# Coupling of Gas-Phase Chemistry in RegCM

Concepts and Modeling

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Workshop on Aerosol-Climate Interactions:

Mechanisms, Monitoring, and Impacts in Tropical Regions

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Hurghada-Egypt

# OBJECTIVES

- Atmospheric chemistry Model Structure
- Gas-phase chemistry in RegCM

# Out-lines

- Emissions
- Photolysis
- Depositions
- Chemical Mechanisms
- Aerosols Mechanisms

# Emissions

- Emissions components

A-Biogenic Emissions

e.g wild fire, forest emissions

B-Anthropogenic Emissions

e.g Industrial emissions, Vehicle emissions. Man made fires.

# Chemical Compositions of Emissions

- Atmosphere has a numerous chemical composition, from inorganic compounds to organic compounds.
- Inorganic like ($H_2SO_4$ , $HNO_3$ , HCL)
- Organic like , Formic acid (HCOOH) , Acetic Acid ($CH_3COOH$)
- Ions ($SO_4^{2-}$ , $NH_4^+$)
- Solids (Dust, Black carbon, Pollens)

# What is a Chemistry Package?

1- Emissions
2- Photolysis
3- Chemical Mechanisms
4- Aerosols processes
5- Dry-deposition
6- Wet-deposition

# Emission driver

- Gunther method for biogenic emissions
- BEIS311 method for biogenic emissions both option support the biogenic emissions for Isoprene and VOC's (ket, xyl, eth, …), they depends on temperature, pressure and short wave radiations inputs.
- Add anthrogenic and biogenic emissions

# Photolysis Driver

- Madronich option
- Fast J. option
- Photolysis driver support the photolysis fields for certain important chemical compounds (O3, NO2, HNO3, HCHO,…)

# Chemical Mechanisms

- Chemical Mechanism means, an approximated set of atmospheric  chemical reactions.
- Such set may be very simple and may be very complex (explicit). Depends on the number of species and reactions employed. The main source of complexity is the implementation of organic species.
- There are three famous chemical mechanisms

- RADM2 (Regional Acidic Deposition Model) (*Stockwell et al.* 1990)
- RACM (Regional Atmospheric Chemistry Mechanism)(*Stockwell et al.* 1997)
- CBM-Z ( Carbon Bond Mechanism-Zaveri) (Zaveri, A. and Peter, K. 1999)

| | RADM2 | RACM |
|---|---|---|
| Stable inorganic species | 14 | 17 |
| Intermediate inorganic species | 4 | 4 |
| Abundant species | 3 | 3 |
| Stable organic species | 26 | 32 |
| Intermediate organic species | 16 | 24 |
| Number of reactions | 157 | 237 |

# Lumping Technique (pros & cons) how to represent VOC's?

- Lumped structure (RADM2 & RACM)

  1-surrogate species have similar reactivity range.

  2-does not conserve carbon mass.

- Lumped molecule (CBM-IV & CBM-Z)

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

  2-conserve carbon mass

# Aerosols Modules

- We have three major Aerosols Modules

1-RPM (Regional Particulate Matter model) (*Binkowski, F. and Shanker* 1995)

2-SORGAM (Secondary Organic Aerosols Model)(*Shell et al. 2001*)

3-MOSAIC (Model for Simulation Aerosols Interaction and Chemistry)(Zaveri. 1999)

# Aerosols Model Modules

- Any aerosols model must have the following components to simulate aerosol formation accurately
  - a- size distribution module (modal/sectional)
  - b- nucleation module
  - c- coagulation module
  - d- condensation/evaporation module
  - e- dry/wet deposition module

The difference between aerosol models depends on how the model simulate each components.

# RPM

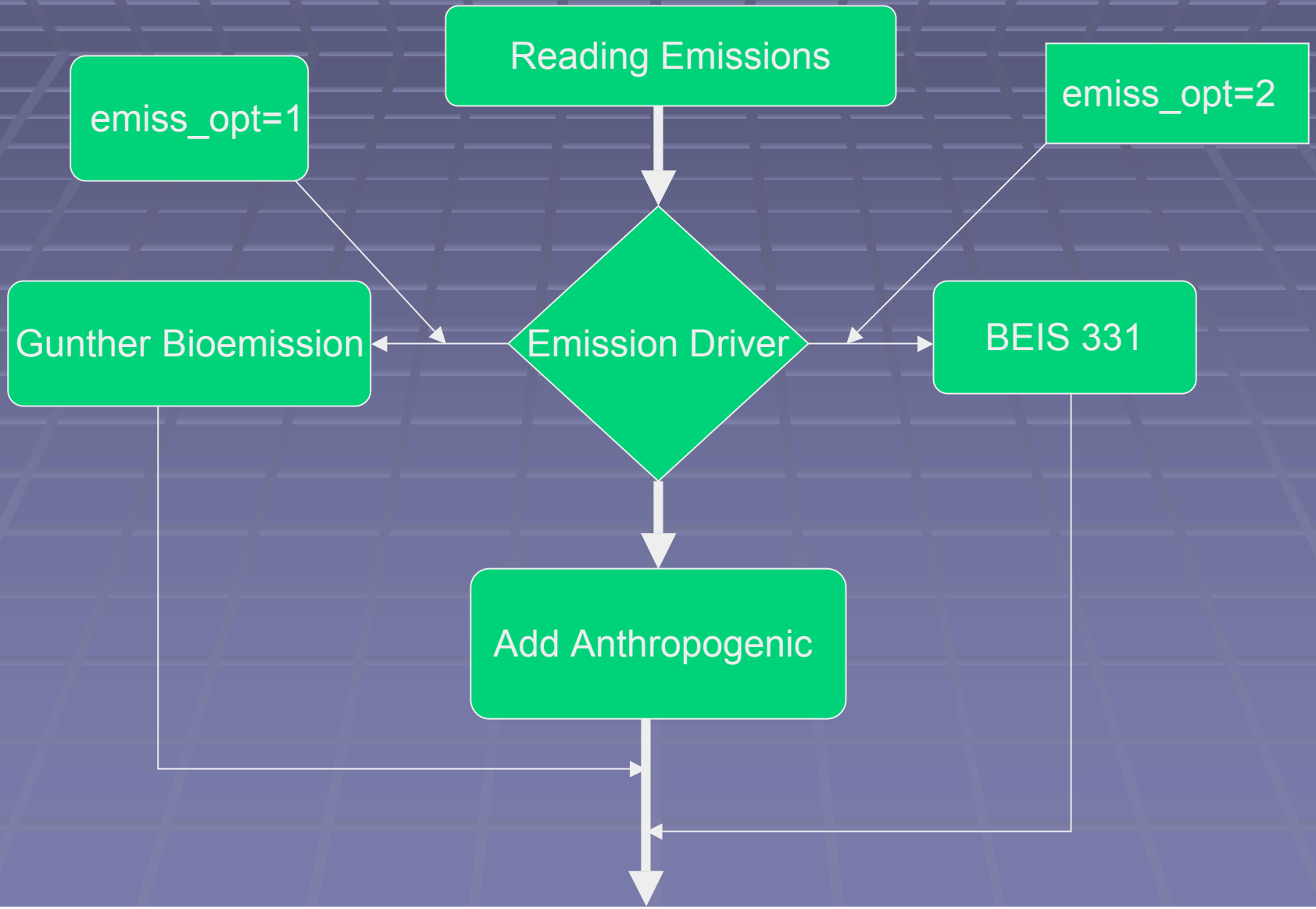
- RPM simulates the chemistry, transport and dynamics of sulfuric acid aerosol resulting from primary emissions and the gas phase oxidation of sulfur dioxide.
- RPM uses a bimodal (two mode) lognormal distribution to represent aerosols.
- RPM is an equilibrium model based on fundamental thermodynamics.

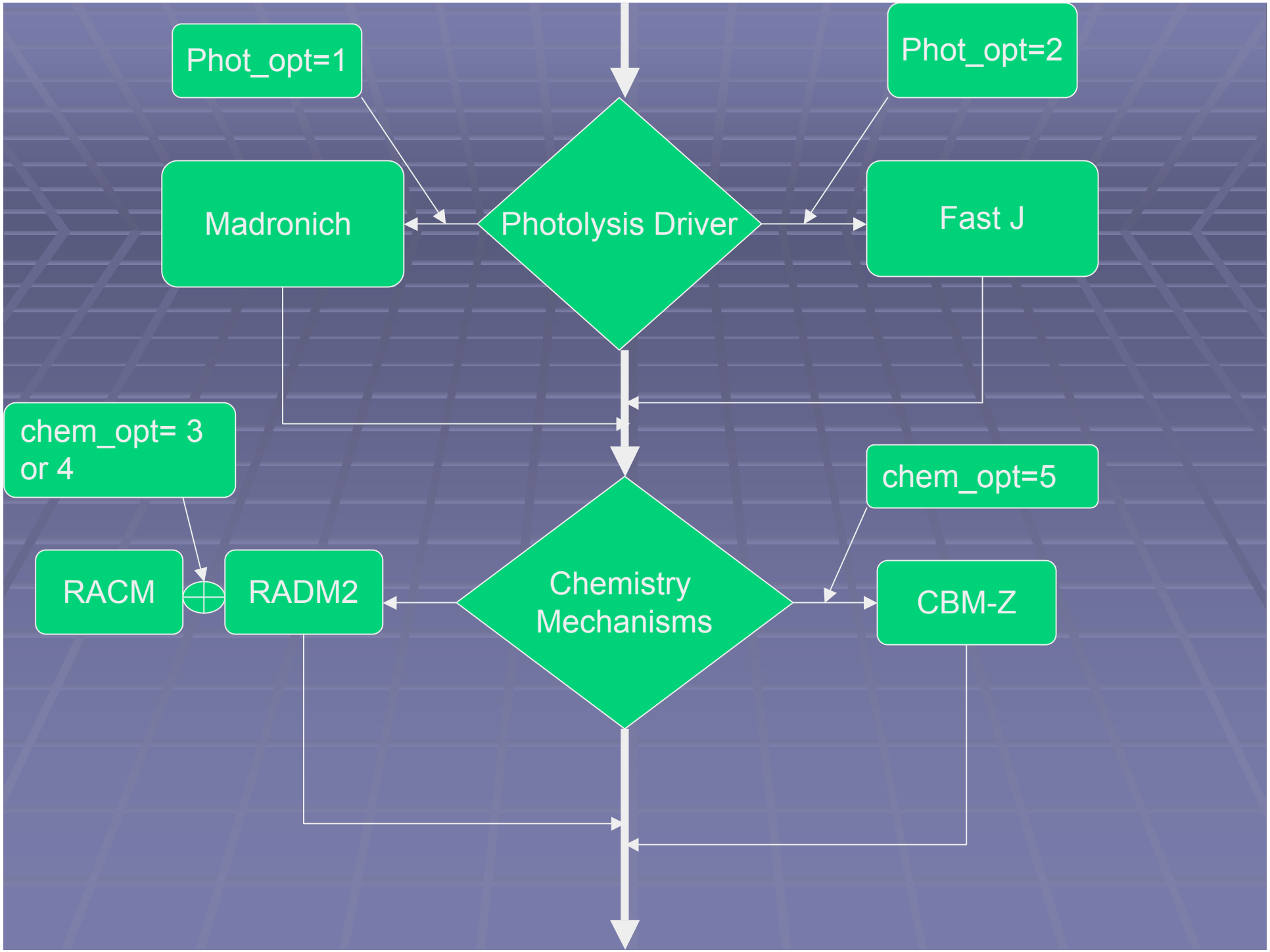
# SORGAM

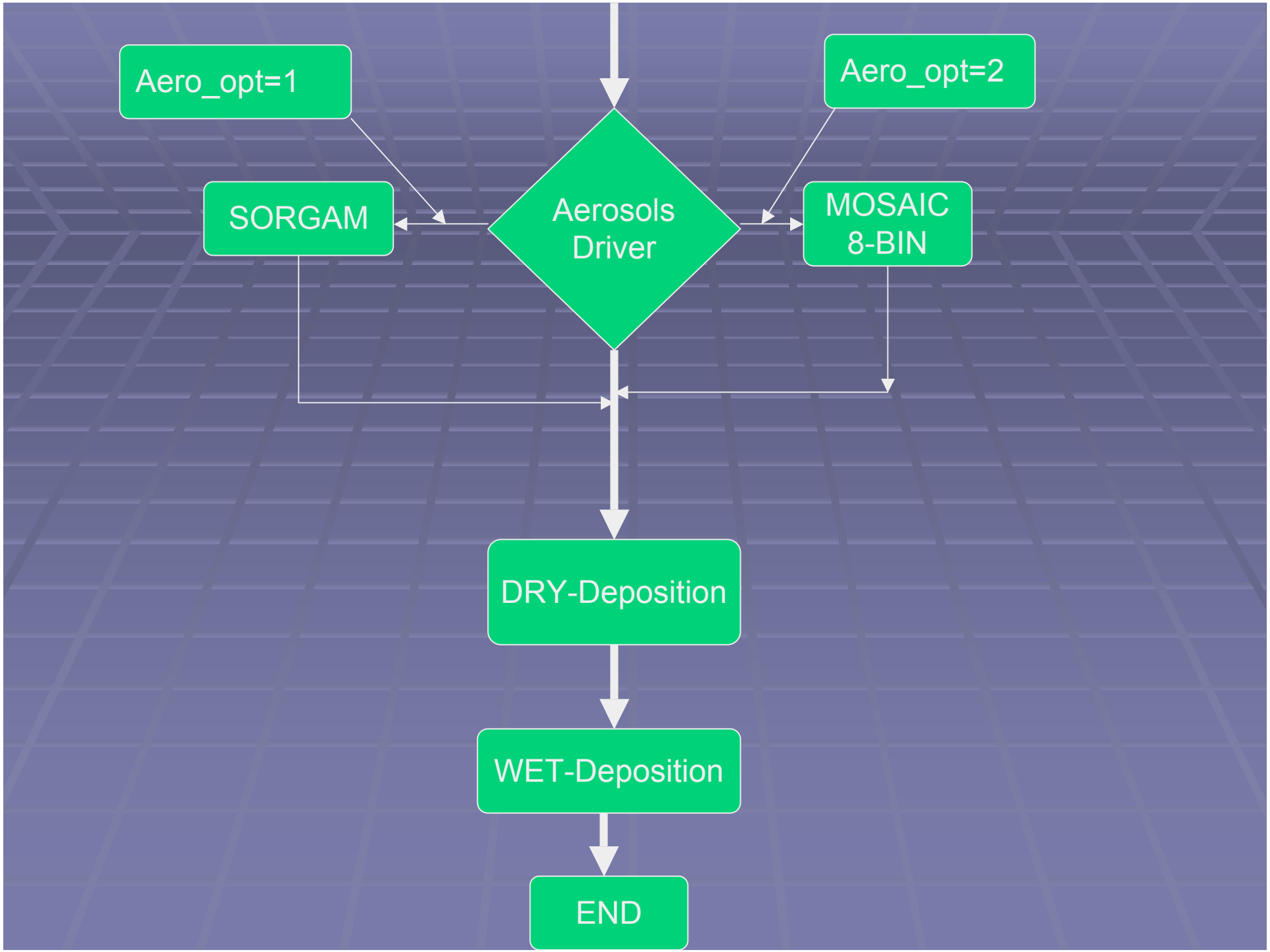
- What is *Secondary Organic Aerosols?*

  Primary organic aerosol is emitted directly into the atmosphere, whereas secondary organic aerosol (SOA) is formed in the atmosphere by gas-to-particle partitioning.

# Chemistry Flow Chart




Phot_opt=1
Phot_opt=2
Madronich
Photolysis Driver
Fast J
chem_opt= 3
or 4
chem_opt=5
RACM
RADM2
Chemistry
Mechanisms
CBM-Z


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

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

- Chemistry Mechanisms includes hundreds of reactions and dozens of chemical species (e.g RACM has 237 reactions and 77 species).
- Solving the corresponding huge systems of ODE requires highly efficient numerical integrators, and costly code developments and updates.

# KPP (cont.)

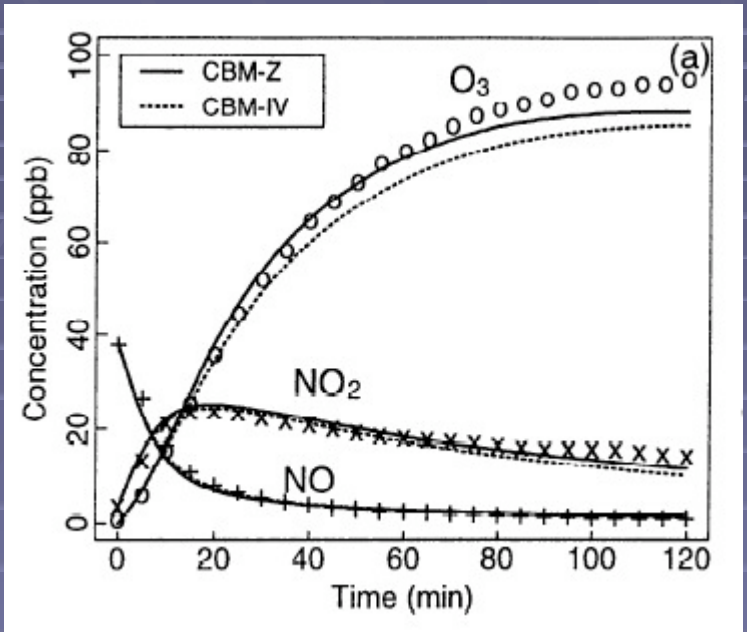
- Automatic Code generation has become widely used tool to overcome the above problems.
- KPP needs only three files (user defined) one for the set of mechanism equations, one for definitions of species and the last one for initialization and inline code.
- KPP will process such files and produce a complete package for simulation of such mechanisms.

# KPP (cont.)

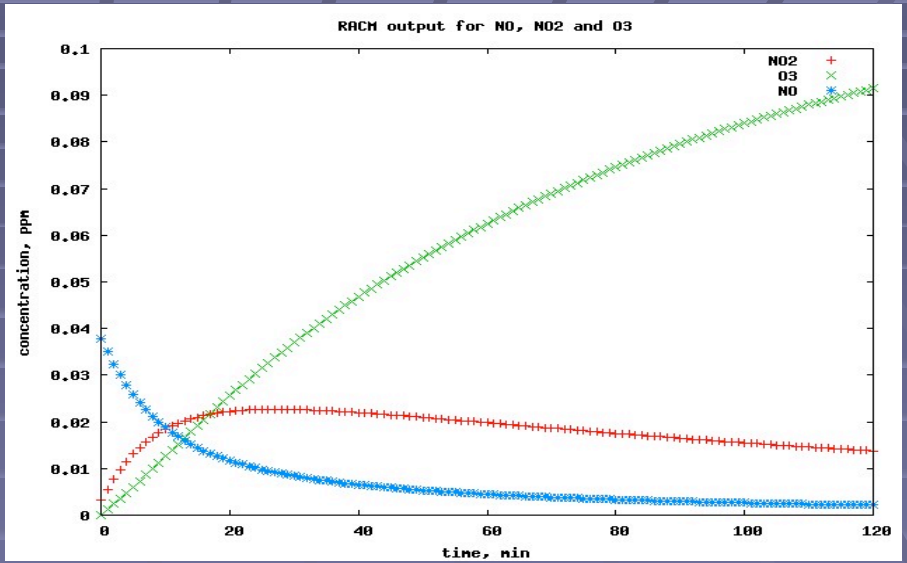
- KPP used to produces the chemical mechanisms for the gas-phase (RADM2, CBM-Z and RACM).

We use the Data of smog (environmental) chamber, to verify the output of KPP, (Simonaitis R. et al. 1997)

# KPP verification

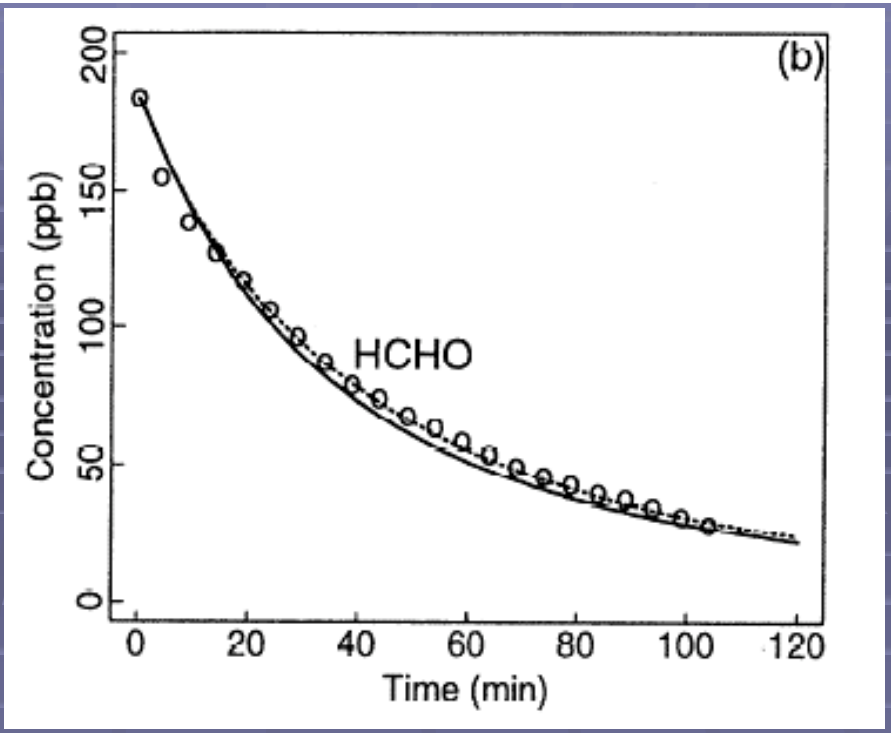



Chamber Data

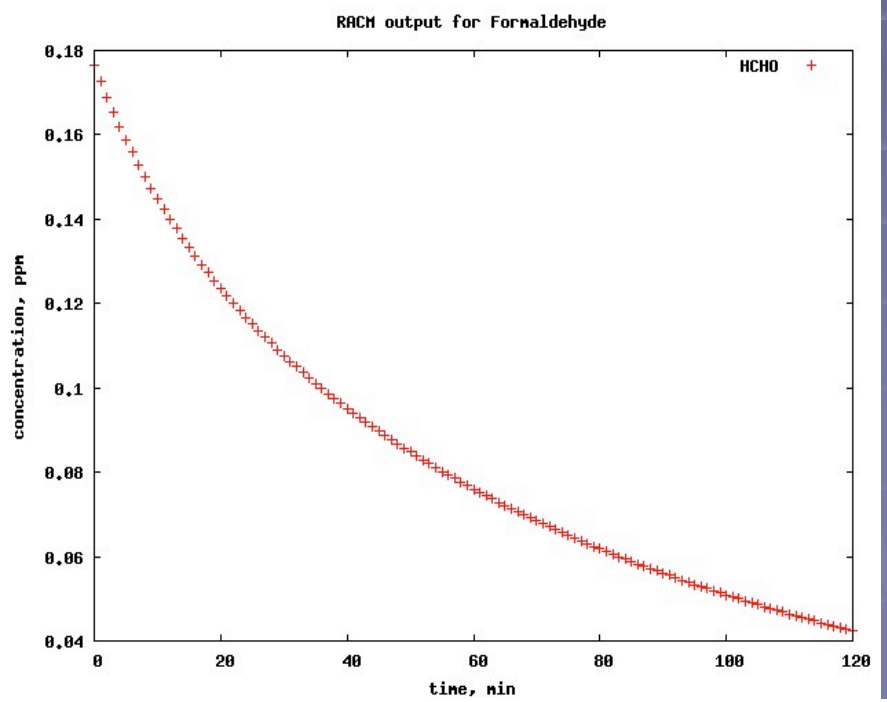


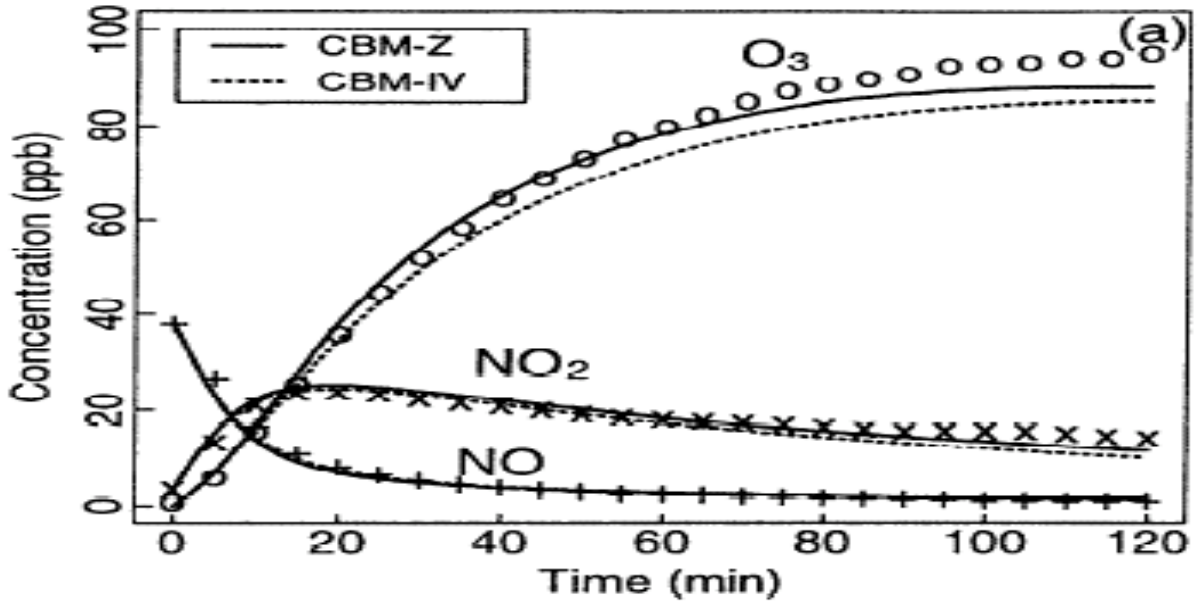

RACM output

Chamber Data




RACM output



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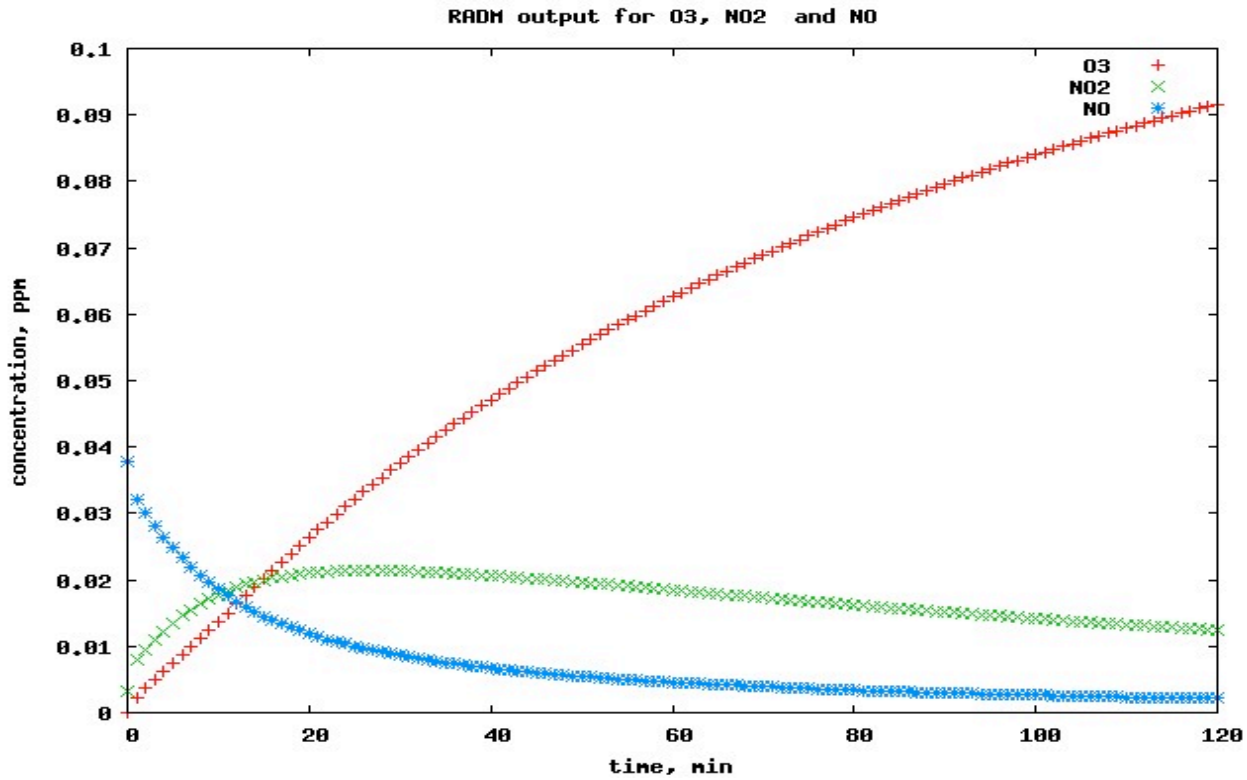
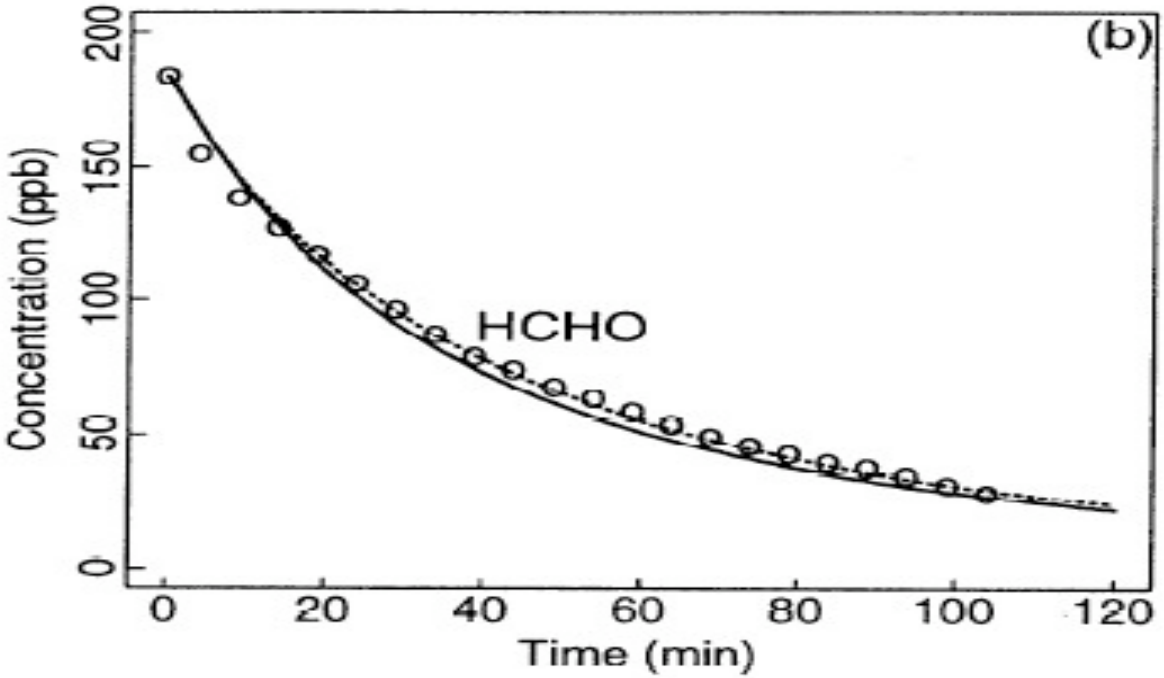



RADM2 output

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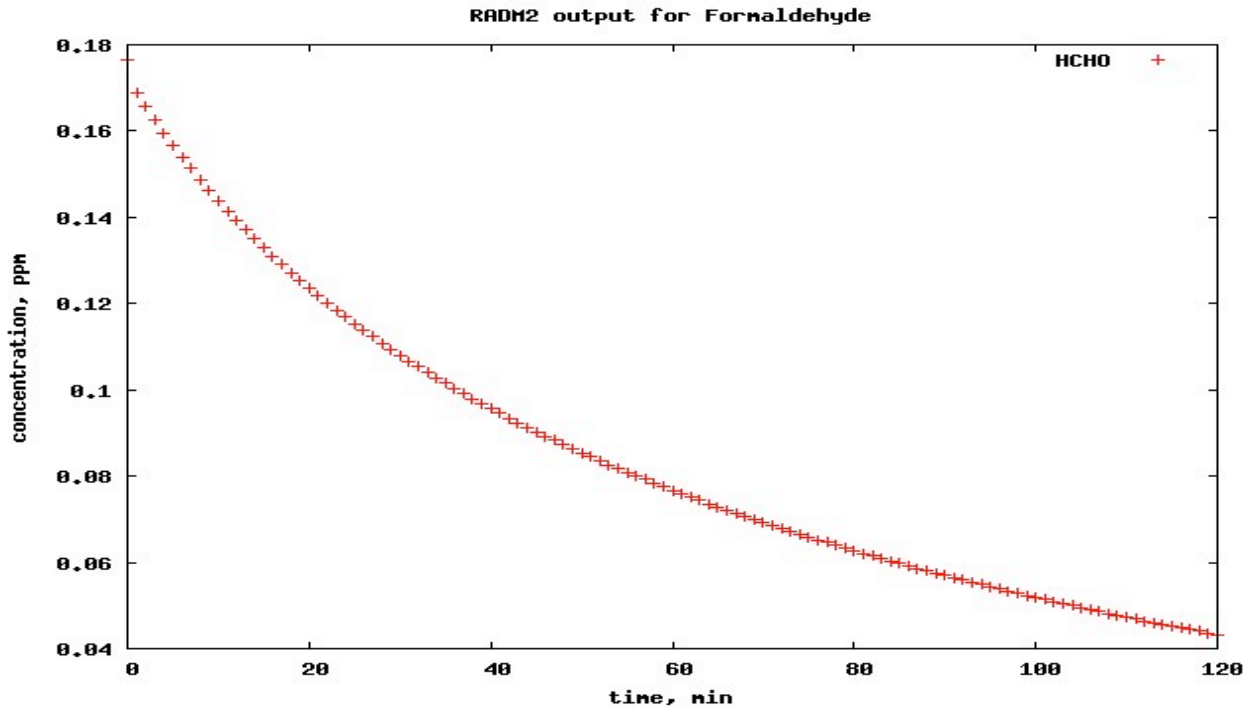
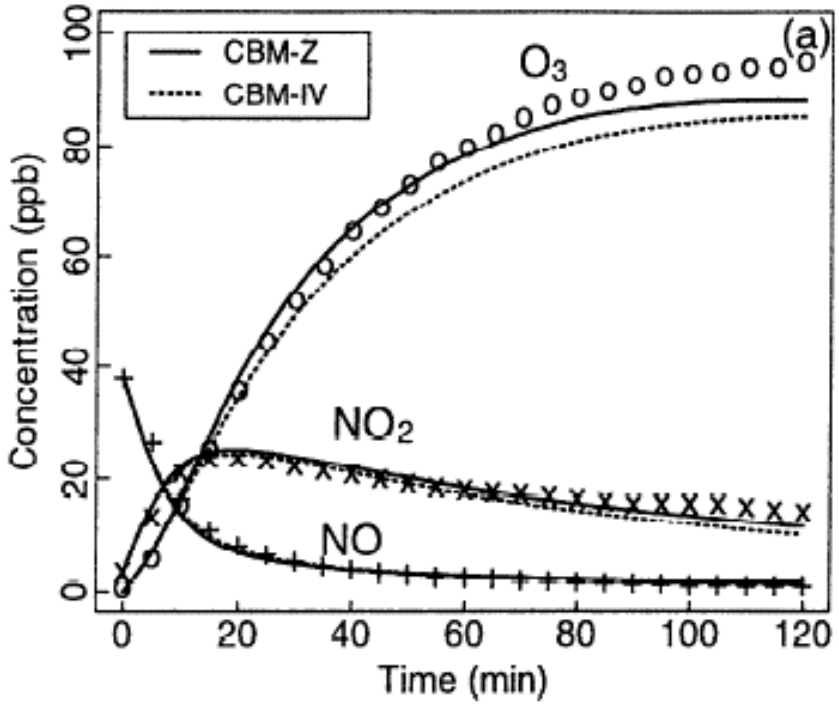
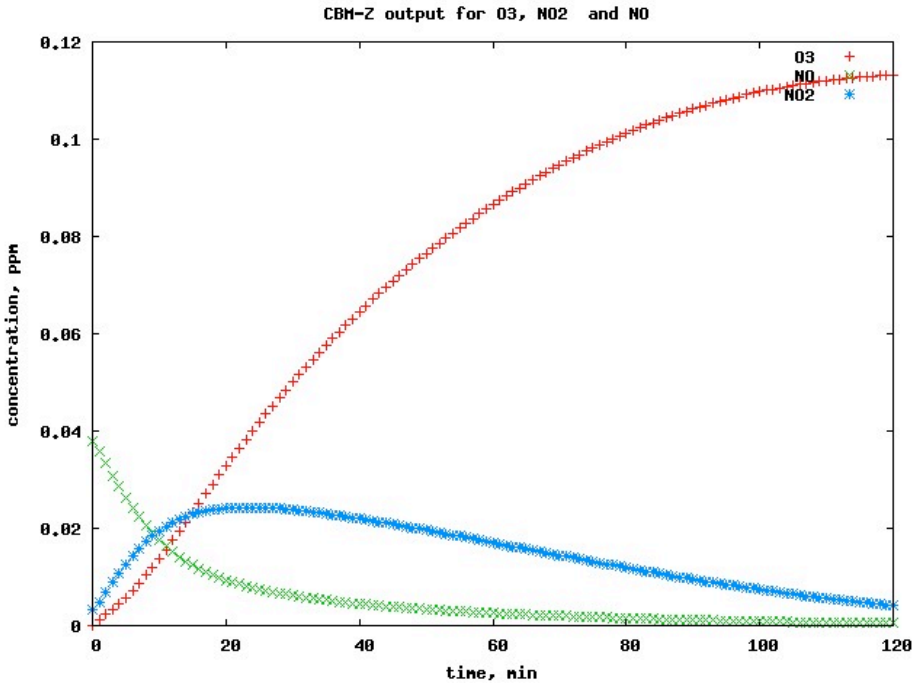


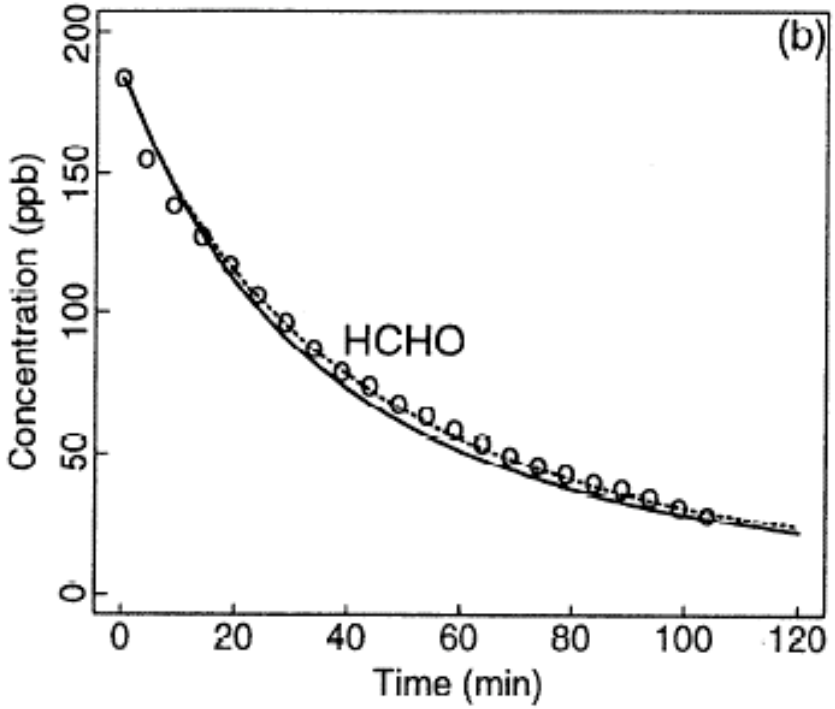

RADM2 output



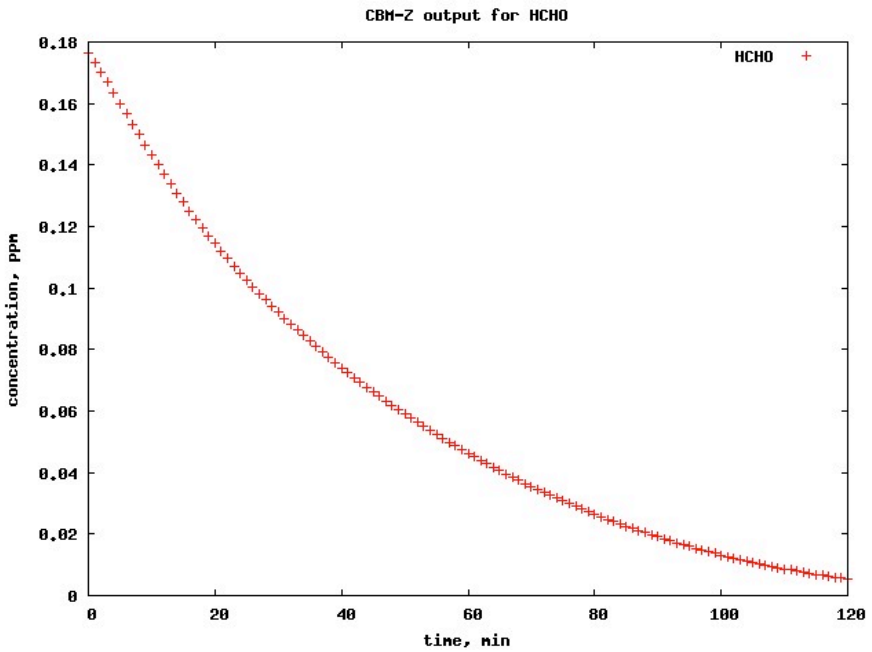




Chamber Data + CBM-Z

CBM-Z KPP output




Chamber Data +
CBM-Z




CBM-Z KPP

# Coupling of Gas Phase with RegCM

# Emission Inventories

1. RETRO 0.5° X 0.5° (1960-2000)

2. EDGAR 3.2FT2000 1° X 1° (2000)

3. POET 1° X 1° (1990-2003)

4. GFED 1° X 1° (1997-2005)

# RETRO

RETRO species

Biogenic {CO, BC, CH4, ACETONE, ETHAN, ISOPRENE, N2O, NH3, OC, PM2.5, SO2, …}

Anthropogenic {ACIDS, ALCOHOLS, BENZENE, CO, ETHER, NOx, PROPANE, …}

# POET

POET species

Biogenic { ACET, CHOH, CO, NOx, …}

Anthropogenic { ACET, CHOH, CO, NOx,…}

# GFED

GFED species

Biogenic {BC, C, CH4, CO, H2, N2O, NMHC, NOx, OC, PM2.5, …}

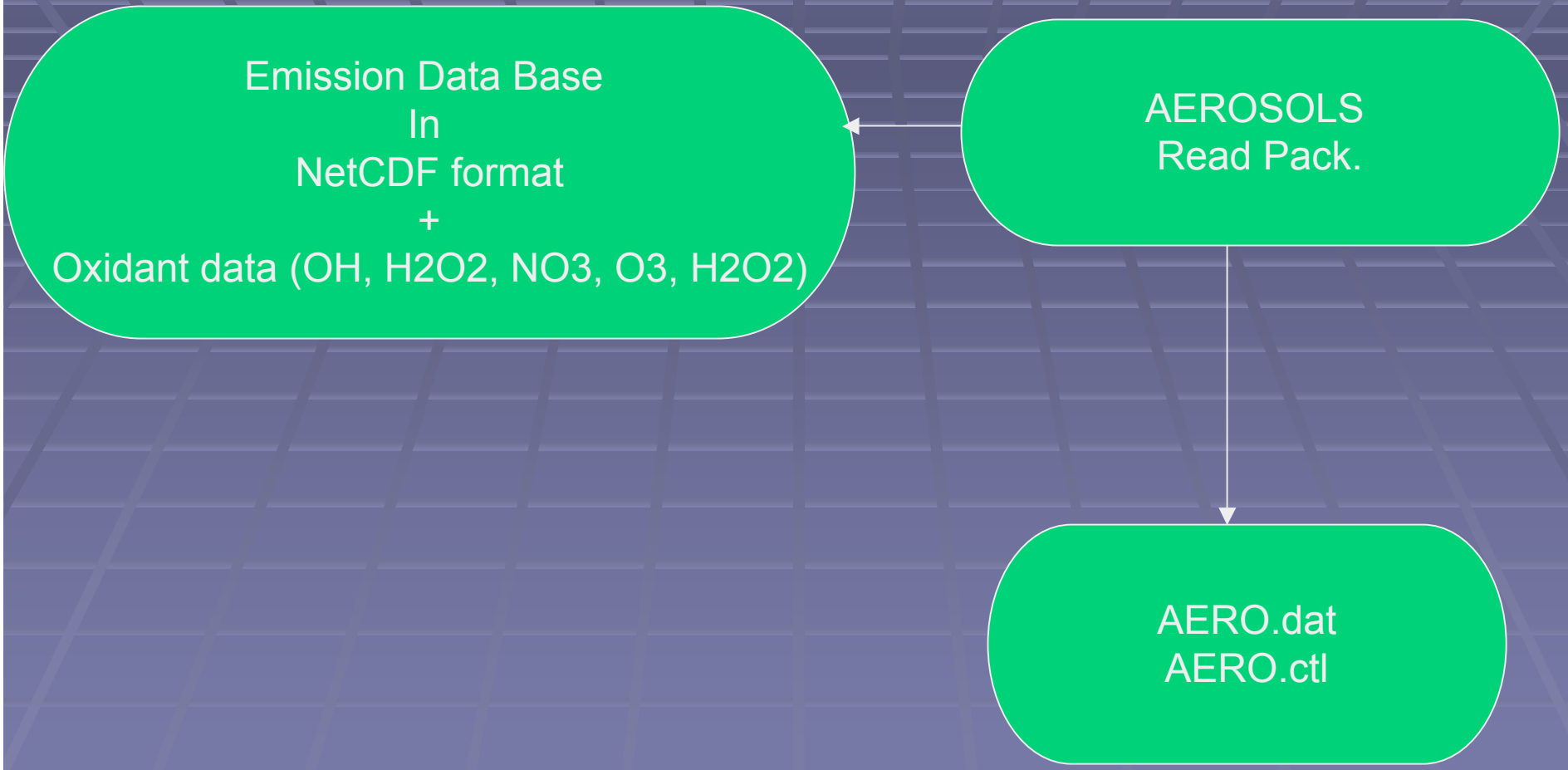
# EDGAR

EDGAR species

Biogenic {BC, CH4, CO, CO2, DMS, OC, SO2,…}

Anthropogenic { BC, CH4, CO, CO2, SO2…}

# Emission Data Base



# Namelist

```
PARAMETER (NSPC1A=1)     !Anthropogenic RETRO
PARAMETER (NSPC2=1)      !POET
PARAMETER  (NSPC4B=1)    !Biogenic EDGAR

DATA ELE_RETROA / 'NOX‘/

DATA ELE_POET / 'ch2o'/

 DATA ELE_EDGARA /'so2'/
```

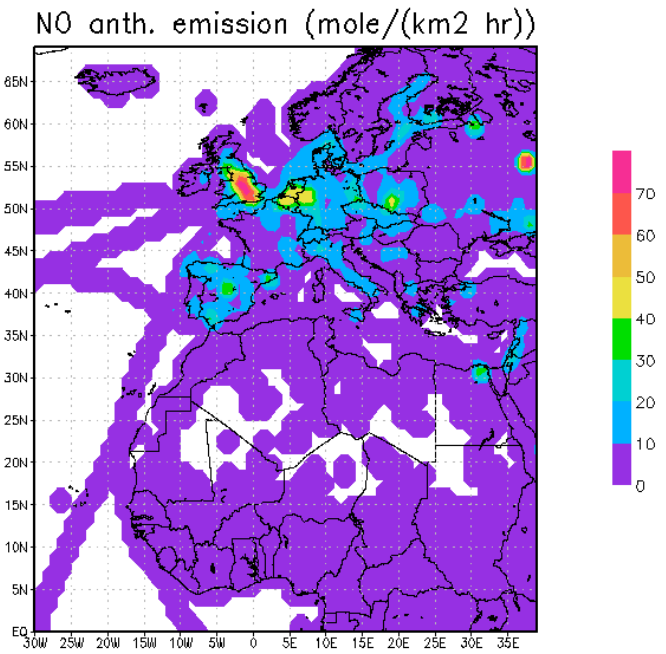
# AERO.ctl

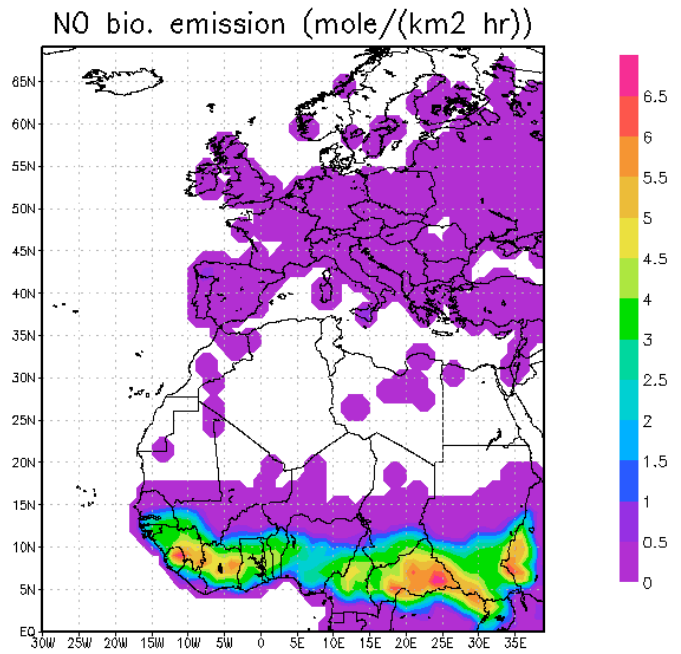
a_NOX 0 99 Anthropogenic emission, RETRO

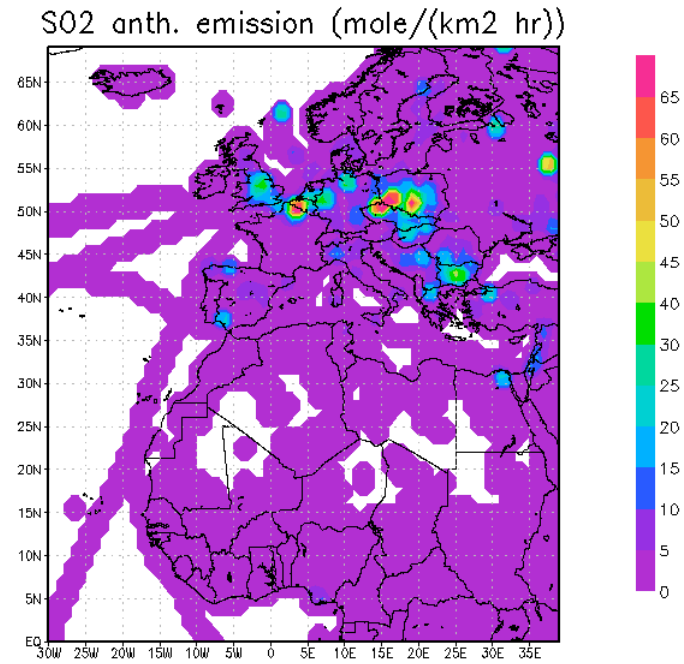
a_ch2o 0 99 Anthropogenic emission, POET

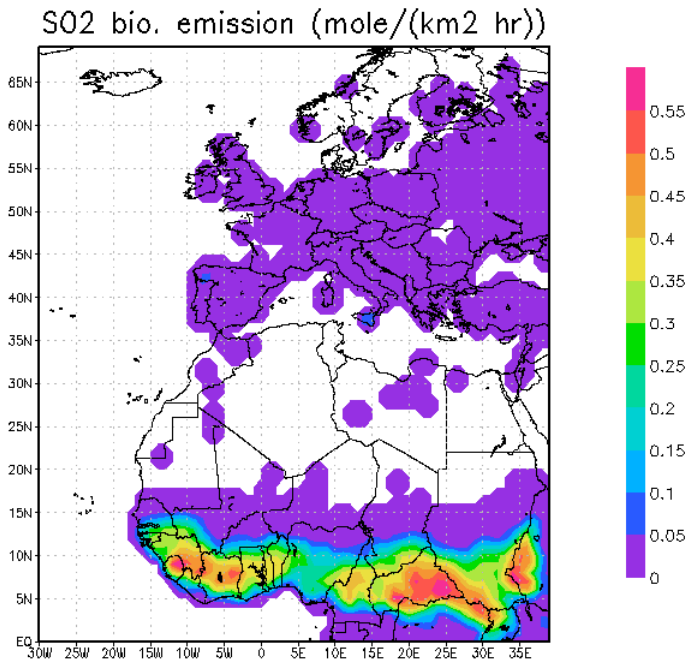
a_so2 0 99 Anthropogenic emission, EDGAR

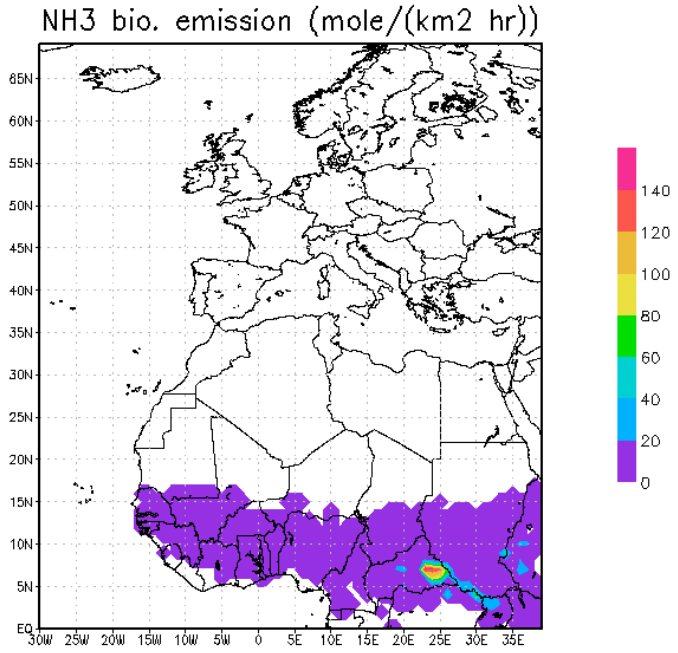
# Emissions Inputs



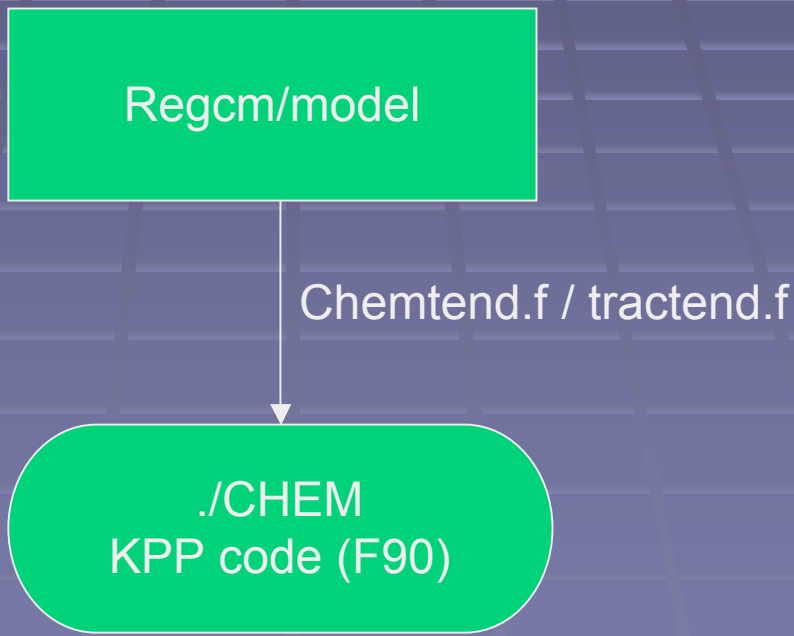




SO2 anth. emission (mole/(km2 hr))
85N
60N
55N
50N
45N
40N
35N
30N
25N
20N
15N
10N
5N
EQ
30W 25W 20W 15W 10W 5W 0 5E 10E 15E 20E 25E 30E 35E
65
60
55
50
45
40
30
25
20
15
10
5
0
GrADS: COLA/IGES
2007-08-02-13:10


SO2 bio. emission (mole/(km2 hr))
85N
60N
55N
50N
45N
40N
35N
30N
25N
20N
15N
10N
5N
EQ
30W 25W 20W 15W 10W 5W 0 5E 10E 15E 20E 25E 30E 35E
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
GrADS: COLA/IGES
2007-08-02-13:10


NH3 bio. emission (mole/(km2 hr))
85N
60N
55N
50N
45N
40N
35N
30N
25N
20N
15N
10N
5N
EQ
30W 25W 20W 15W 10W 5W 0 5E 10E 15E 20E 25E 30E 35E
140
120
100
80
60
40
20
0
GrADS: COLA/IGES
2007-08-02-13:06

# Gas Phase in RegCM

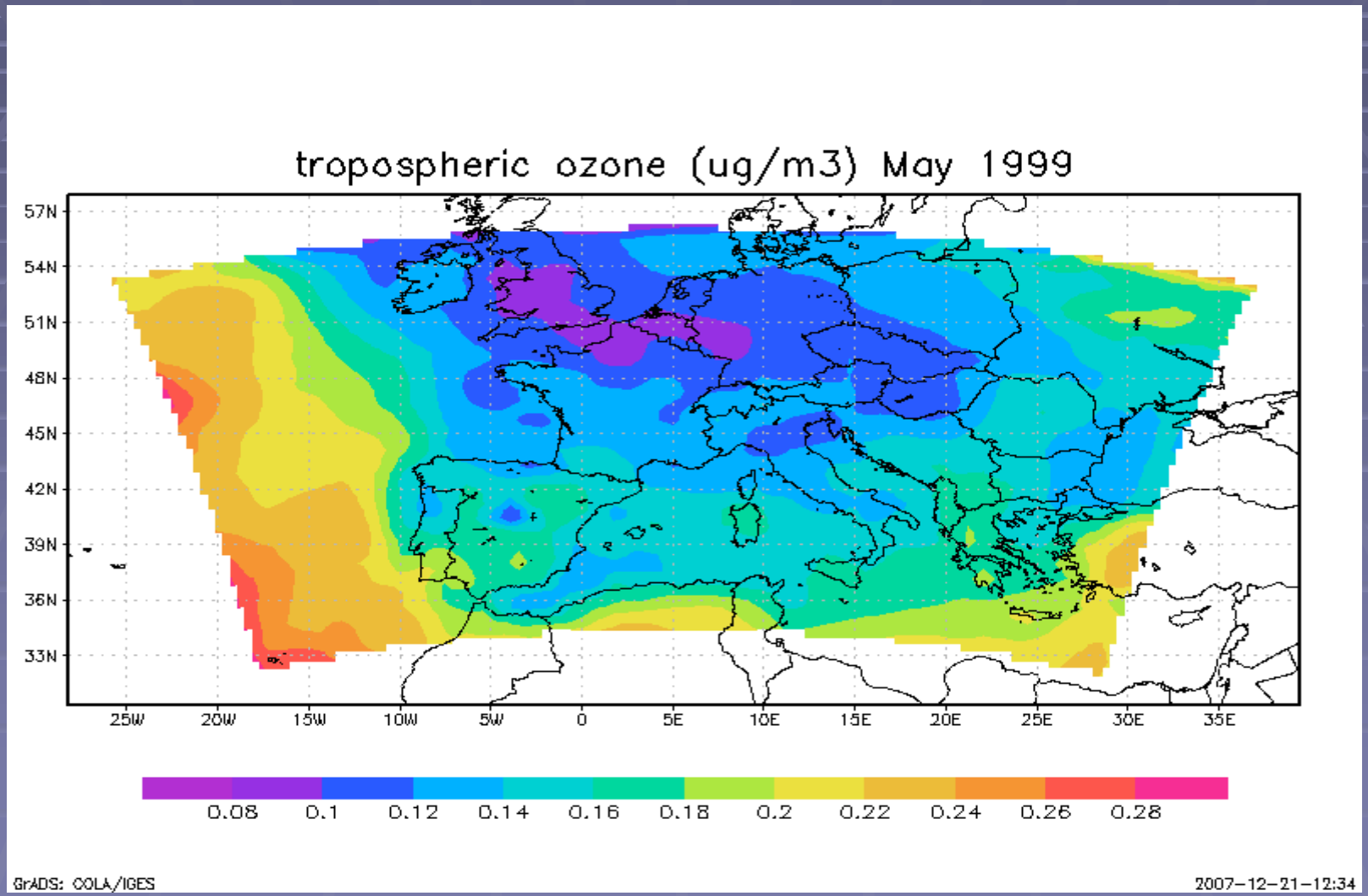


# Number of advected Species (10)

regcm.in

- Sulfur dioxide (SO2)
- Nitrogen dioxide (NO2)
- DMS
- HCHO
- Ozone (O3)
- Sulfuric acid (H2SO4(g))
- Nitric Acid (HNO3(g))
- MSA
- OH
- H2O2

# O3 production



# *References*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2. Shell, B., I.J. Achermann, H. Hass, F. S. Binkowski, A. Ebel, 2001: Modeling the formation of secondary organic aerosol within a comprehensive air quality model system

# *Reference con.*


3. Rahul A. Zaveri, Richard C. Easter, and Leonard K. Peters, A comutationally efficient Multicomponents Equilibrium Solver for Aerosols (MESA), 2005 *JGR* vol. 110, D24203

4- Binkowski, Francis S., and Uma Shankar, The Regional Particulate Matter Model

1-Model description and Preliminary results. 1995, *JGR* vol. 100, 26191-26209

# *Reference con.*

5- Sandu, A., R. Sander, Technical note: simulating chemical systems in Fortratn90 and Matlab with the Kinetic PreProcessor KPP-2.1, 2006, Atmos. Chem. Phys., 6 187-195

6-Stockwell, W., Middleton, P., Chang, S., The Second Generation Regional Acid Deposition Model Chemical Mechanism for Regional Air Quality Modeling. 1990 *JGR* vol. 95 16343-16367.

# *Reference con.*

7-Zaveri, R., L., Peters, A new lumped structure photochemical mechanism for large-scale applications. 1999, *JGR* vol.104, 30387-30415

# THANK YOU