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Implementation of gas-phase chemistry within RegCM

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Implementation of Gas-Phase chemistry in RegCM

(Climate-Chemistry Interaction, CCI)

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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

Gas-phase chemistry
- \( \text{NO}_2 + h\nu \rightarrow \text{O}_3 \)
- \( \text{O}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{O}_2 \)
- \( \text{H}_2\text{O} + \text{NO}_2 \rightarrow \text{HNO}_3 \)

Meteorological transport

Transport

Cloud processes
- Aqueous chemistry
  - \( \text{H}_2\text{O}_2 + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 \)

Wet deposition

Dry deposition

Environment

Emissions
- \( \text{NO}_x \)

Hydrocarbons

Biogenic compounds

Earth System Physics, The Abdus Salam International Centre for Theoretical Physics
Air Quality
Forcing
Climate
Emissions
Forcing
Boundary Layer Processes and Chemical Transformations
Chemical Transformations
Connections
Impacts
Feedbacks
Processes
Mitigation
Scales

Local/urban ~1-10^2 km
Regional ~10^3 km
Global ~10^4 km

Megacities
Air Quality
Climate

Days - weeks
Years - decades

1 s - 1 hr
Timescales of ozone chemistry

Global chemistry. Dominated by \( \text{NO}_x + \text{CH}_4 + \text{sunlight} \). 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 \( \sim \)500 km.

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

\[
\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2
\]
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

Dynamics
Radiation

Chemistry
Photolysis

Tagging:
diagnostical
chemistry
scheme

All feedbacks included

No feedbacks

Earth System Physics, The Abdus Salam International Centre for Theoretical Physics
Models and future scenario

**Anthropogenic emissions (IPCC A1B scenario)**

- MOZART4 (Chem. BC)
- ECHAM5 (Met. BC)

**RegCM-Chem**
- Detailed ozone-NOx-VOC-aerosol chemistry

**GHG**
- Radiative forcing

**Climate Change**
- Global Emissions

**Air pollutants & their precursors**
- Natural emissions
- Chemistry, transport, deposition, etc

**Regional Climate/Chemistry interaction (RCCI)**

*Earth System Physics, The Abdus Salam International Centre for Theoretical Physics*
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

Reading Emissions

- emiss_opt=1
  - MAGEDN
    - Biogenic Emission
  - Add Anthropogenic

- emiss_opt=2
  - EM_ENV
Photolysis Driver

Phot_opt=1

Look_up_table

Phot_opt=2

Fast J

chem_opt=3
or 4

Geos-CHEM
Condensed

CBM-Z
Condensed

chem_opt=5

KPP

CBM-Z, Geos-CHEM, RACM,
RADM2, CBM-xx,
## Emissions Inventories

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Description</th>
<th>Time Period</th>
<th>Resolution</th>
<th>Frequency</th>
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</thead>
<tbody>
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<td>RETRO</td>
<td>Biomass burning and anthropogenic</td>
<td>1960-2000</td>
<td>0.5° X 0.5°</td>
<td>monthly</td>
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<tr>
<td>POET</td>
<td>Biomass burning, anthropogenic and biogenic</td>
<td>1990-2000</td>
<td>1° X 1°</td>
<td>annually</td>
</tr>
<tr>
<td>EDGAR</td>
<td>Biomass burning, anthropogenic and biogenic</td>
<td>2000</td>
<td>1° X 1°</td>
<td>annually</td>
</tr>
<tr>
<td>GFED v2</td>
<td>Biomass burning</td>
<td>1995-2005</td>
<td>1° X 1°</td>
<td>annually</td>
</tr>
</tbody>
</table>
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 is 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
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).
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°C in SE England.
- How frequent will such summers be in the future?
<table>
<thead>
<tr>
<th></th>
<th>KPP_CBMZ (by KPP)</th>
<th>KPP_GEOS (by KPP)</th>
<th>Updated-GEOS (by sanford sillman)</th>
<th>KPP_RACM (by KPP)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NO. of Species</strong></td>
<td>58</td>
<td>175</td>
<td>175</td>
<td>75</td>
</tr>
<tr>
<td><strong>No. of Reaction</strong></td>
<td>134</td>
<td>533</td>
<td>533</td>
<td>237</td>
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<tr>
<td><strong>Solvers</strong></td>
<td>Rosenbrock</td>
<td>Rosenbrock</td>
<td>Radical balance solver</td>
<td>Rosenbrock</td>
</tr>
<tr>
<td><strong>Lumping Technique</strong></td>
<td>Lumped structure</td>
<td>Lumped molecule</td>
<td>Lumped molecule</td>
<td>Lumped molecule</td>
</tr>
<tr>
<td><strong>No. of Transported species</strong></td>
<td>19</td>
<td>19</td>
<td>19</td>
<td>19</td>
</tr>
</tbody>
</table>
Daily Average for 88 stations

[Graph showing daily average for 88 stations with legends for different data sets: Observation, SILL, KFP_SESE, KFP_SEME]
Daily Maximum averaged over 88 stations
CPU time
Model vs. Observation stations
Effects of clouds on ozone and photolysis
cross section for cloud fraction at noon
O3 Cross-sec (ppb) [ (with-without) cloud ] at noon
NO2 → O3P photolysis diff(with−without)cloud at noon
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.
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

**Meteorology**
- Transport
  - Advection: Bott/Easter
  - Vertical Turbulent Mixing
  - Convective Cloud Mixing: Walcek-Taylor/Berkowitz

**Emission**
- GAS Phase Chemistry (Rate constants NASA, 1997)
  - $\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4$
  - $\text{DMS} + \text{OH} \rightarrow \text{DMS}$ chem Yin/Seinfeld
  - $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2$ (limited by Mozart)

**Oxidant**
- AQUEOUS Phase Chemistry
  - $\text{SO}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{SO}_4$ Schwartz
  - $\text{SO}_2 + \text{O}_3 \rightarrow \text{H}_2\text{SO}_4$

- IN CLOUD Activation:
  - Proportional to LWVF, max 0.5

- DRY DEPOSITION
  - Time, location dependent: Wesely

- WET DEPOSITION
  - Exponential decay in cloud

Flow:
- SO2
- SO4
- DMS
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 parameterisation**:
  - Cumulus – Groll (1993)
  - Radiation – CCM3 (Kiehl et al. 1996)
  - PBL – Holtag et al. (1990)
  - Dust module – Zakov et al. (2006)
Sulfur Dioxide mass load (burden)  mg/m2
Sulfate mass load (burden)  mg/m²

SO₄²⁻ mass burden (mg/m²) 2000–2006  DJF

SO₄²⁻ mass burden (mg/m²) 2000–2006  MAM

SO₄²⁻ mass burden (mg/m²) 2000–2006  JJA

SO₄²⁻ mass burden (mg/m²) 2000–2006  SON
DMS mass load (burden)  mg/m²
DMS Contribution to Sulfate aerosols
Climate feedback
Top-Atmosphere Radiative Forcing W/m²
Surface Radiative Forcing W/m²
• Thank you for your attention