ECHMERIT
an online coupled Hg model

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ECHMERIT - structure

ECHMERIT
ECH – ECHAM5
MER – MERCURY
IT – ITALY
Modelling Concept

GCM: Meteorology & Transport

CBM-z & Hg-chemistry
Fast-J photolysis
emissions & deposition & ...

benefits from on-line coupling:

=> higher temporally resolved meteorology
=> higher level of consistency (grid, resolution, transport scheme, ...)
=> no interpolation needed

meteorological variables, etc.
chemical species concentrations
Simulated processes

- Aqueous phase chemistry
- Gas phase chemistry
- Transport processes
- Wet deposition
- Dry deposition
- Ocean emission
- Soil and biosphere emission
- Anthropogenic emissions
### State-of-the-art models

<table>
<thead>
<tr>
<th>Model</th>
<th>Area</th>
<th>Meteo</th>
<th>Horizontal Resolution</th>
<th>Vertical Resolution</th>
<th>Gas/Aqueous</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEHM</td>
<td>hem</td>
<td>offline</td>
<td>2.5x2.5 degrees</td>
<td>20</td>
<td>gas</td>
</tr>
<tr>
<td>MSCE-HM-Hem</td>
<td>hem</td>
<td>offline</td>
<td>2.5x2.5 degrees</td>
<td>8</td>
<td>both</td>
</tr>
<tr>
<td>CTM-Hg</td>
<td>glob</td>
<td>offline</td>
<td>8x5 degrees</td>
<td>9</td>
<td>both</td>
</tr>
<tr>
<td>GEOS-chem</td>
<td>glob</td>
<td>offline</td>
<td>4x5 degrees</td>
<td>30</td>
<td>both</td>
</tr>
<tr>
<td>GRAHM</td>
<td>glob</td>
<td>online</td>
<td>variable grid</td>
<td></td>
<td>gas</td>
</tr>
<tr>
<td>ECHMERIT</td>
<td>glob</td>
<td>online</td>
<td>flexible (T21-T163)</td>
<td>19 or 31</td>
<td>both</td>
</tr>
</tbody>
</table>

**major reactants (in gas and/or aqueous phase)**

<table>
<thead>
<tr>
<th>Model</th>
<th>Reactants</th>
<th>Source</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEHM</td>
<td>O$_3$,SO$_2$,Cl$^-$</td>
<td>offline calculation/constant</td>
<td>Christensen et al, 2003</td>
</tr>
<tr>
<td>MSCE-HM-Hem</td>
<td>OH$_3$,O$_3$,Cl$_2$,Cl,SO$_3$</td>
<td>monthly means (MM)</td>
<td>Travnikov, 2005</td>
</tr>
<tr>
<td>CTM-Hg</td>
<td>OH,$_3$O,H$_2$O$_2$,HOCI,OH$^-$,SO$_3$,HCl,Cl$_2$,Br,BrO</td>
<td>offline calculation/observed (MM)</td>
<td>Seigneur et al., 2001,2004</td>
</tr>
<tr>
<td>GEOS-chem</td>
<td>OH,O$_3$</td>
<td>offline calculation (MM)</td>
<td>Bey et al., 2001</td>
</tr>
<tr>
<td>GRAHM</td>
<td>O$_3$,OH,Br,BrO,Br$_2$,Cl$_2$,Cl</td>
<td>offline calculation/observed (MM)</td>
<td>Dastoor&amp;Larocque, 2004</td>
</tr>
<tr>
<td>ECHMERIT</td>
<td>O$_3$,OH,H$_2$O$_2$,Br,Br$_2$,Cl,$_2$Cl,HOCl,HOCl$^-$,(SO$_3$)$_2$,Cl$^-$</td>
<td>online calculation</td>
<td>Jung et al., in preparation</td>
</tr>
</tbody>
</table>
Latest Model Improvements

- Strictly sequential operator splitting of emission, advection, convection, chemistry and deposition
- Mass conserving convective mass flux correction => To avoid negative tracer concentrations that occur in ECHAM5 transport scheme in regions with strong gradients (source regions, lowest model layers)
- New chemical solver (SEULEX more stable than Rosenbrock2)
Model Changes

- Online calculated emissions (soil, vegetation) at the moment not activated => need further testing

- => Biomass burning emission, ocean emissions, biosphere and soil emissions mapped to CO emissions
Model setup

- Horizontal resolution: T42 (2.81 degrees)
- Vertical resolution: 19 layers
- Lower boundary: AMIP monthly mean SST
- ECMWF reanalysis data for nudging of meteorological fields
Emissions input

=> POET Emissions (1°x1°)
(http://www.aero.jussieu.fr/projet/ACCENT/POET.php)

=> Hg Emissions: AMAP (1°x1°)
http://www.amap.no/

=> GEIA Emissions (SO₂)
(http://www.geiacenter.org/)

Hg₀ emissions [Mg/m²/year]
Emissions input

Ocean and biosphere/soil emissions
=> scaled with CO emissions (POET)
=> annual sum: 3000 tons (ocean), 1669 tons (biosphere&soils)

=> overestimation of emissions in southern hemisphere
underestimation in northern hemisphere
=> representative annual global emission sum
Emissions input

Biomass burning emissions
=> scaled with CO emissions (POET)
=> annual sum: 675 tons

=> overestimation of emissions in southern hemisphere
underestimation in northern hemisphere
=> representative annual global emission sum
Model evaluation

dry deposition velocities [cm/s]
up: SO2
down left: O3
down right: HgO
Model evaluation

Ozone concentration [ppb] compared to EMEP stations

February 2001

Eskaldemuir, UK

Vreedepeel, Netherlands

Frederiksborg, Denmark
Model evaluation

Ozone concentration [ppb] compared to EMEP stations

July 2001

Bassum, Germany

Topolniky, Slovakia

C.N.R. Institute for Atmospheric Pollution, Division of Rende, Italy
http://www.cs.iia.cnr.it/
Model evaluation

Ozone concentration [ppb] compared to EMEP stations (monthly means)

=> good performance in mid-latitudes
=> improvements needed in polar regions
Model evaluation

Work in progress: analysis and validation of ozone vertical profiles!
Model Evaluation - Ozone

Seasonal surface ozone [ppb]

DJF

MAM

JJA

SON
Model evaluation

=> ozone: underestimated in winter, overestimated in summer
=> TGM: underestimated in all seasons except of summer
Model evaluation - TGM

TGM [ppq] in surface layer:
right: annual mean
down left: JJA
down right: SON

http://www.cs.iia.cnr.it/
Model evaluation

wet & dry deposition [ng/m²]

Annual precipitation [mm]
Open Question – problems in global mercury chemistry modelling
While regional and hemispherical models are to an extent constrained by boundary conditions, which facilitate maintaining the modelled Hg concentration field over the domain, global models require a balance between emission and deposition in order to reproduce measurements, (scarce though they are).
Deposition vs. Emission

Therefore the emissions databases are required to be accurate (there is some debate about the quality of available emissions databases), as are the processes which promote Hg deposition, namely atmospheric oxidation (over which there is also much debate).
Rapid re-emission

Within a number of global models an empirical rapid re-emission of deposited Hg is invoked which is proportional to the deposition flux. This is likely to be a reflection of a real process, as emissions from soil after precipitation have been observed to increase. However it is a process which is not understood and for which there is no theory to relate emission strength to model parameters.
Constraining models

The most important requirement to improve model validation and reduce model uncertainty is a much wider network of Hg monitoring sites, especially in the southern hemisphere. This is being addressed to an extent by GEO task (HE-0902d).

“The GEO Sub-Task for Global Monitoring Plan for Atmospheric Mercury aims to develop a global monitoring network for mercury by harmonizing standard operating procedures for monitoring mercury and its compounds in air, atmospheric deposition, water, soil, sediments, vegetation and biota.”
Still mercury-chemistry reactions taking place in the global atmosphere are not even doubtlessly known.
How to work on this problem?
Box model experiments

Sensitivity testing for:
- Meteorological input
- Rate constants
- Chemical schemes
- Time stepping
- ...

Much less computer power demand than full 3-d simulations.
1 box model run vs. 150.784 box model runs per time step in ECHMERIT (2.5°, 19 layers)
3D-sensitivity experiments

Hg$^0$ concentration [ppq] using Hg+O$_3$ reaction rate constant of Pal and Ariya (2004) and reaction with OH
3D-sensitivity experiments

Hg+O₃ reaction rate constant of Hall (1995), without oxidation with OH
versus
Hg+O₃ reaction rate constant of Pal & Ariya (2004), with oxidation with OH

Difference [ppq] in Hg⁰ concentrations
March 2001, after 3 months simulation
linked to O₃ and surface temperature pattern
3D-Sensitivity experiments

**with OH reaction versus without OH reaction**

both: Hg+O$_3$ reaction rate constant of Hall (1995)

Difference [ppq] in Hg$^0$ concentrations

March 2001 after 3 months simulation

linked to maximum OH concentration patterns
Conclusions & Outlook

- first evaluation of ECHMERIT successful

ongoing work:
- extensive model validation
- improvement of biosphere and ocean emissions
- further Hg chemistry sensitivity studies
- testing different chemistry schemes (also box model studies)
- full-chemistry HTAP experiments
- inclusion of bromine species (Br/BrO climatology?)

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Thanks!

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