Modelling atmospheric chemistry with the CAABA/MECCA box model

Rolf Sander

Max-Planck Institute for Chemistry, Mainz, Germany

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Agenda

- PART I: THEORY
  - General Introduction to CAABA/MECCA
  - Running CAABA/MECCA: A demonstration
- LUNCH 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).

Model Description: MECCA Chemistry

- Comprehensive set of chemical reactions:
  - Gas phase: 204 species and 409 reactions
  - Aqueous phase: 89 species and 147 reactions
- Numerical integration via the KPP program (Sandu and Sander, 2006)
- 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 including Mainz Isoprene Mechanism 2 (MIM2) from Taraborrelli et al. (2009)
- Possibility to add reactions from Master chemical mechanism (MCM), Saunders et al. (1997)
- 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

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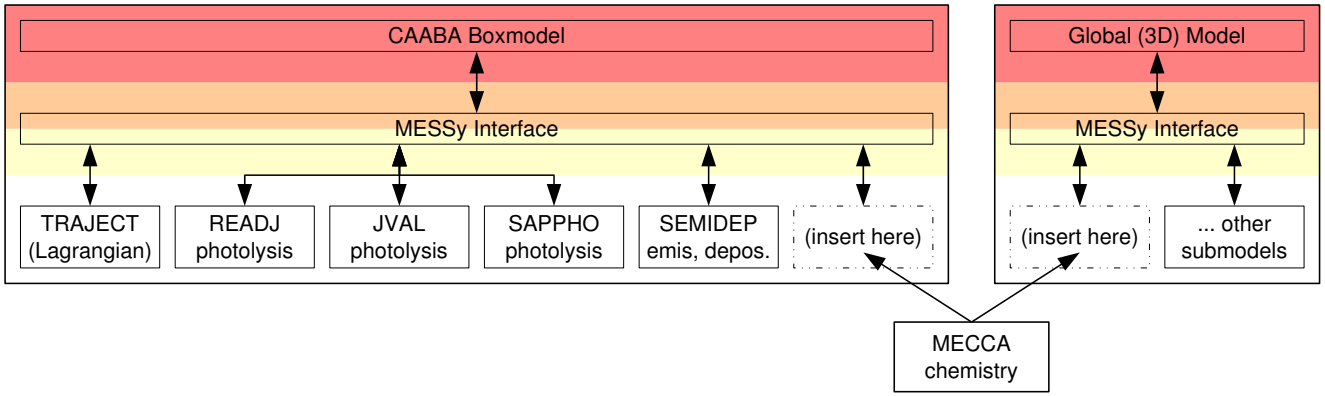
- Reference information: 2626 = JPL recommendation (2011)

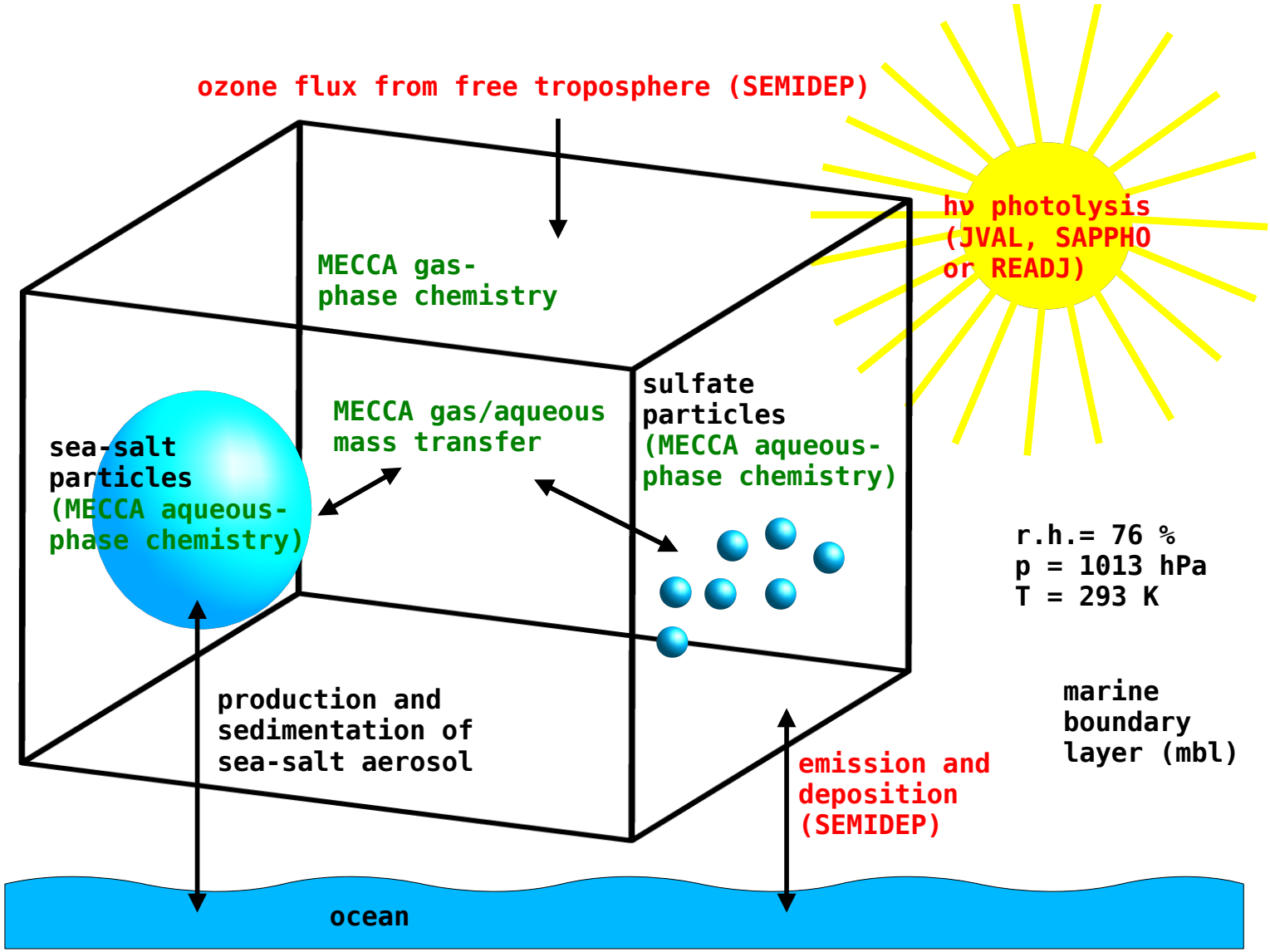
Model Description: CAABA/MECCA Modularity

- 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

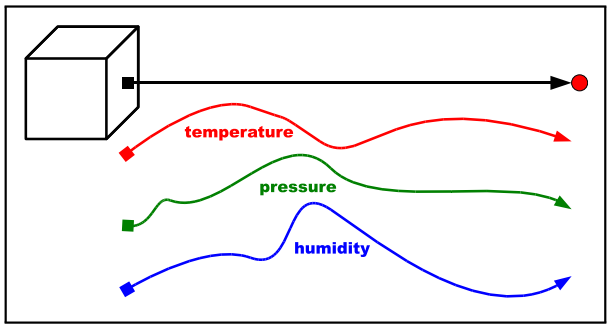
Model Description: The CAABA Box Model



Model Description: Box Model Modes

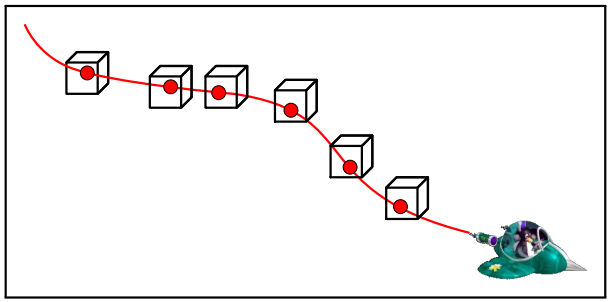
Box mode:

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



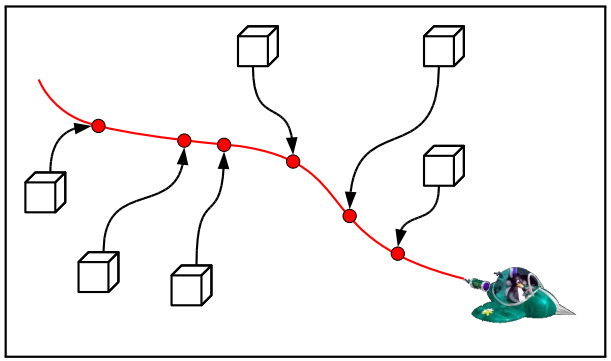
Steady-state mode:

- initialize with measured long-lived species
- let model run into steady state conditions
- one model run for each measured data point



Trajectory mode:

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



Monte-Carlo mode:

- variation of rate coefficients

Namelists

- 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

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- Make code additions available (which can eventually be incorporated into main CAABA/MECCA code)

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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