

Modelling atmospheric chemistry with the CAABA/MECCA box model

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CAABA/MECCA workshop
Mainz

Agenda

- **PART I: THEORY**

- General Introduction to CAABA/MECCA
- Running CAABA/MECCA: A demonstration

- **BREAK**

- **PART II: PRACTICE**

- The virtual machine
- Running the model
- Plotting the results
- Performing sensitivity studies
- Adapting the model to your project

Introduction

- Many atmospheric chemistry models have been developed in the past decades.
- Models vary strongly in complexity and efficiency.
- Each aimed at a particular goal, e.g. tropospheric or stratospheric chemistry. . .
- Often no clear separation between meteorological and chemical part of the model.
- When merging different chemistry mechanisms, often incompatibilities between codes occur.
- MESSy contains the comprehensive and flexible atmospheric chemistry module

MECCA

(Module Efficiently Calculating the Chemistry of the Atmosphere).

MECCA Chemistry

- 699 gas phase species:
 - 1789 reactions
 - 384 photolysis reactions
- 89 aqueous phase species:
 - 145 reactions
 - 47 gas-aqueous mass transfer reactions
 - 34 acid/base and other equilibria
- Basic O_3 , CH_4 , HO_x , and NO_x chemistry
- Tropospheric halogen (Cl, Br, I) and sulfur (S) chemistry from Sander and Crutzen (1996) and von Glasow et al. (2002)
- Tropospheric non-methane hydrocarbon (NMHC) chemistry and MOM isoprene/terpene mechanism (Taraborrelli et al., 2009)
- Stratospheric chemistry based on the model of Steil et al. (1998) and the Mainz Chemical Box Model (Meilinger, 2000)
- Rate coefficients updated according to recent JPL and IUPAC recommendations

MECCA Chemistry

- Only one master file (gas.eqn) for all gas-phase reactions, e.g.:
 $\text{O}_2 + \text{O} = \text{O}_3 : \{ \% \text{UpStTrG} \}$
 $3.3\text{E-}11 \{ \S 1.1 \} * \text{EXP}(55./\text{temp}) ; \{ \& 3245 \}$

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 - Up = upper atmosphere
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MECCA Chemistry

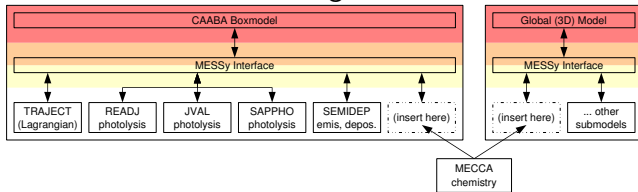
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- Reference information: 3245 = JPL recommendation (2015)

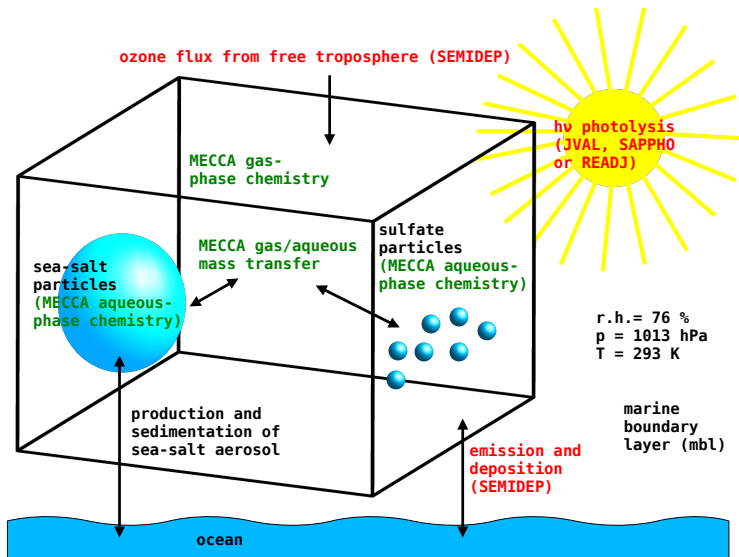
CAABA/MECCA Modularity

- Very modular structure (MESSy standard by Jöckel et al. (2005))
- Link to different meteorological base models



- CAABA = Chemistry As A Boxmodel Application
- Extensive testing in a box model
- Develop parameterization
- Run parameterization in global model runs

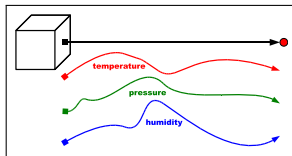
The CAABA Box Model



Box Model Modes

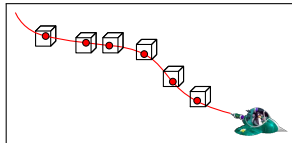
Box mode:

- static: constant T , p , rh
- dynamic: Lagrangian along trajectory, variable T , p , rh



Steady-state mode:

- initialize with measured long-lived species
- let short-lived species (e.g., OH, HO₂) run into steady state conditions
- multirun: one run for each measured data point

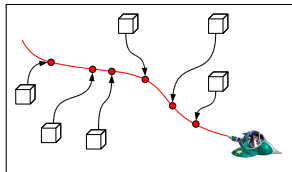


Trajectory mode:

- initialize with data from global model
- model runs along trajectory
- multirun: one run for each measured data point

Monte-Carlo mode:

- variation of rate coefficients



Namelist

- Control the behaviour of a CAABA/MECCA model run:
 - temperature, pressure, humidity
 - model start and duration
 - output interval
 - select submodels (MECCA, JVAL, SEMIDEP, TRAJECT, ...)
 - scenarios
 - steady-state stop?
 - trajectory file?
- Default: use the same namelist as last time
- For testing: `caaba_simple.nml`

Scenarios

- describe boundary conditions:
 - photolysis
 - initialization
 - emission
 - dry deposition
- available scenarios:
 - **MBL, OOMPH:** MBL chemistry
 - **FF_ANTARCTIC, FF_ARCTIC:** frost flowers and polar ODEs
 - **FREE_TROP, HOOVER:** free troposphere
 - **STRATO, MTCHEM:** stratosphere and above
 - **LAB, LAB_C15:** laboratory conditions (reaction chamber)
 - **MIM2:** for isoprene chemistry (Taraborrelli et al., 2009)
 - **???:** add your own...
- select your scenario in namelist file

Further Information

- Web page:
<http://www.mecca.messy-interface.org>
- CAABA/MECCA model description paper:
Sander et al. (2011), GMD, 4, 373-380
<http://www.geosci-model-dev.net/4/373>
- User manual:
[manual/caaba_mecca_manual.pdf](#)
- GPL License

NEXT:

On-screen demo of model run

- Jöckel, P., Sander, R., Kerkweg, A., Tost, H., and Lelieveld, J.: Technical Note: The Modular Earth Submodel System (MESSy) – a new approach towards Earth System Modeling, *Atmos. Chem. Phys.*, 5, 433–444, <http://www.atmos-chem-phys.net/5/433>, 2005.
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- Steil, B., Dameris, M., Brühl, C., Crutzen, P. J., Grewe, V., Ponater, M., and Sausen, R.: Development of a chemistry module for GCMs: First results of a multiannual integration, *Ann. Geophys.*, 16, 205–228, 1998.
- Taraborrelli, D., Lawrence, M. G., Butler, T. M., Sander, R., and Lelieveld, J.: Mainz Isoprene Mechanism 2 (MIM2): an isoprene oxidation mechanism for regional and global atmospheric modelling, *Atmos. Chem. Phys.*, 9, 2751–2777, <http://www.atmos-chem-phys.net/9/2751>, 2009.
- von Glasow, R., Sander, R., Bott, A., and Crutzen, P. J.: Modeling halogen chemistry in the marine boundary layer, 1. Cloud-free MBL, *J. Geophys. Res.*, 107D, 4341, doi:10.1029/2001JD000942, 2002.