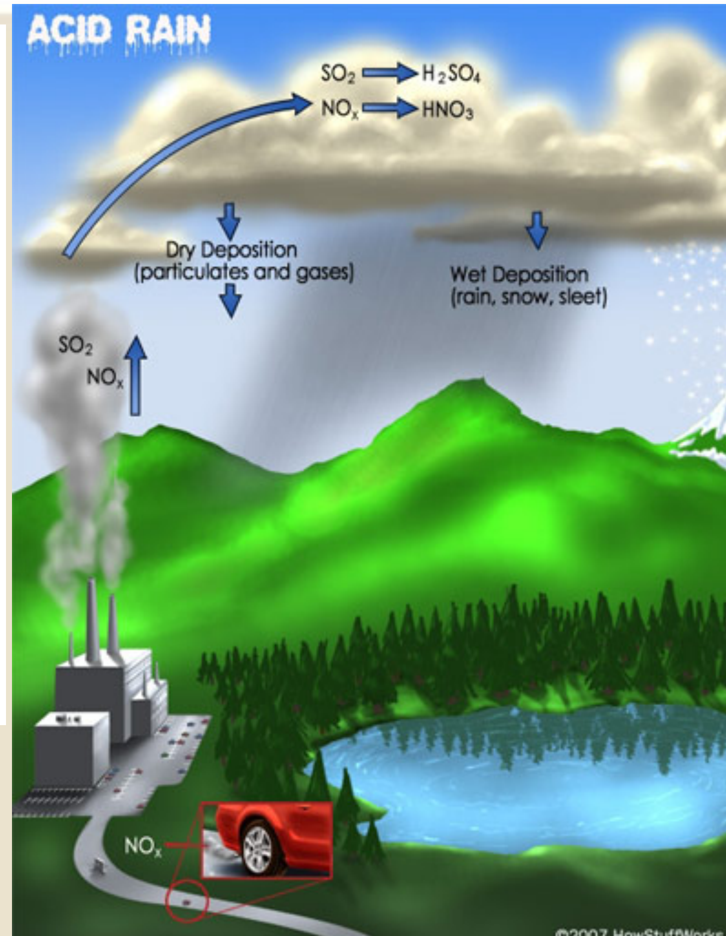


Why Chemistry Modeling?
Basic Components

Green House Gases: CO_2, CH_4, H_2O, O_3, CFC

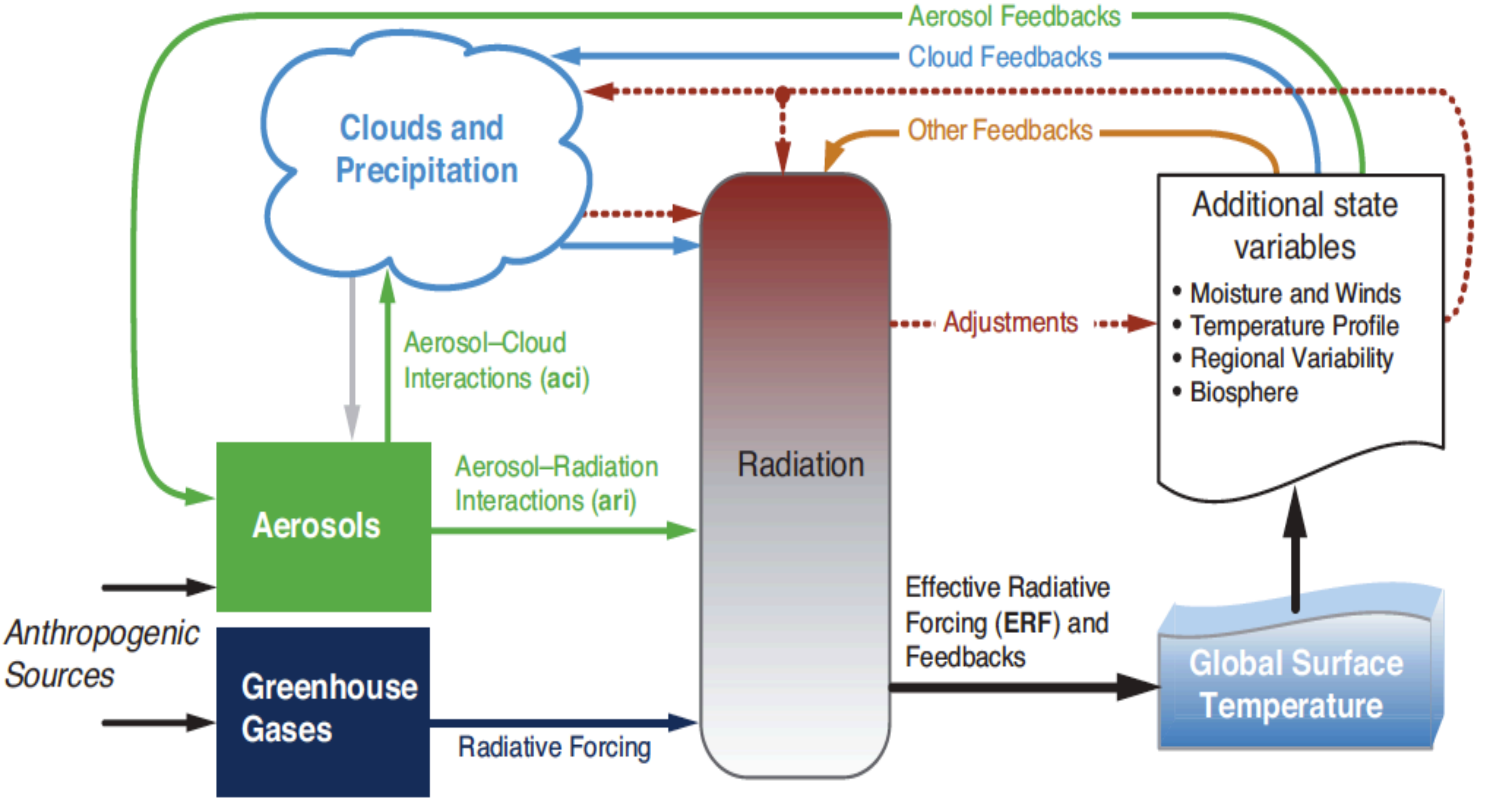


Acids: H_2SO_4, HNO_3, HCL



Aerosols: Sulfate, OC, BC, Dust, SOA

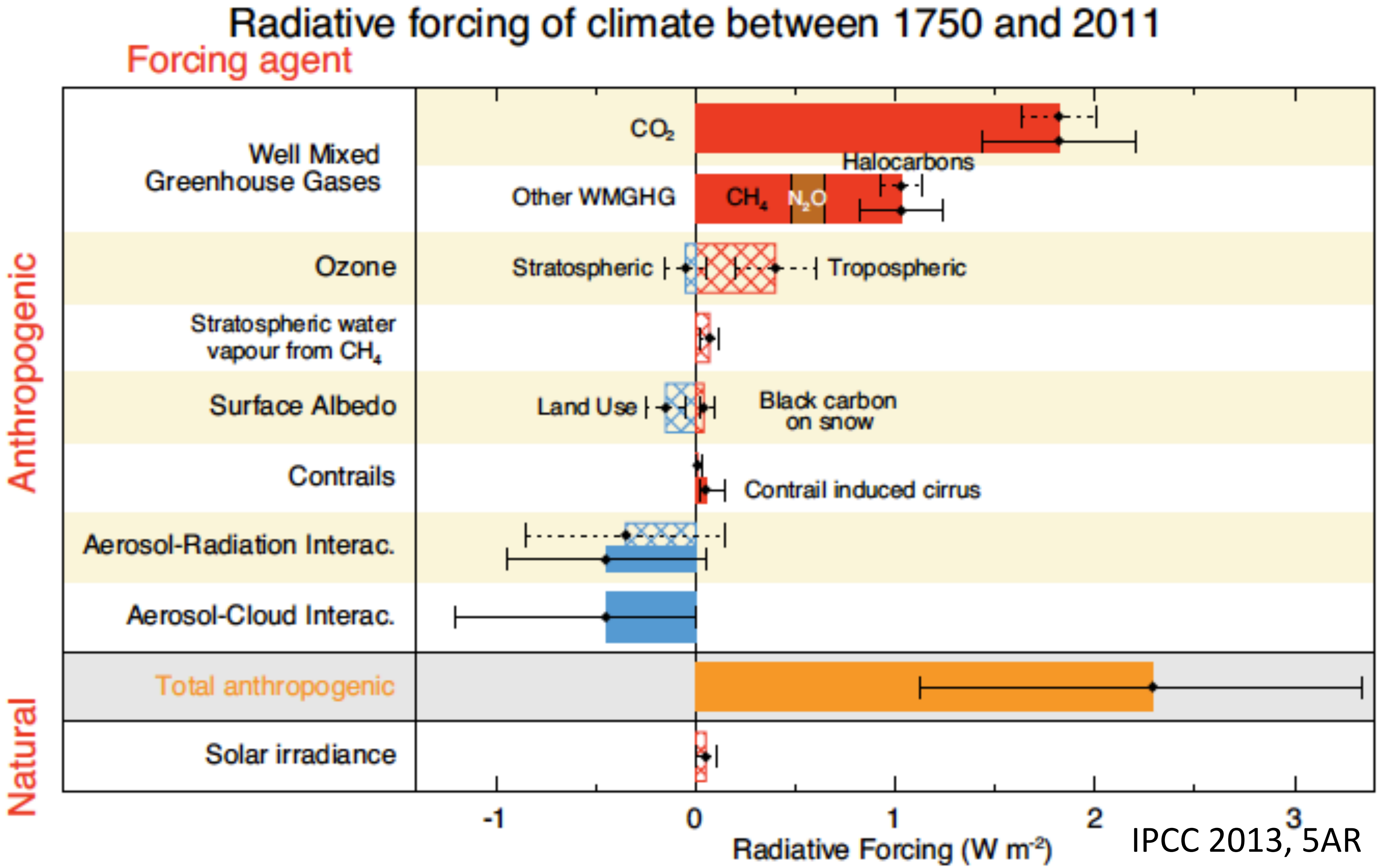
$$\frac{dV}{dt} + fk \times V + \nabla\Phi + \frac{RT}{p}\nabla p = 0$$



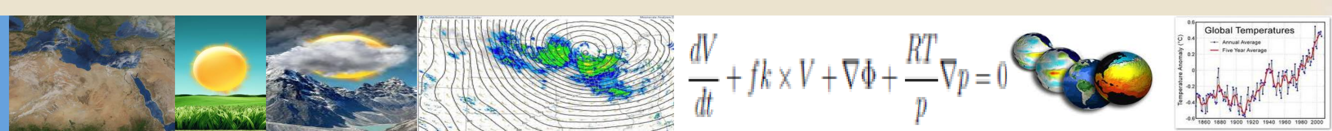
IPCC 2013, 5AR

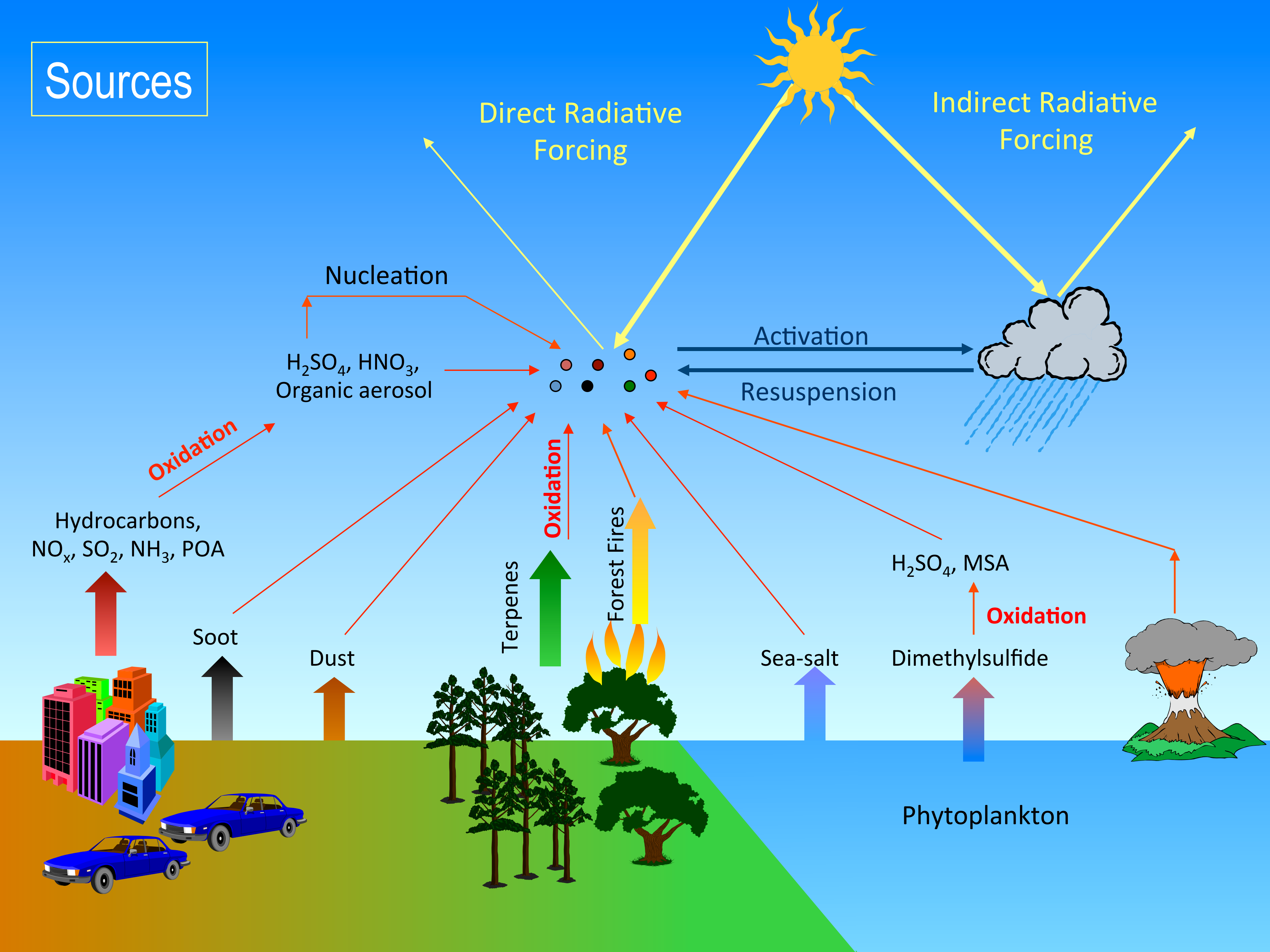
Irradiance Changes from Aerosol-Radiation Interactions (**ari**)

Irradiance Changes from Aerosol-Cloud Interactions (**aci**)



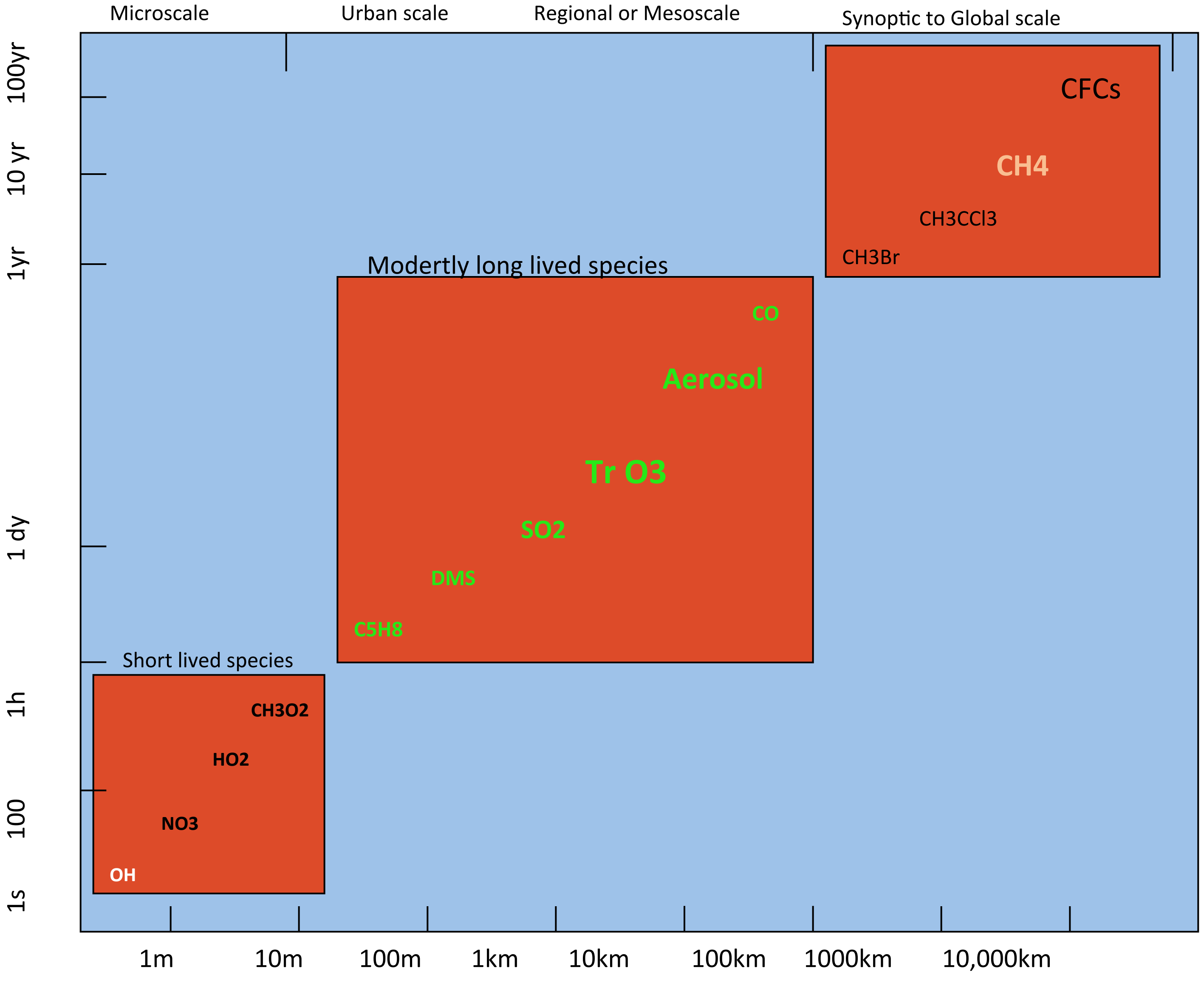
IPCC 2013, 5AR





Sources
Direct Radiative Forcing
Indirect Radiative Forcing
Nucleation
H_2SO_4, HNO_3,
Organic aerosol
Activation
Resuspension
Oxidation
Hydrocarbons,
NO_x, SO_2, NH_3, POA
Soot
Dust
Terpenes
Oxidation
Forest Fires
Sea-salt
H_2SO_4, MSA
Oxidation
Dimethylsulfide
Phytoplankton

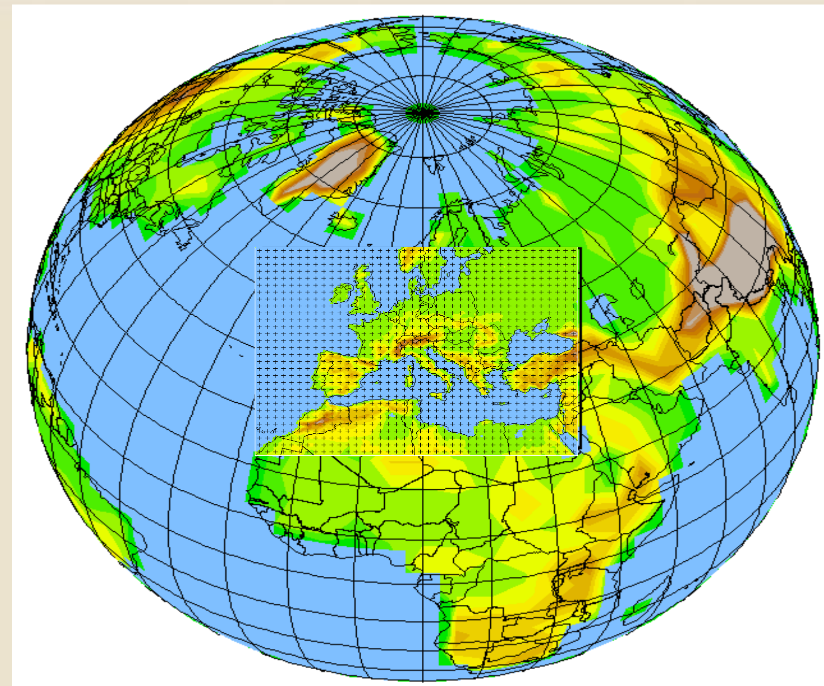
Spatial and Temporal Scales for atmospheric composition



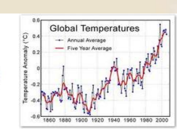
RegCM4 Regional Climate Model

Global Climate model is an Initial Value problem (we need to specify the initial values and then let the model goes forward)

Regional climate model is boundary value problem (we need to know the boundary conditions for the whole period of simulation) and the model will deduce the fine details (the added value) .



$$\frac{dV}{dt} + fk \times V + \nabla\Phi + \frac{RT}{p}\nabla p = 0$$



RegCM4.5 framework

$$\frac{\partial \chi}{\partial t} = -\overline{V} \cdot \nabla \chi + F_H + F_V + T_{CUM} + S_\chi - R_{w,ls} - R_{w,cum} - D_{dep} + \sum Q_p - Q_l$$

Re-analysis & GCM data

ERA40,
ERA_ENTRIM, NCEP
Re
MPI, Hadgem, etc.

GCTM data

MOZART
(6 hourly or
Climatology)

Emission data

Emission Inventories:
IIASA and RCPs

Pre-Processing

ICBC: prepare Meteorology and chemistry Initial condition and Boundary conditions for the whole period of Integration

EMISSIONS: Prepare emissions data by interpolate and regrid global emission data to the Model grid.

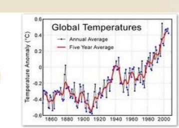
Model

Dynamic

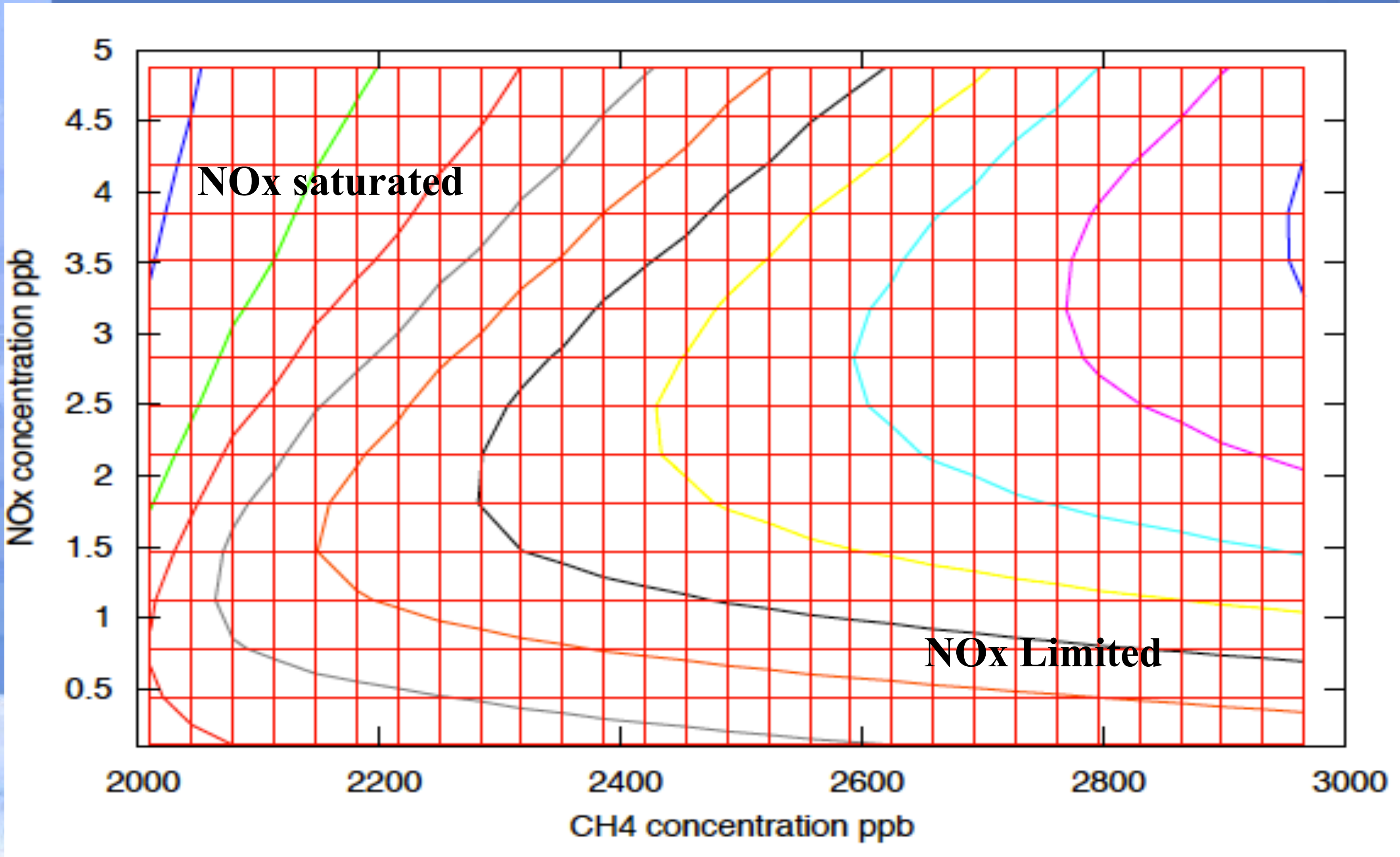
- Radiation
- Convection
- PBL
- Land Surface
- Tracers Tendencies
  - H. Advection
  - V. Advection
  - H. Diffusion
  - Cumulus transportation
  - Wet Deposition
  - Dry Deposition
  - Emission rate

Chemistry solver (KPP)

$$\frac{dV}{dt} + fk \times V + \nabla\Phi + \frac{RT}{p}\nabla p = 0$$



NOx-VOC-Ozone (source of air pollution)



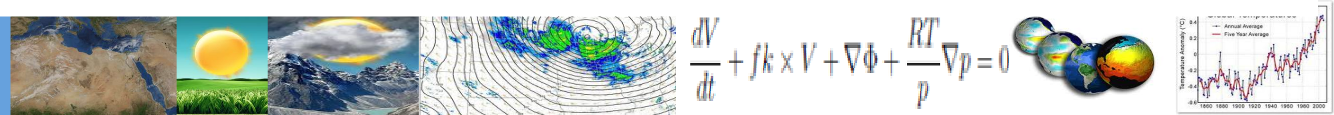
What is CBMZ chemical mechanism?

Inorganic Chemistry

$NO_2 + h\nu \xrightarrow{O_2} NO + O(^3P)$	J_{NO_2}
$NO_3 + h\nu \longrightarrow 0.89NO_2 + 0.89O(^3P) + 0.11NO$	J_{NO_3}
$HNO_2 + h\nu \longrightarrow OH + NO$	J_{HNO_2}
$HNO_3 + h\nu \longrightarrow OH + NO_2$	J_{HNO_3}
$HNO_4 + h\nu \longrightarrow HO_2 + NO_2$	J_{HNO_4}
$O_3 + h\nu \longrightarrow O(^3P)$	J_{O_3a}
$O_3 + h\nu \longrightarrow O(^1D)$	J_{O_3b}
$H_2O_2 + h\nu \longrightarrow 2OH$	$J_{H_2O_2}$
$O(^1D) + O_2 \longrightarrow O(^3P) + O_2$	$3.2 \times 10^{-11} \exp(70/T)$
$O(^1D) + N_2 \longrightarrow O(^3P) + N_2$	$1.8 \times 10^{-11} \exp(110/T)$
$O(^1D) + H_2O \longrightarrow 2OH$	2.2×10^{-10}

Paraffin Chemistry

$CH_4 + OH \xrightarrow{O_2} CH_3O_2$	$T^{0.667} 2.8 \times 10^{-14} \exp(-1575/T)$
$C_2H_6 + OH \longrightarrow ETHP$	$T^2 1.5 \times 10^{-17} \exp(-492/T)$
$PAR + OH \longrightarrow RO_2$	8.1×10^{-13}
$CH_3OH + OH \longrightarrow HCHO + HO_2$	$6.7 \times 10^{-12} \exp(-600/T)$



Olefin chemistry

$ETH + O_3 \longrightarrow HCHO + 0.22HO_2 + 0.12OH + 0.24CO + 0.24CO_2 + 0.52HCOOH$	$1.2 \times 10^{-14} \exp(-2630/T)$
$ETH + OH \longrightarrow XO_2 + 1.56HCHO + HO_2 + 0.22ALD2$	$F(1.0(-28), 0.8, 8.8(-12), 0.0)$
$OLET + O_3 \longrightarrow 0.57HCHO + 0.47ALD2 + 0.33OH + 0.26HO_2 + 0.08H_2 + 0.07CH_3O_2 + 0.06ETHP + 0.03RO_2 + 0.13C_2O_3 + 0.04MGLY + 0.03CH_3OH + 0.06CH_4 + 0.01C_2H_6 + 0.31CO + 0.22CO_2 + 0.22HCOOH + 0.09RCOOH - 1.06PAR$	$4.2 \times 10^{-15} \exp(-1800/T)$

Carbonyl Chemistry

$HCHO + h\nu \xrightarrow{O_2} 2HO_2 + CO$	J_{HCHOa}
$HCHO + h\nu \longrightarrow CO$	J_{HCHOb}
$HCHO + OH \xrightarrow{O_2} HO_2 + CO$	1.0×10^{-11}
$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	$3.4 \times 10^{-13} \exp(-1900/T)$

Aromatic Chemistry

$TOL + OH \longrightarrow 0.08XO_2 + 0.2HO_2 + 0.12CRES + 0.8TO_2$	$2.1 \times 10^{-12} \exp(322/T)$
$XYL + OH \longrightarrow 0.5XO_2 + 0.55HO_2 + 0.8MGLY + 1.1PAR + 0.45TO_2 + 0.05CRES$	$1.7 \times 10^{-11} \exp(116/T)$

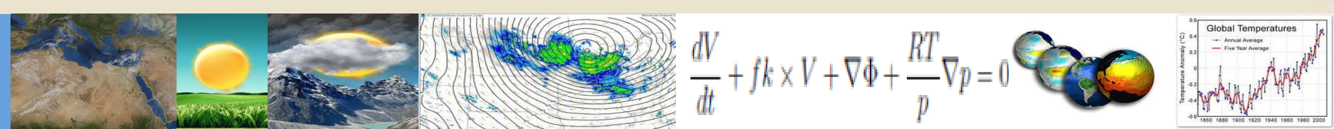
Isoprene Chemistry

$ISOP + OH \longrightarrow ISOPP + 0.08XO2$	$2.55 \times 10^{-11} \exp(409/T)$
$ISOP + O_3 \longrightarrow 0.6HCHO + 0.65ISOPRD + 0.27OH + 0.07CO + 0.39RCOOH + 0.07HO_2 + 0.15ALD2 + 0.2XO_2 + 0.2C_2O_3$	$1.2 \times 10^{-14} \exp(-2013/T)$
$ISOP + NO_3 \longrightarrow ISOPN$	$3.0 \times 10^{-12} \exp(-446/T)$

$$\frac{d[X_i]}{dt} = \sum_i \text{source} - \sum_i \text{sink}$$

Number of reaction	**132**
Total number of Species	58
Number of transported species	30
Number of Alkane	3 (CH4, C2H6, PAR)
Number of Alkene	3+1(Isoprene)
Number of Aromatic	3 (TOLU, XYL, CRES)

Calculating the time evolution of gas-phase chemistry requires an integration of a set of stiff ordinary differential equations and is among the most computationally expensive operations performed in a climate chemistry model.



Global Emission

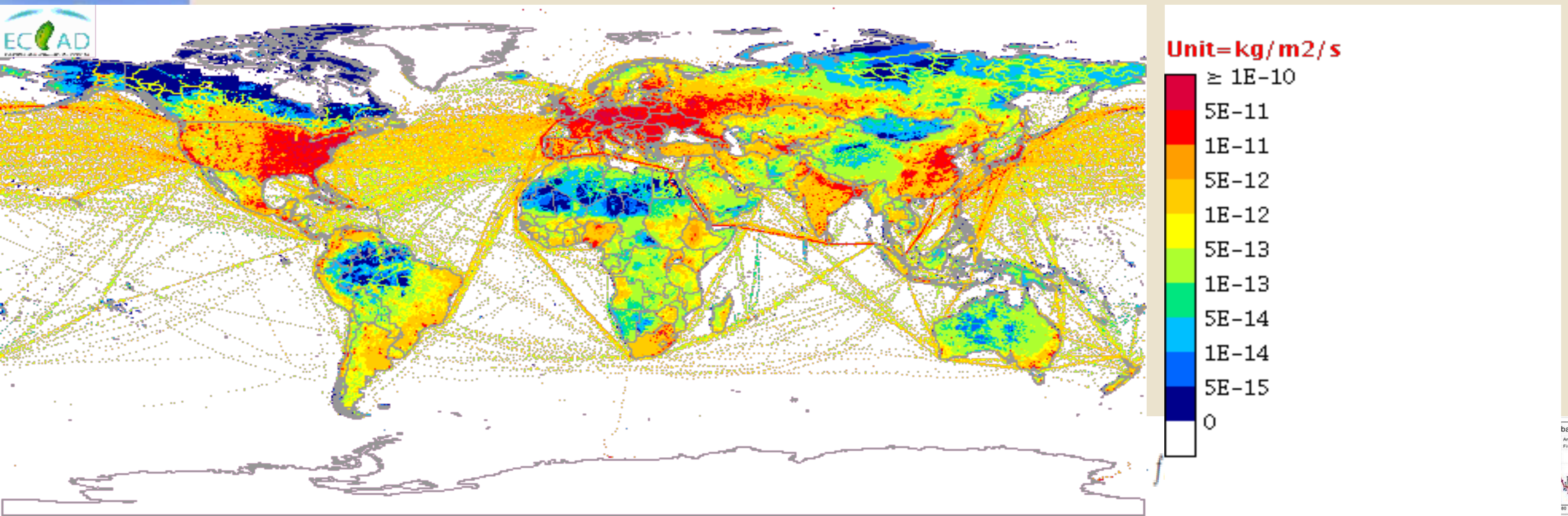
IIASA emission is global 0.5 degrees resolution, which has nine substances, SO2, total VOC, CH4, CO, NOx, NH3, BC, OC, PM2.5 and it is consistent with RCP (Representitive Concentration Pathway) sectors (industry, energy, transport, etc.)

IIASA emissions available for 2005, 2010, 2030, and 2050

1-RegCM4.5 interpolate and regrid these global map to the model grid.

2-derives the corresponding VOCs in a consistent way from the Total VOC.

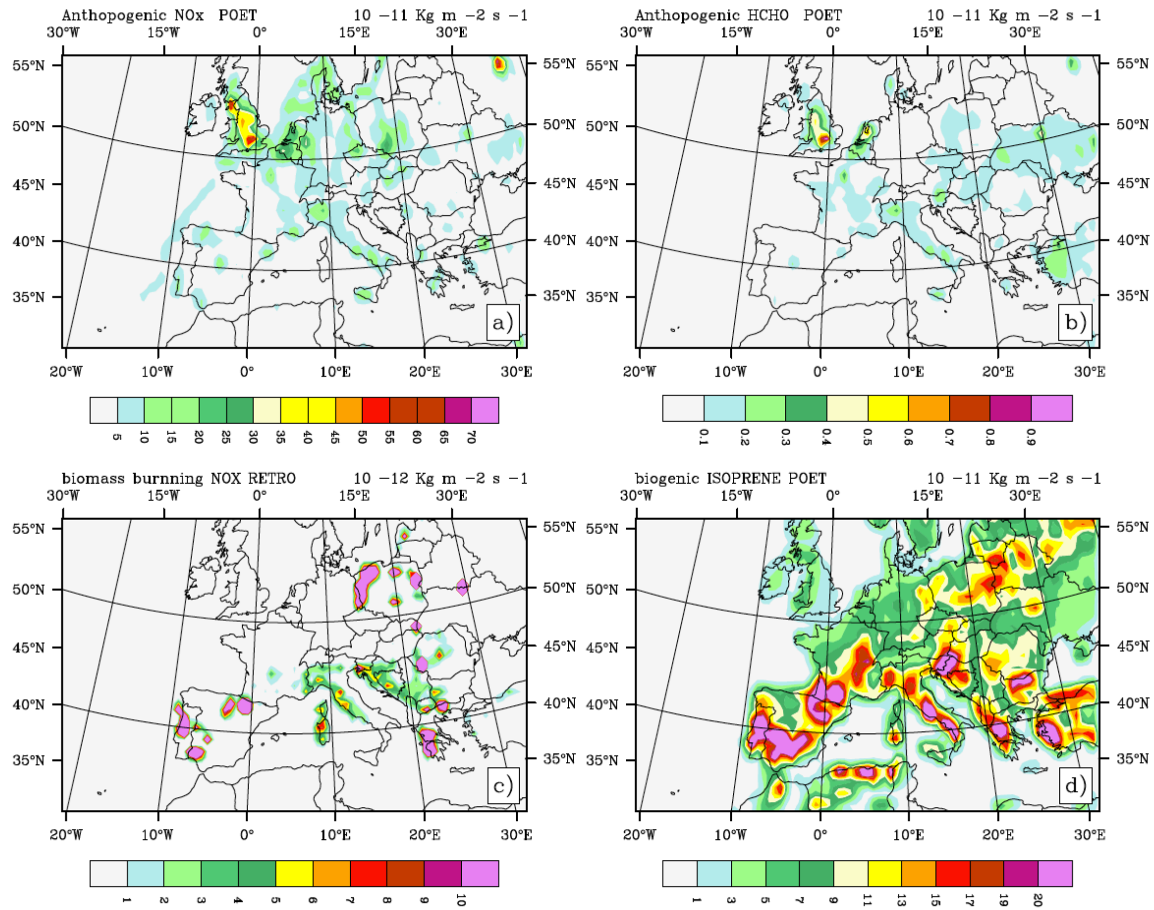
Anthropogenic Nox 2005



RegCM4.5 framework (cont.)
Emissions data (IIASA emission)

Sample data represents the emissions used by RegCM4.5

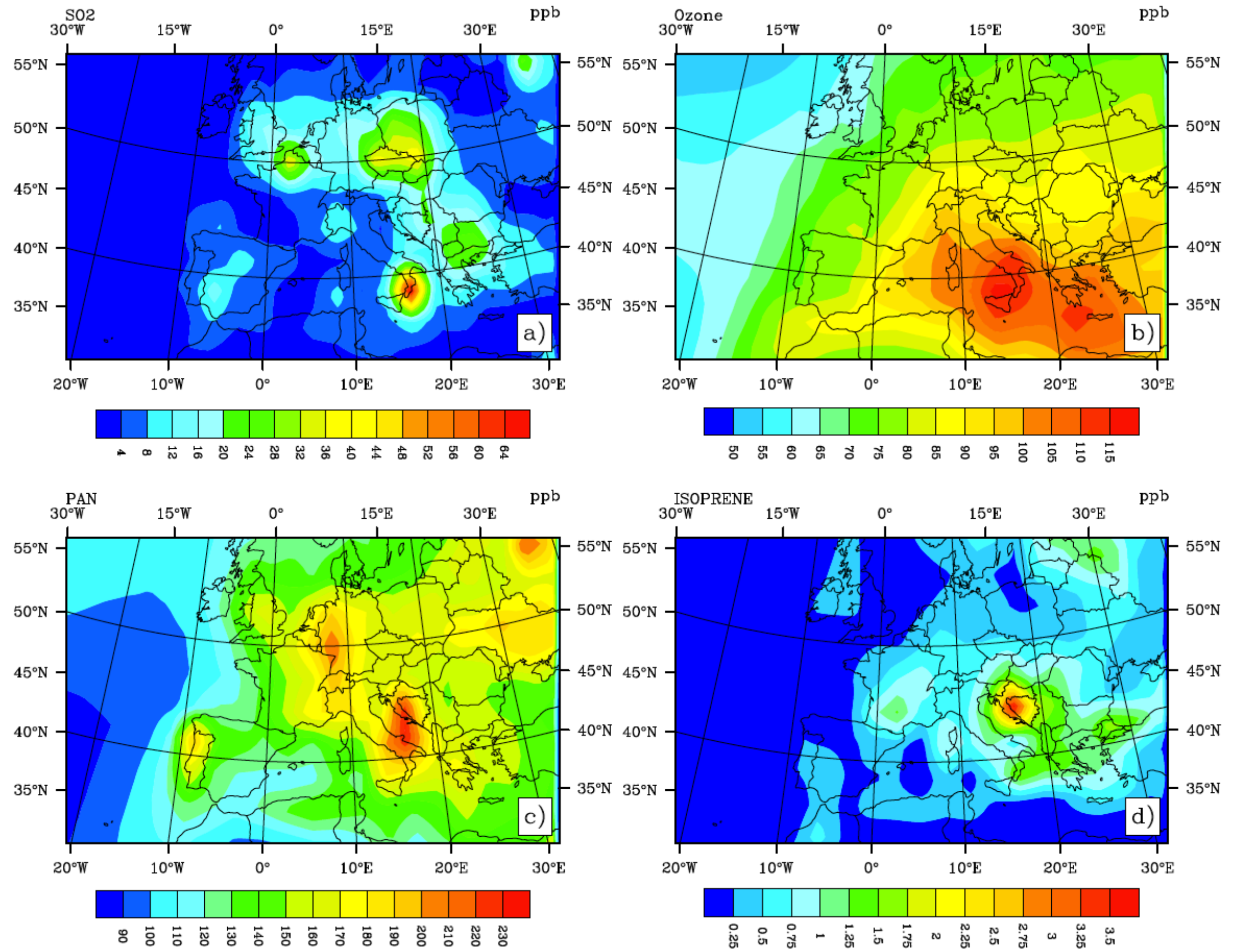
a)Anth. NOx
b)Anth. HCHO
c)Biomass NOx
d) Biogenic ISOPRENE



RegCM4.5 (cont.)
Chemistry Boundary Conditions

Sample from chemistry boundary conditions file, represents SO2, Ozone, PAN, ISOPRENE.

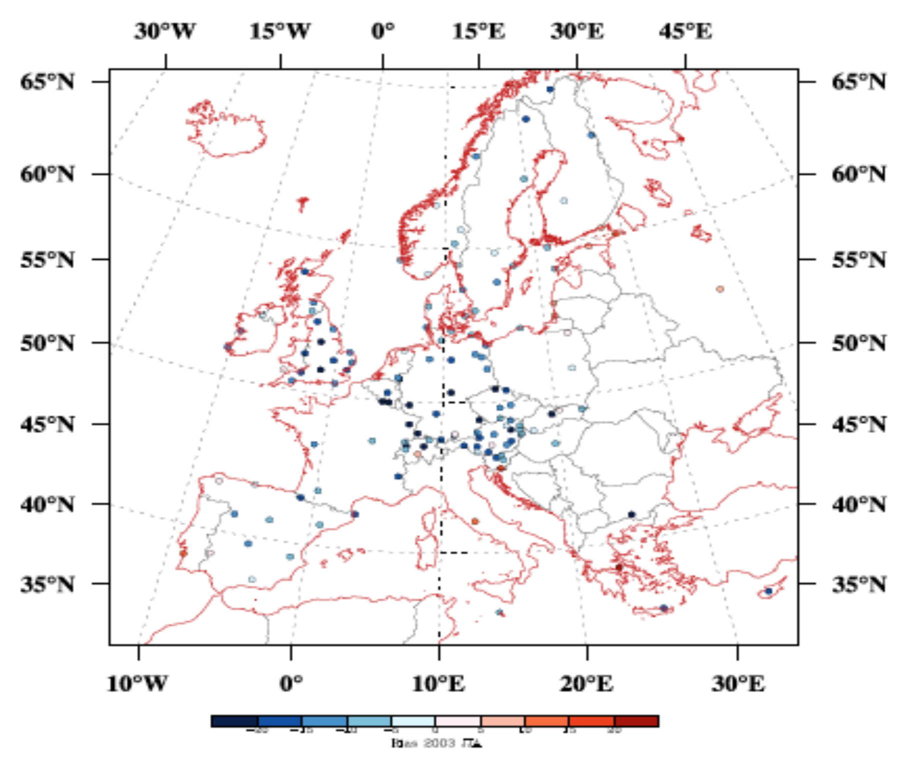
MOZART global chemistry model has been used to provide the initial and boundary condition for RegCM4.5
There are two option
1-use 6 hourly boundary conditions
2-use climatology of 10 year (1999-2009)



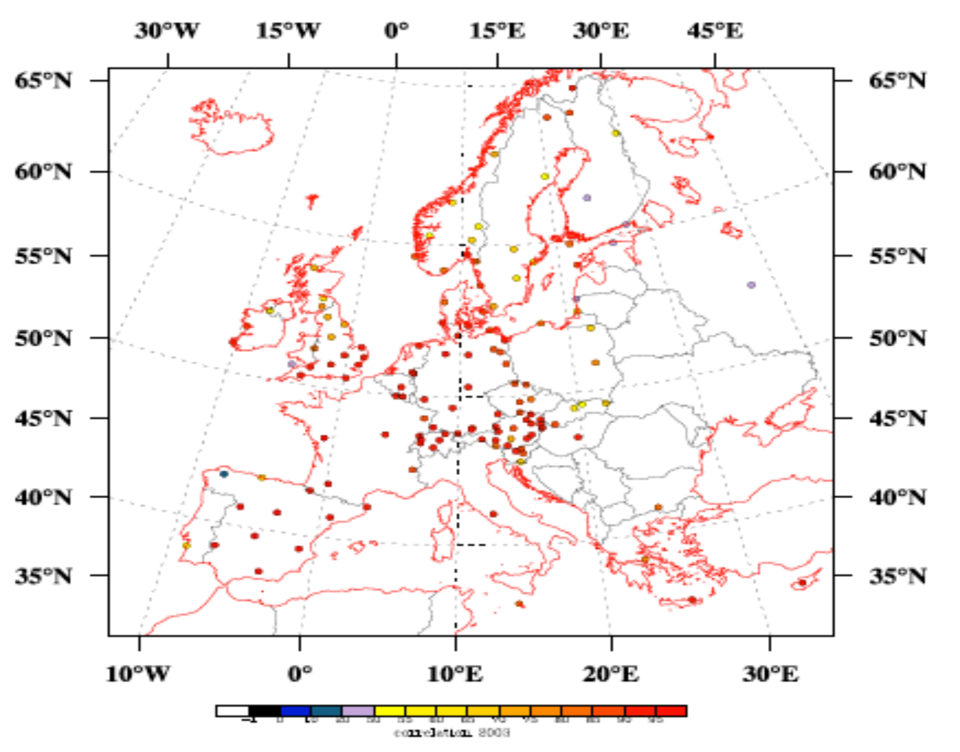
Ozone simulation

Ozone simulation: present and future climatology

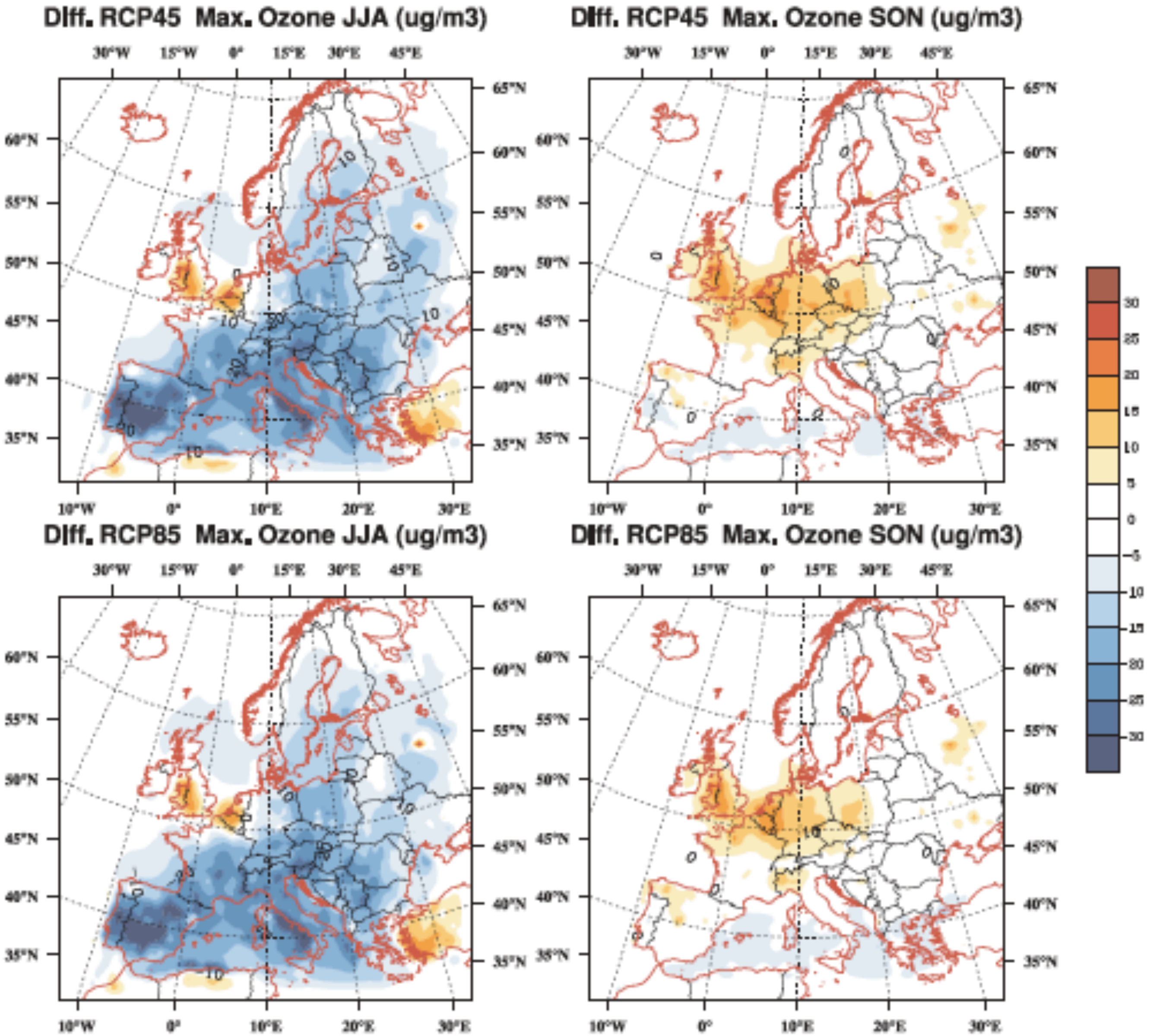
Surface ozone evaluation against EMEP network, for 2003



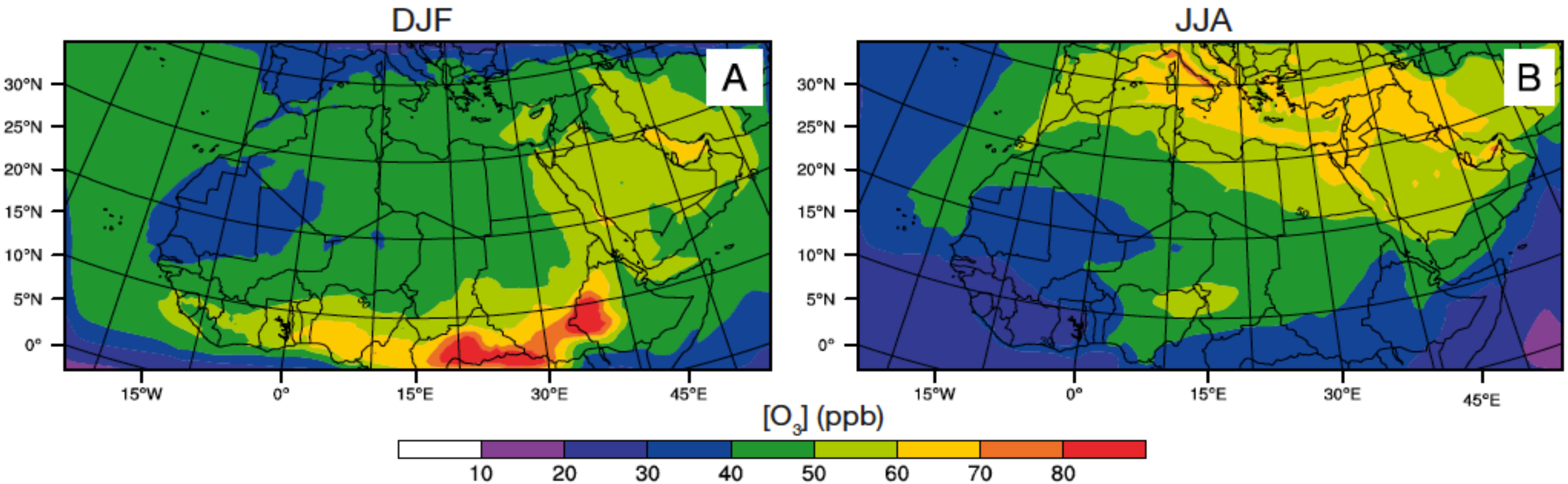
Surface ozone bias JJA 2003

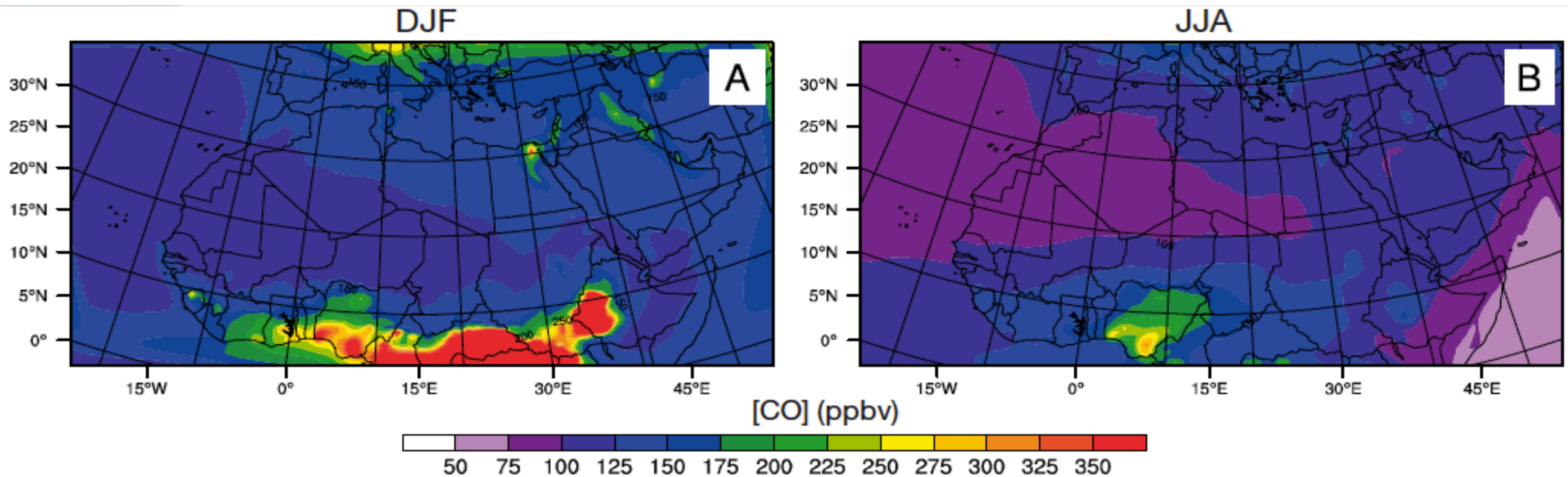


Surface Ozone correlation 2003



Future scenarios of ozone (2045-2055) Using RCP4.5 and RCP8.5 With the future emission of IIASA 2050

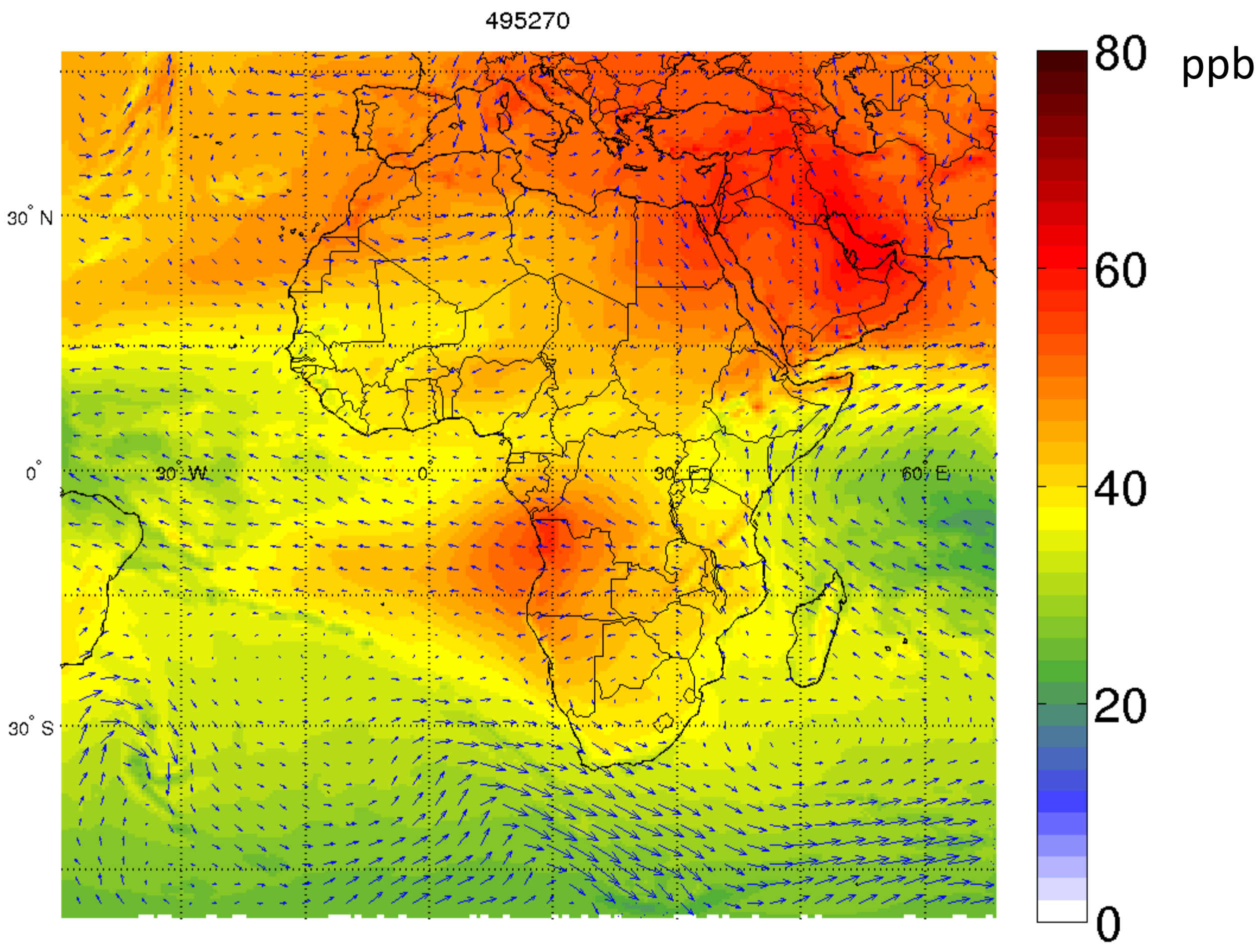




Steiner et al, 2014 CR.

Ex: Simulated Ozone concentration evolution at 750 hpa – June 2006

African biomass burning producing high concentration of troposheric ozone over the tropical Atlantic (a well known seasonal anomaly of global atmospheric chemistry)



Aerosol simulation

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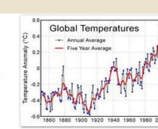
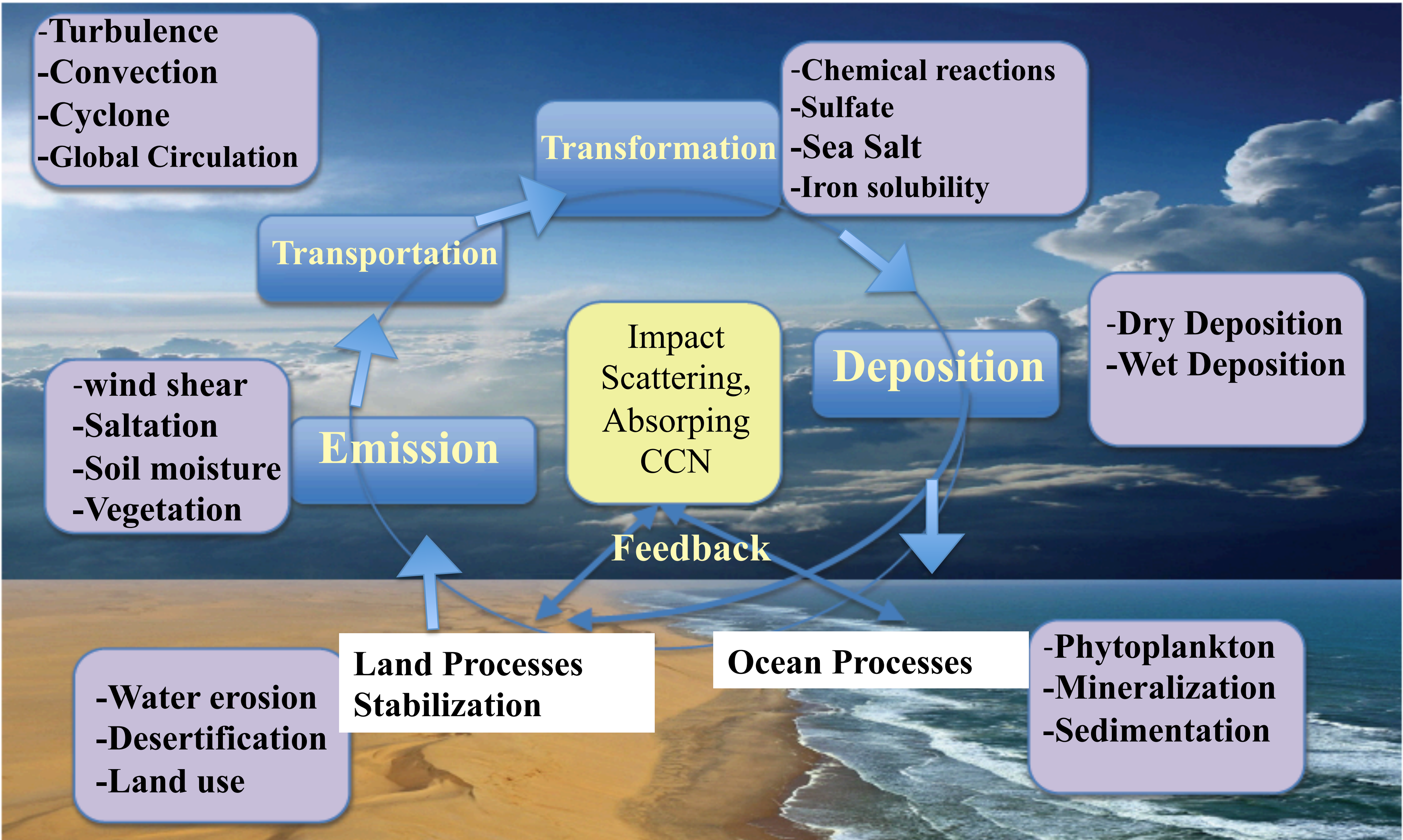


Dust Processes (Dust life cycle)

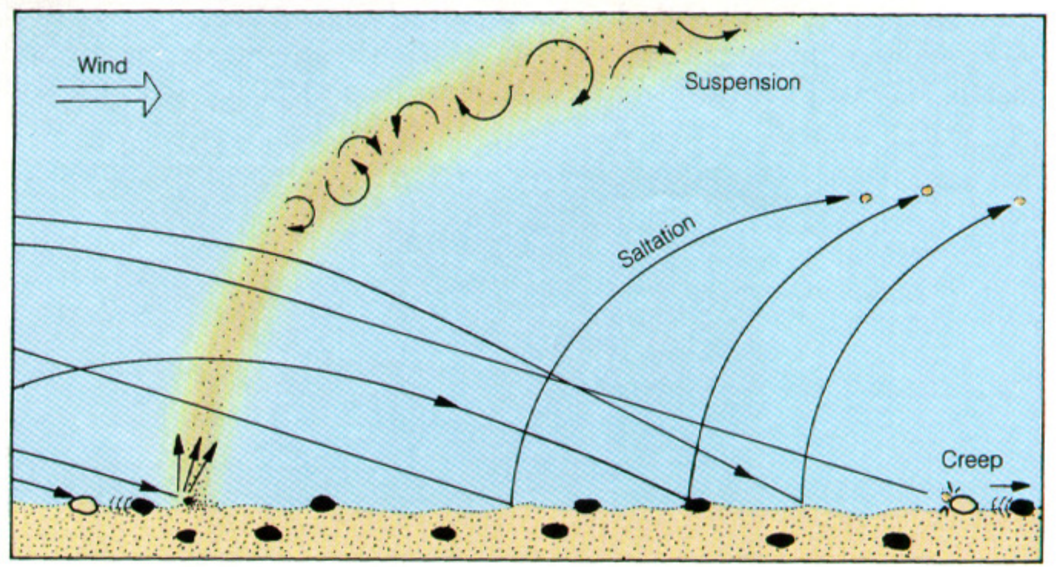


Shao et al 2010, Aeolian research

Physical Processes in a Dust Storm (Saltation and Sandblasting)

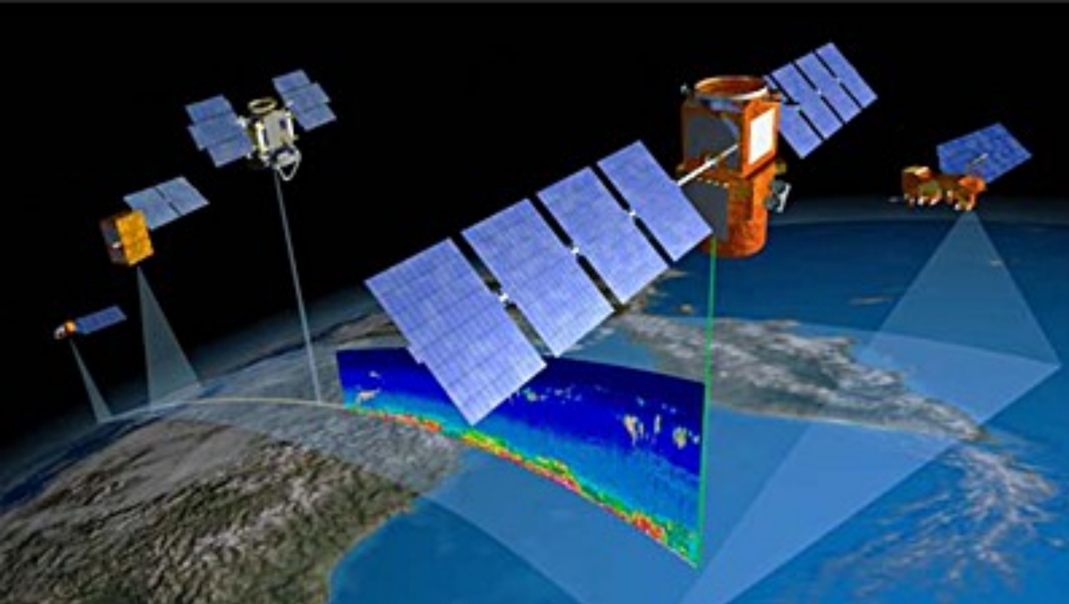
- The forces acting on the dust particles are:
  1-particle weight; 2-wind shear stress; 3-interparticle cohesion force.
- Saltation of large particles is initiated when the friction velocity exceed the threshold value. (**Saltation**)
- Large particles bombard fine particles aggregates causing breaking of the binding force within the aggregate and leading to suspension. (**Sandblasting**)

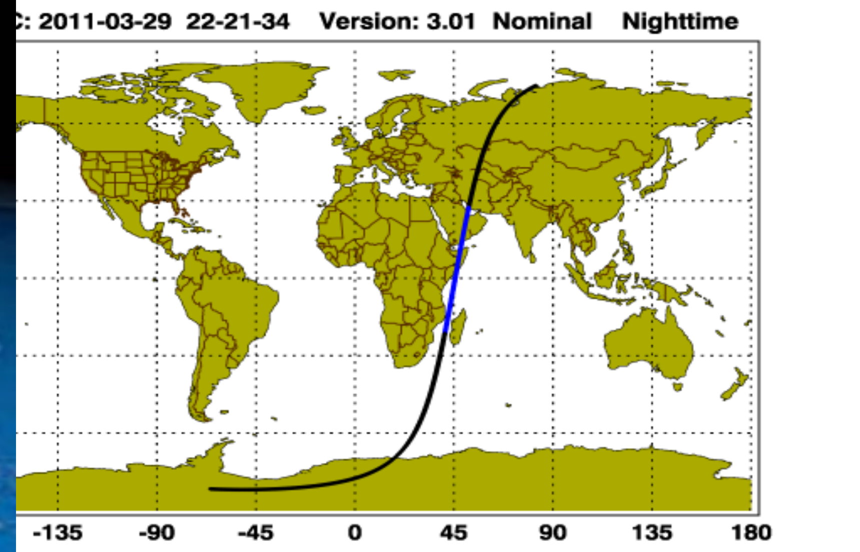
The vertical dust flux is proportional to the horizontal dust flux, which in turn depends on friction velocity.



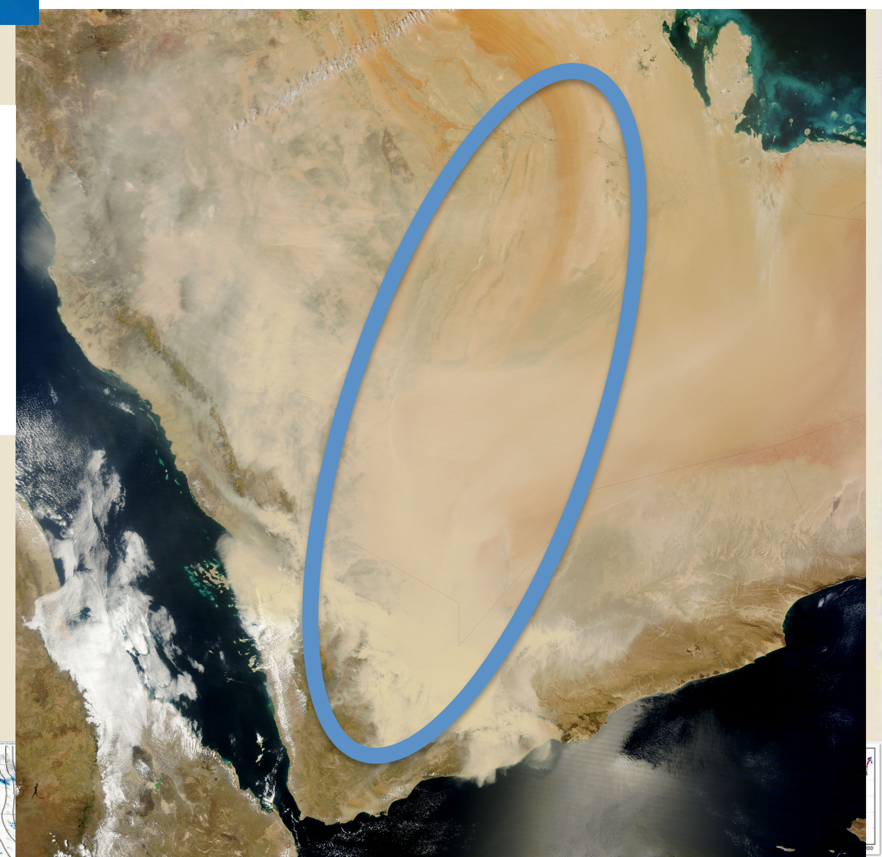
$$\frac{dV}{dt} + fk \times V + \nabla\Phi + \frac{RT}{p}\nabla p = 0$$


NASA Earth Observatories
Jason-1
Landsat 7
QuikSCAT
ERBS
ACRIMSAT
Aqua
Terra
TOPEX/Poseidon
TRMM
SAGE III/METEOR-3M
UARS
SORCE
GRACE
SeaWiFS
EP-TOMS
NMP/EO-1
ICESat
Aura

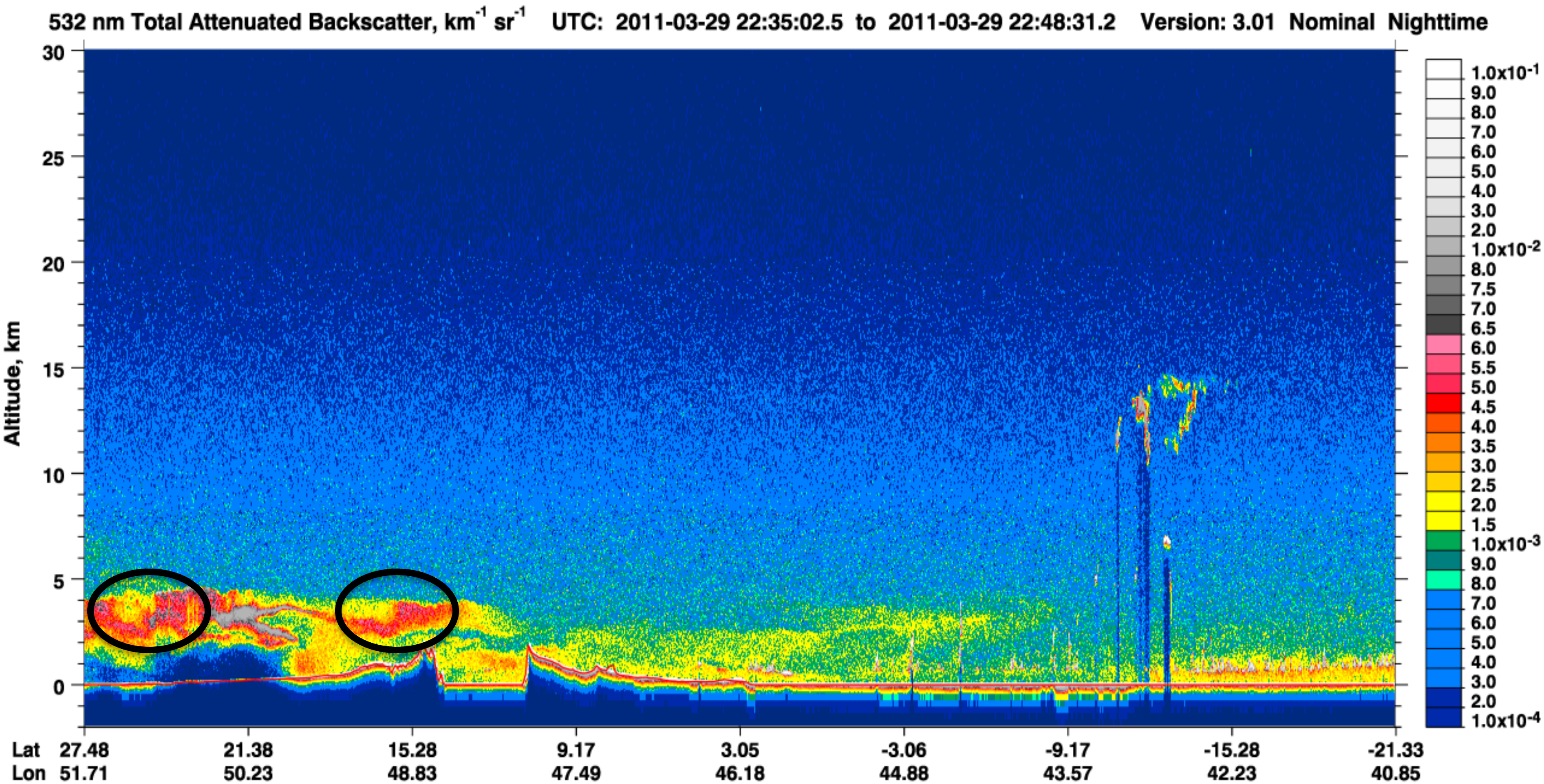




CALIPSO
The Cloud Aerosol Lidar and Infrared Pathfinder Satellite Observation



The Abdus Salam International Centre for Theoretical Physics

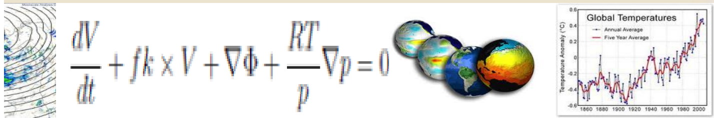


Detailed Information can be retrieved from CALIPSO

1-Aerosol concentration and height

2-Aerosol type (Absorbing or Scattering)

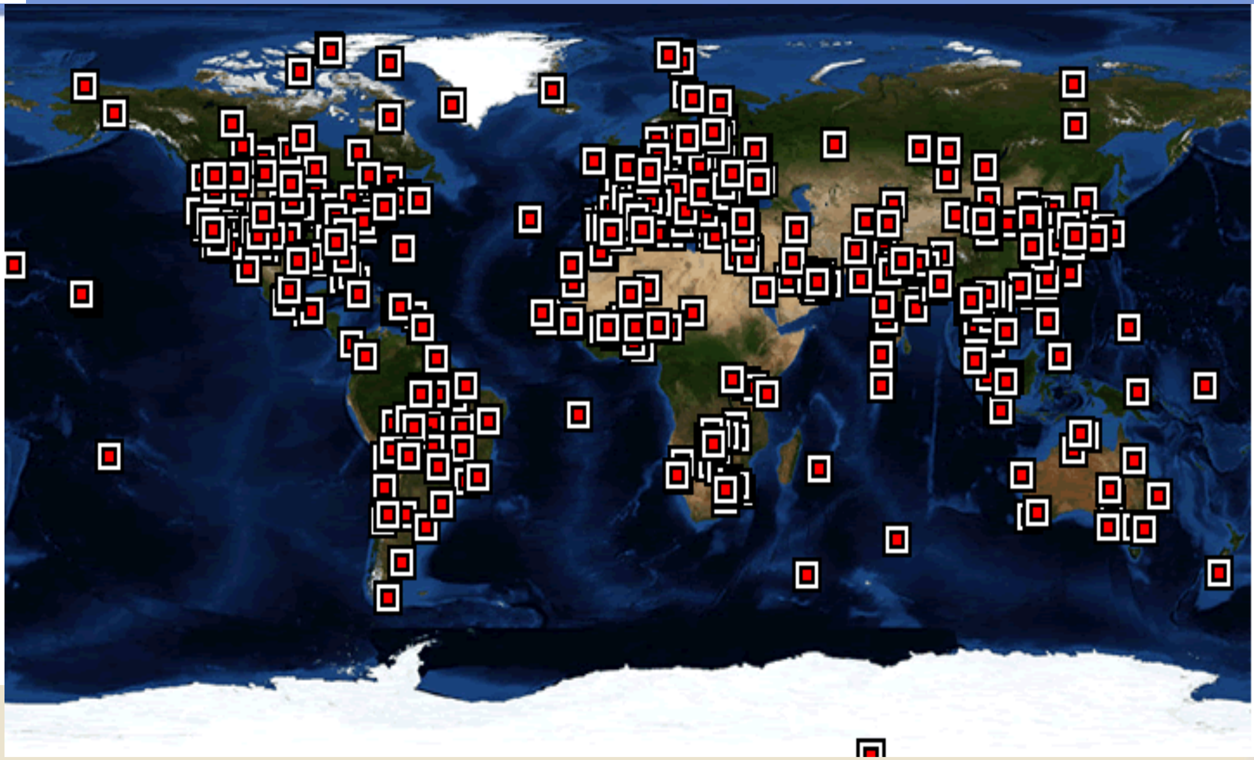
3-Aerosol shape (spherical or non-spherical)



AErosol **RO**botic **NET**work (**AERONET**)

http://aeronet.gsfc.nasa.gov/

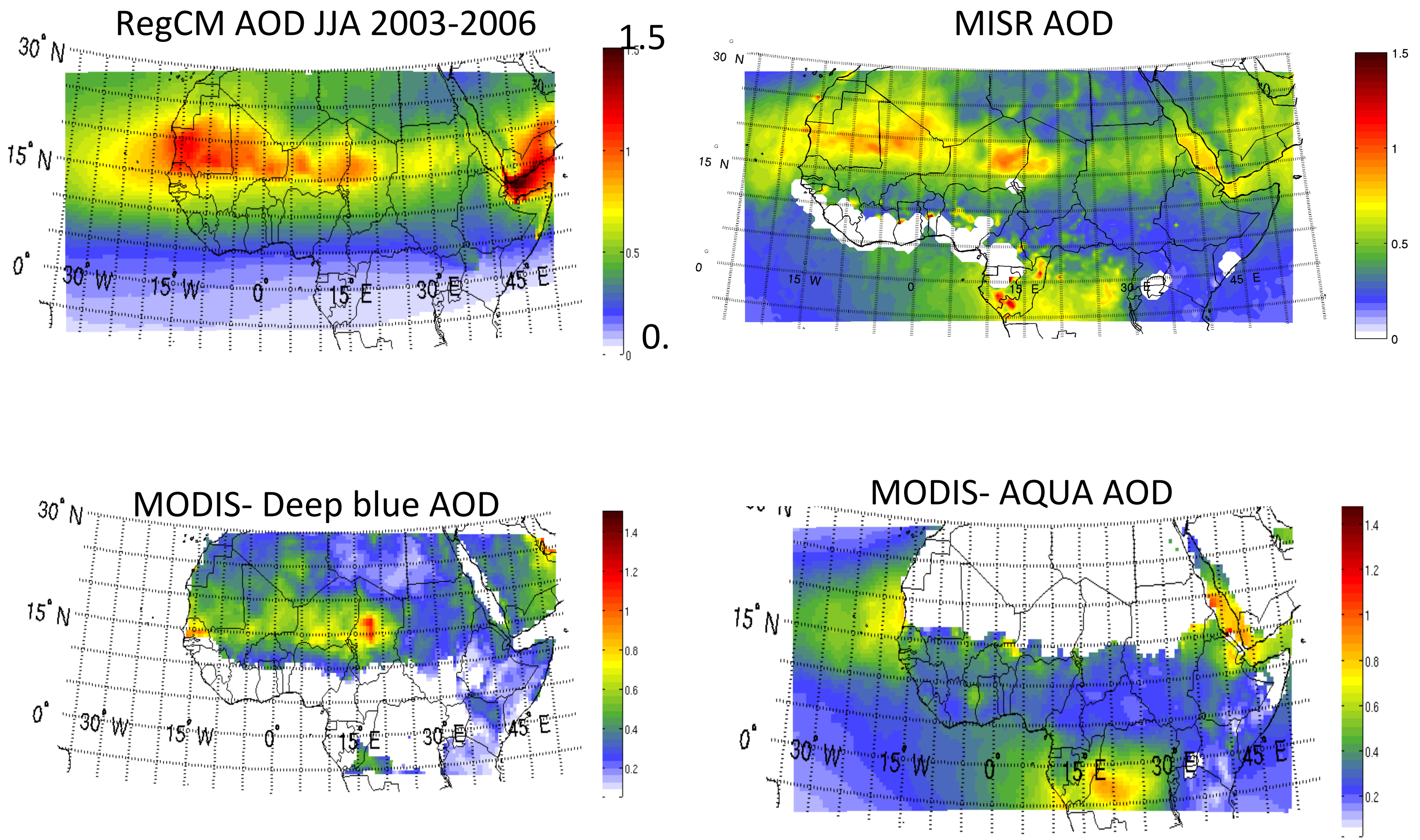
AERONET provides the most valuable information about the atmospheric aerosols.



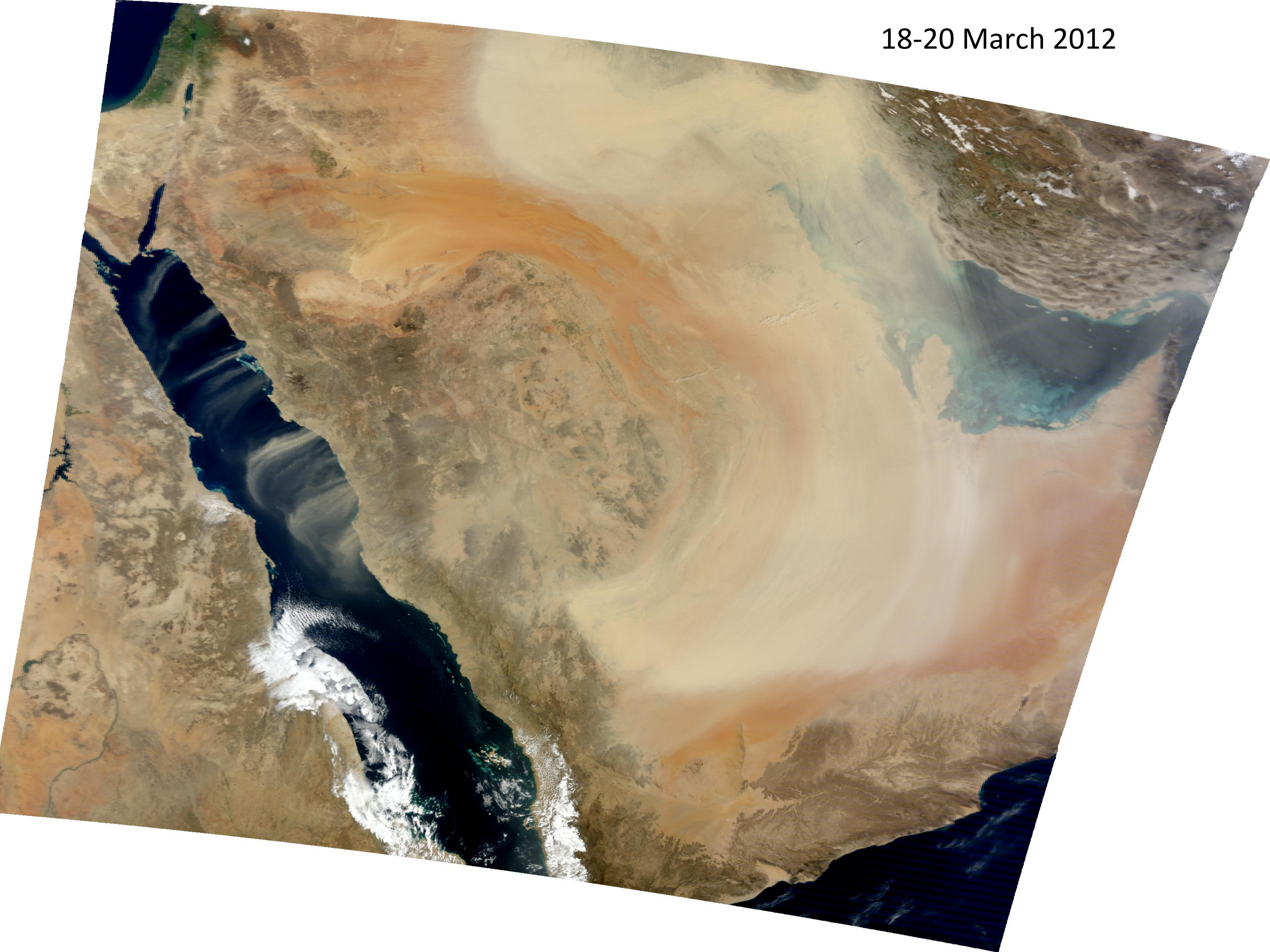
1-The aerosol optical depth (aerosols densities)

2-The aerosol size distribution (aerosols type)

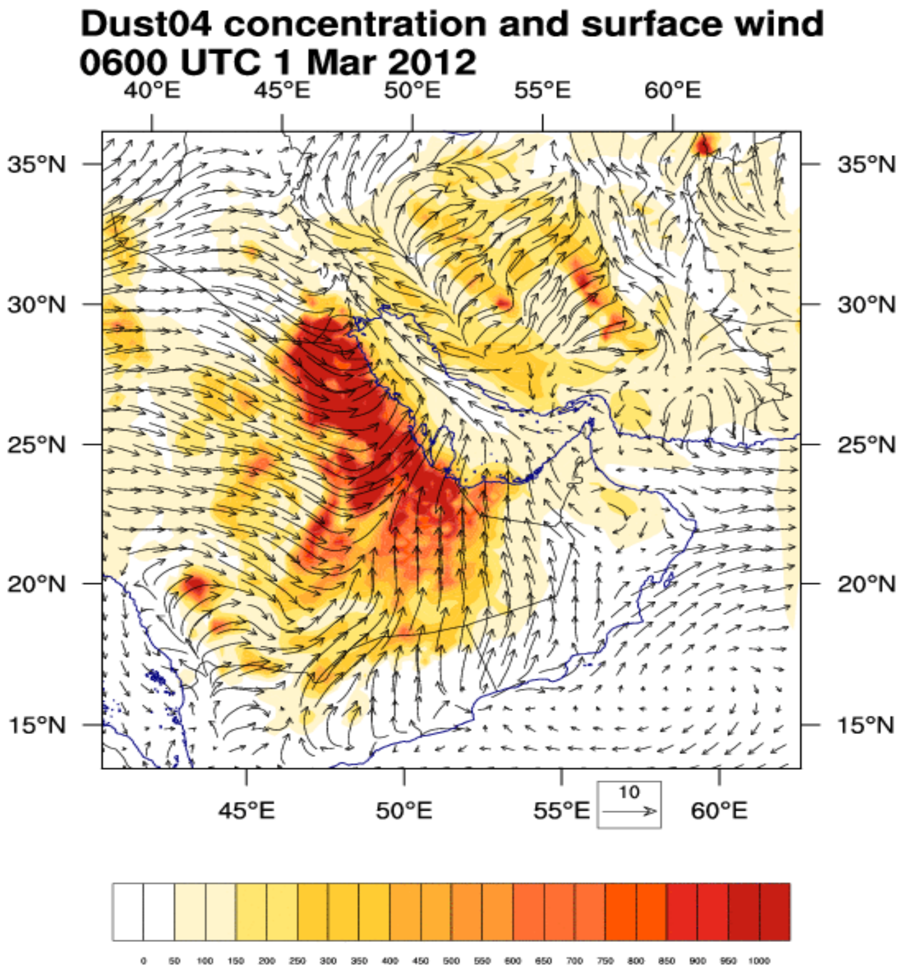
3-The aerosol radiative effects (Cooling and heating rates)

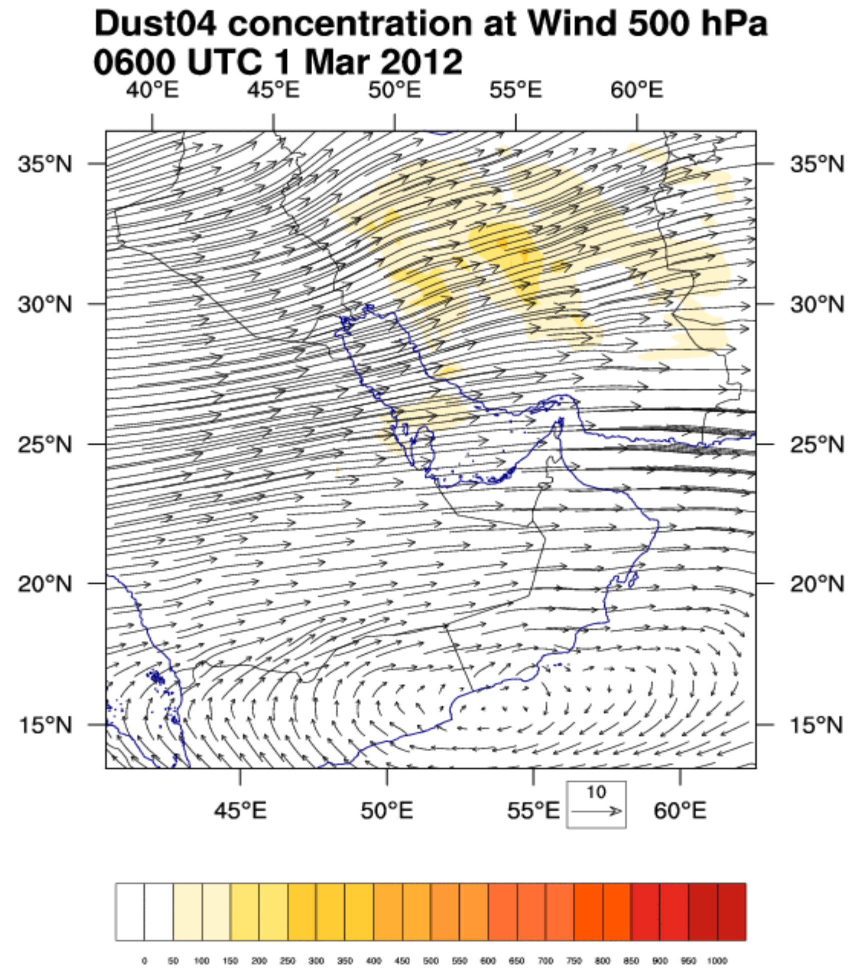


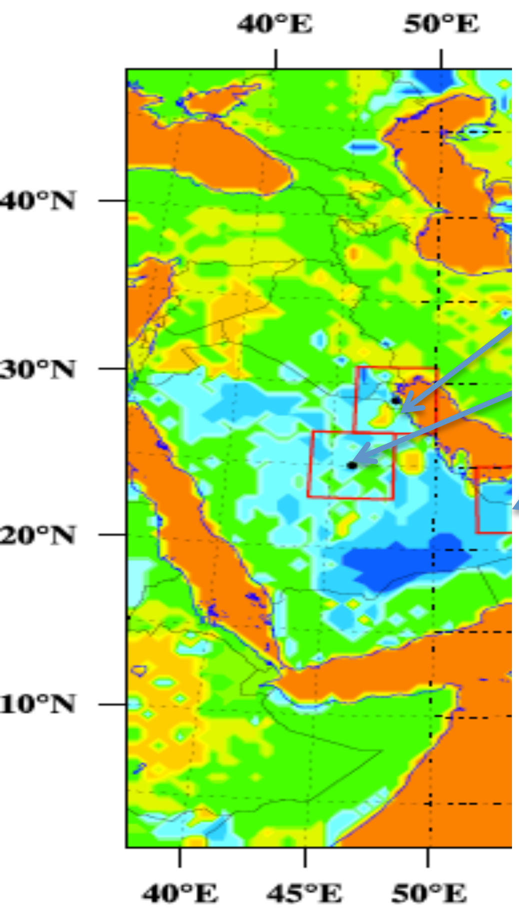
Solomn et al, 2012 CR.

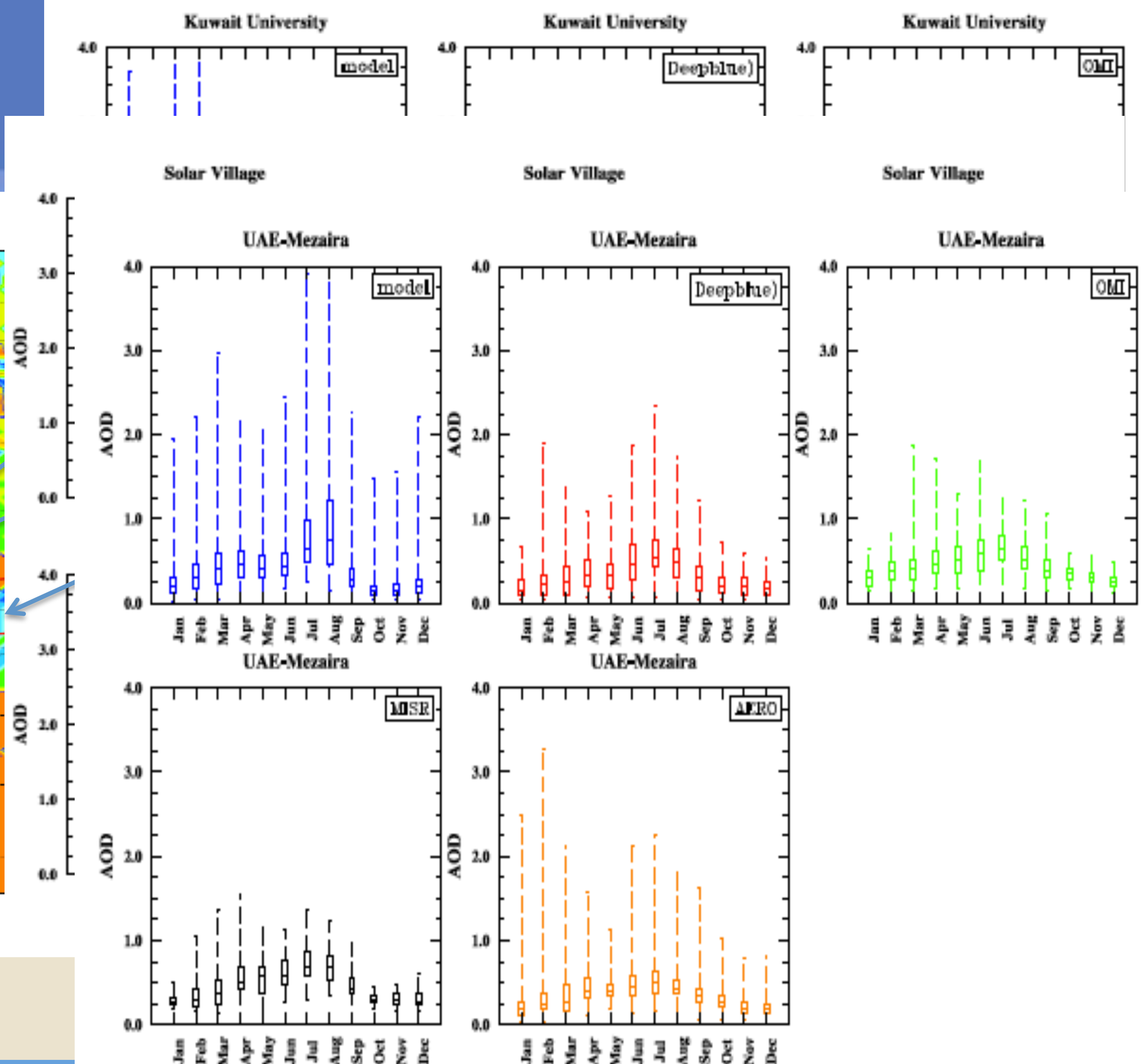

18-20 March 2012

Surface and Upper Air Wind in Spring






40°E
50°E
40°N
30°N
20°N
10°N
40°E
45°E
50°E


Kuwait University
model
Deepblue)
OMI
Solar Village
UAE-Mezaira
model
Deepblue)
OMI
MISR
AERO
AOD
4.0
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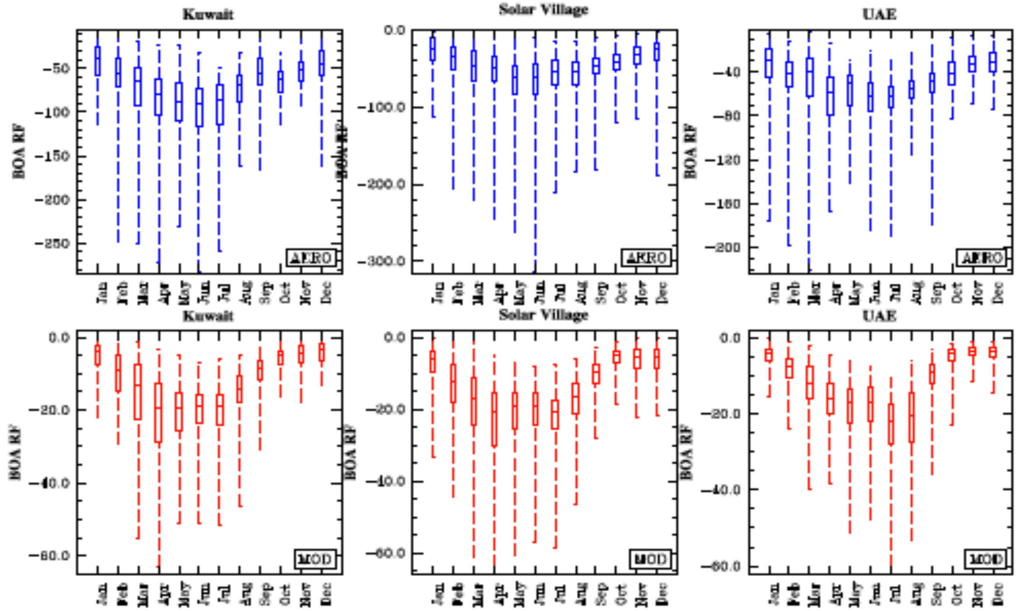
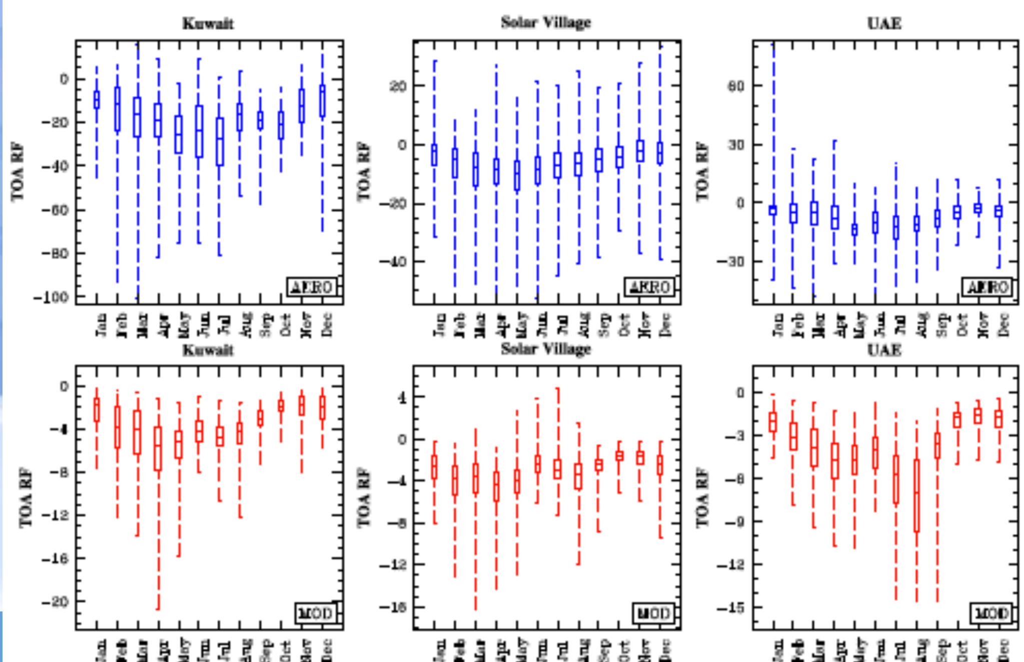
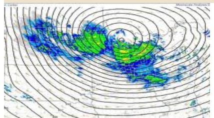


The Bottom of the atmosphere radiative forcing
Blue is the AERONET, RED is model
The model underestimates the Radiative forcing in BOT and TOA



The Top of the atmosphere radiative forcing
Blue is the AERONET, RED is model

This result shows a pronounced difference between northern and southern climatology of dusty season



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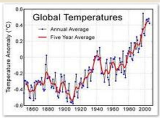
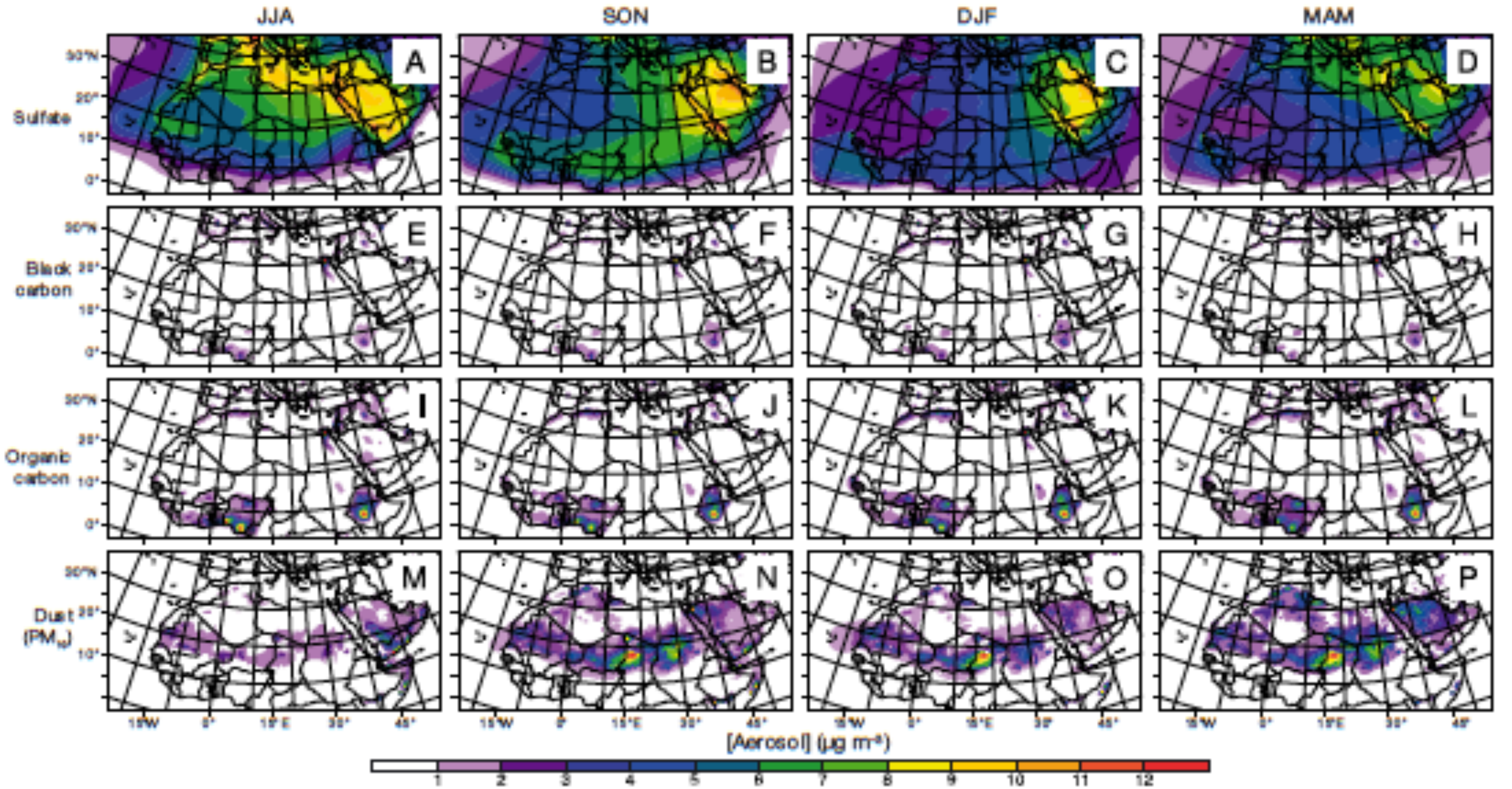
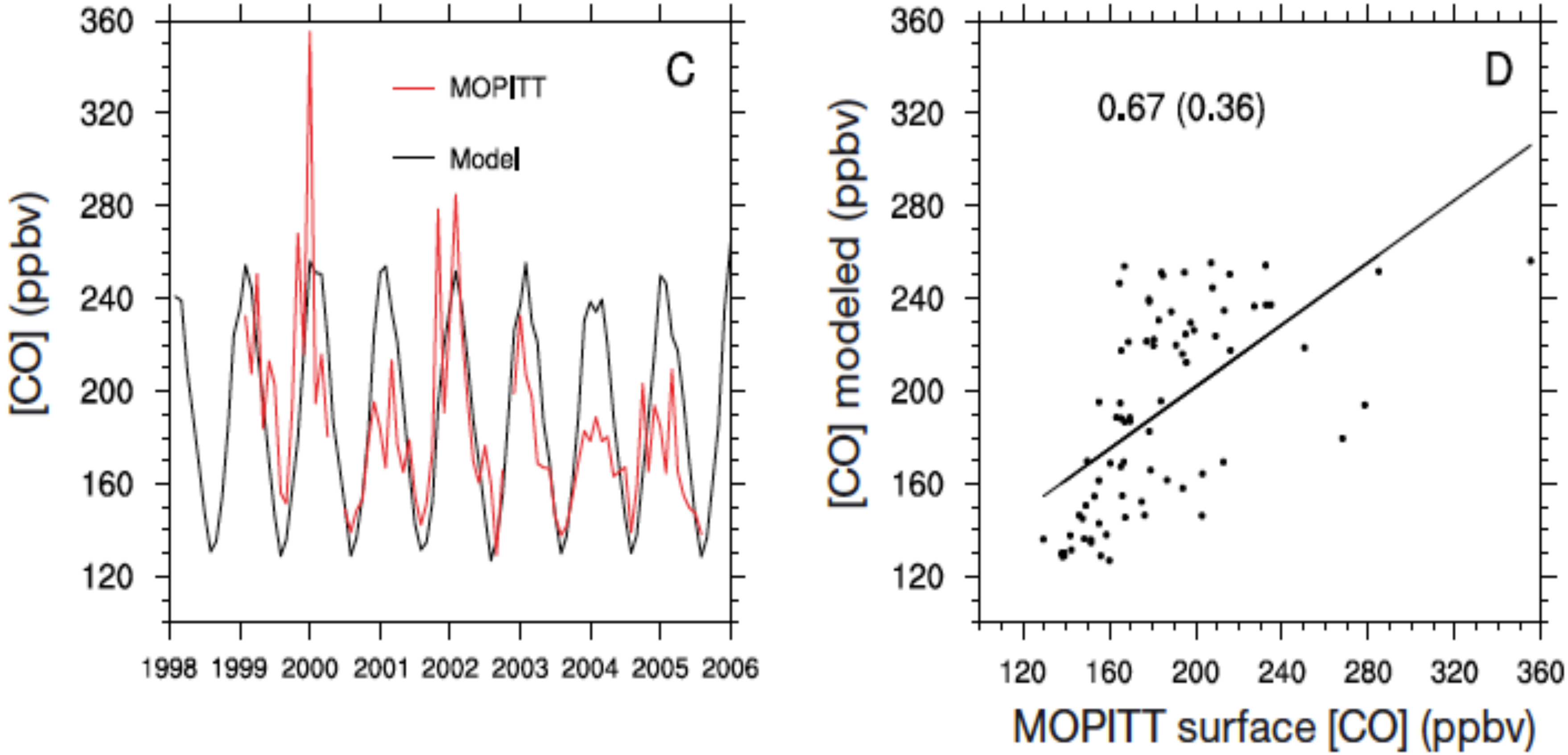




Steiner et al, 2014 CR.



Comparison between Stallite data MOPITT and model output over Great Cairo.

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Thank you for your attention