**Geoscientific
Model Development
Discussions**

The atmospheric chemistry box model CAABA/MECCA-3.0gmdd

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Abstract

We present version 3.0gmdd of the atmospheric chemistry box model CAABA/MECCA. In addition to a complete update of the rate coefficients to the most recent recommendations, a number of new features have been added: chemistry in multiple aerosol size bins; automatic multiple simulations reaching steady-state conditions; Monte-Carlo simulations with randomly varied rate coefficients within their experimental uncertainties; calculations along Lagrangian trajectories; mercury chemistry; more detailed isoprene chemistry; tagging of isotopically labeled species. Further changes have been implemented to make the code more user-friendly and to facilitate the analysis of the model results. Like earlier versions, CAABA/MECCA-3.0gmdd is a community model published under the GNU General Public License (GPL).

1 Introduction

In a previous publication by Sander et al. (2005), we presented the multi-purpose atmospheric chemistry model MECCA (Module Efficiently Calculating the Chemistry of the Atmosphere). Since its release, the code development has branched with different modelers adding and using different new features (Stickler et al., 2006; Xie et al., 2008; Taraborrelli et al., 2009; Riede et al., 2009; Keene et al., 2009; Gromov et al., 2010; Kubistin et al., 2010). We have now merged these additions into the most recent model version and make the revised code available to the research community. This code merger also makes it possible to combine model features that were previously only available in different branches of the development.

The code has a modular structure with the chemistry part strictly separated from box-model specific calculations. Unfortunately, the name MECCA has been used in the past for both the box model as well as for the chemistry mechanism. This led to confusion because the MECCA chemistry can not only be used in a box model but also in global models (e.g., Jöckel et al., 2010). For clarity, the box model is now called

CAABA (Chemistry As A Boxmodel Application). The relation of CAABA to MECCA is illustrated in Fig. 1. When referring to the combination of the CAABA box model with MECCA chemistry, the term "CAABA/MECCA" is used. In Sect. 2 we decribe the CAABA box model, and in Sect. 3 we show features recently added to the MECCA chemistry code.

Like earlier versions, CAABA/MECCA-3.0gmdd[1] is a community model published under the GNU General Public License (GPL, http://www.gnu.org/copyleft/gpl.html). The model code can be found in the electronic supplement. In addition to the complete code, a list of chemical reactions (including rate coefficients and references) and a user manual are available in the manual/ directory of the supplement. For further information and updates, the MECCA web page at http://www.mecca.messy-interface.org should be consulted.

2 CAABA model description

2.1 Main features

In the base configuration, CAABA represents an air parcel (i.e., a box) in the marine boundary layer, as shown schematically in Fig. 2. In addition to chemical reactions, the model calculates entrainment, emission, deposition, and the photolysis of chemical species. These processes are coded as individual submodels, which are connected to CAABA via the Modular Earth Submodel System (MESSy) interface by Jöckel et al. (2005), as shown in Fig. 1.

Exchange with air masses outside of the box (entrainment, emission, detrainment, deposition) is calculated by the submodel SEMIDEP (simplified emission and deposition). For box model calculations, there is no difference between entrainment

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[1]The name of this version indicates that it is used for the interactive discussion in GMDD. If necessary, bug fixes can still be made. We plan to release the final version CAABA/MECCA-3.0 together with the final paper in GMD.

from above and emissions from below. Thus these processes can be treated in the same way. Assuming a well-mixed marine boundary layer of height z_{mbl} (cm), the change in concentration Δc ($cm^{-3} s^{-1}$) can be calculated from the emission (or entrainment) flux J_e ($cm^{-2} s^{-1}$) as:

$$\Delta c = J_e / z_{mbl} \tag{1}$$

The concentration change Δc due to deposition depends on the concentration c (cm^{-3}) and the deposition velocity v_d ($cm\,s^{-1}$):

$$\Delta c = c \cdot v_d / z_{mbl} \tag{2}$$

CAABA contains 3 submodels which can provide rate coefficients J (s^{-1}) for photolytical reactions (also called "J-values"):

- The submodel SAPPHO (simplified and parameterized photolysis rates) provides a simple function:

$$J = a \cdot \exp\left(\frac{-b}{\cos\vartheta + c}\right) \tag{3}$$

Here, ϑ is the solar zenith angle. The three parameters a (s^{-1}), b (dimensionless), and c (dimensionless) are defined for each photolysis reaction. This method has also been used in previous model versions.

- The submodel JVAL calculates J-values using the method of Landgraf and Crutzen (1998). Its implementation into the MESSy system will be described in a separate publication (Sander et al., 2011).

- Finally, the submodel READJ reads J-values from a file. This option is useful for either applying measured J-values, or offline-calculated J-values obtained from another model.

2.2 Multiple simulations and the steady-state mode

In the base configuration, CAABA/MECCA calculates the temporal evolution of the chemistry inside an air parcel. This is ideal for sensitivity studies analyzing the effect of individual reactions inside a large chemical mechanism. To make measurements that can be compared directly with these model results, it would be necessary to follow an air parcel, e.g. by attaching instruments to a balloon that is drifting with the wind. Often, however, measurements during a campaign consist of data originating from different air masses. To allow a comparison of these measurements with model results, we have added two features to CAABA. The first is the "steady-state mode", which automatically terminates a simulation when a selected species reaches steady-state, i.e. when its concentration change is less than a user-defined threshold. A useful application of this mode is to fix the physical boundary conditions and the concentrations of long-lived species (e.g., alkanes, alkenes) to their measured values and then calculate steady-state values of short-lived species (e.g., OH, HO_2). A comparison of the simulated short-lived species to their measured values yields insight how well our understanding of the complex reaction mechanism is. Since this approach requires one simulation for each data set measured at a given time, a second feature has been added to CAABA: multiple simulations. Here, the code loops over measured data sets. For each data set, it first reads input data for the simulation (measured concentrations and offline-calculated photolysis rate coefficients), and then starts a CAABA simulation which terminates when a steady state is reached. This is illustrated in Fig. 3a where a box simulation is made for each data set of air-borne measurements. This approach, which had already been implemented in previous model versions (de Reus et al., 2005; Stickler et al., 2006; Kubistin et al., 2010), is now available officially in the current version of CAABA. Although it usually makes sense to combine multiple simulations with the steady-state mode, each of them could also be used independently.

2.3 Lagrangian trajectories

With the submodel TRAJECT by Riede et al. (2009), CAABA can simulate atmospheric chemistry along pre-calculated Lagrangian trajectories. In contrast to the steady-state mode (Sect. 2.2) with fixed physical boundary conditions for each simulation,
₅ TRAJECT varies longitude, latitude, pressure, temperature, relative humidity, and optionally radiation with time during the simulation along each trajectory (Fig. 3b). Exchange with surrounding air masses (mixing) is currently not considered in CAABA/TRAJECT.

In addition to the general functionality of a trajectory-box model, CAABA/TRAJECT
₁₀ simulations also offer a method to analyse results from global models. For that purpose, the trajectory-box model can be configured for maximum consistency with the global model, i.e., trajectories are based on the global model wind fields and the same chemical mechanism is chosen. When comparing the trajectory-box model output to the global model results along the trajectories, any deviation can then be attributed to
₁₅ mixing during trajectory travel time (and subsequent chemistry). Consequently, it is possible to separate and quantify the contributions of transport, mixing and chemistry onto the concentrations of chemical species in the global model, as described in detail by Riede et al. (2009).

2.4 Stratospheric model simulations

₂₀ The chemistry mechanism contains reactions for all levels of the atmosphere, including the stratosphere and mesosphere. These are routinely used when MECCA is coupled to a global 3-D model (e.g., Jöckel et al., 2006). The CAABA/MECCA box model, however, has almost exclusively been used for simulations focusing on the lower troposphere. As a new feature, CAABA now offers an easy way to switch to
₂₅ a stratospheric scenario. Here, the chemistry is initialized with values typical for 20 hPa. Photolysis rate coefficients are calculated in the JVAL submodel, based on the vertical profiles of ozone, water vapor, pressure and temperature. These profiles have been

updated and extended up to a level of 1 Pa (≈80 km altitude) using results from Jöckel et al. (2006). An application of CAABA/MECCA in the stratosphere and mesosphere has recently been presented by Baumgaertner et al. (2010).

2.5 Executing CAABA on a virtual machine

The CAABA/MECCA software has been written for UNIX/Linux operating systems, it does not run natively under MS-Windows. However, it is now possible to run the model inside a virtual Ubuntu Linux machine with the VMware Player software. After the model has run on the virtual Linux machine, the user can access the output under Windows and analyse it there. Information how to obtain the code on a virtual machine is given on the MECCA web page at http://www.mecca.messy-interface.org.

3 MECCA model description

3.1 Multiple aerosol size bins

Previous versions of MECCA were able to calculate aerosol chemistry in one or two size bins. Modeling the marine boundary layer, these were normally assigned to a submicrometer sulfate mode and a supermicrometer sea-salt mode, respectively. Considering the high demand of CPU time for aqueous-phase chemistry, this is already at the limit of complexity for global models (e.g., Kerkweg et al., 2008). However, to study the interaction of gas-phase chemistry with aqueous-phase chemistry in aerosols of different sizes in detail, more than just two aerosol bins are required. To achieve this, we now allow up to 99 aerosol size bins in MECCA. Each size bin is described by its radius (m) and its liquid water content ($m^3 m^{-3}$). These two parameters determine the number concentration of each bin (m^{-3}) in the box model. A lifetime is assigned to each size bin, representing the (size-dependent) loss of particles via sedimentation and dry deposition. Assuming that aerosol production and loss are in steady state, an appropriate production term keeps the aerosol concentration constant during the simulation. Each size bin can be initialized with an individual primary composition

of cations (NH_4^+) and anions (SO_4^{2-}, HSO_4^-, Cl^-, Br^-, I^-, IO_3^-, HCO_3^-). If there is a difference between the amount of cations and anions, it is assumed to consist of chemically inert ions, e.g., Na^+ for sea salt. Transfer between the gas phase and each aerosol size bin is calculated using the mass transfer coefficient k_{mt} (Schwartz, 1986; Sander, 1999). Although there are no direct reactions between aqueous-phase species in different aerosol bins, they are coupled indirectly because they all interact with the same gas phase. MECCA with multiple aerosol size bins has been used recently for a comparison to ship-borne measurements of marine aerosol with a 6-stage cascade impactor (Keene et al., 2009).

3.2 Monte-Carlo simulations

The value of each rate coefficient in the chemical mechanism is associated with an uncertainty. Monte-Carlo simulations are an efficient method to analyse how the model results depend on these uncertainties. A MECCA Monte-Carlo simulation is an ensemble of simulations, each with slightly and randomly varied rate coefficients. The range of model results can be related to the range of the varied input parameters. Such an analysis has been performed with a previous MECCA version by Kubistin et al. (2010) to study the effect of kinetic uncertainties on the production of OH radicals. As another example, Fig. 4 shows how O_3 changes when rate coefficients are varied.

In a MECCA Monte-Carlo simulation, the recommended values of the rate coefficients are varied according to:

$$k_{mc} = k_{rec} \times 10^{(z\,\Delta\log k)} \tag{4}$$

where k_{mc} is the rate coefficient used in the Monte-Carlo simulation, and k_{rec} is the recommended rate coefficient. The measurement uncertainty is given by $\Delta\log k$, and z is a normally-distributed random number centered around zero. $\Delta\log k$ can be taken from data compilations, e.g. Atkinson et al. (2004, 2006, 2007). If it is not known, a value of $\Delta\log k = 0.1$ is assumed. The Marsaglia polar method (http://en.wikipedia.

org/wiki/Marsaglia_polar_method) is used to generate the normally-distributed random numbers z from uniformly distributed random numbers. MECCA uses two options from the submodel MAIN_RND to generate uniformly distributed random numbers: either the Fortran 90 standard subroutine RANDOM_NUMBER or the Mersenne-Twister algorithm (Matsumoto and Nishimura, 1998) can be used. A potential disadvantage of the Fortran 90 standard subroutine is that different compilers will produce different random numbers of different quality. If it is necessary to repeat a Monte-Carlo simulation with exactly the same "random"-numbers, the Mersenne-Twister algorithm should be used.

3.3 Mercury chemistry

Atmospheric gas and aqueous-phase chemistry of mercury has been included by Xie et al. (2008). The main focus of the mechanism development was the oxidation of Hg(0) by O_3, OH, and halogen radicals. These reactions are not only important to explain mercury-depletion events in polar regions, but may have global significance as well (e.g., Steffen et al., 2008; Jöckel et al., 2010). However, it should be noted that the uncertainties of current kinetic laboratory measurements are quite large. Thus, regular updates of the rate coefficients in future versions of MECCA will be necessary.

3.4 Chemistry of organic trace gases

The oxidation mechanism for organic trace gases is significantly different from that in previous versions of MECCA. The main developments are briefly described here.

The self- and cross-reactions of organic peroxy radicals (R^iO_2) are treated following the permutation reaction formalism (Jenkin et al., 1997; Saunders et al., 2003) which is a simplification of the formalism used by Madronich and Calvert (1990). Each individual peroxy radical reacts with a generic RO_2, which represents the sum of all peroxy radicals: $RO_2 = \sum_i R^iO_2$. A pseudo-unimolecular reaction is then assigned to each individual peroxy radical:

$$R^iO_2 \xrightarrow{k_i[RO_2]} \text{products}$$
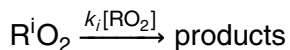
with an averaged rate coefficient k_i that includes the concentration of the generic RO_2.

A new condensed degradation scheme for isoprene (2-methyl-1,3-butadiene, C_5H_8) has been implemented by Taraborrelli et al. (2009). Replacing the Mainz Isoprene
5   Mechanism (MIM) by Pöschl et al. (2000), the new scheme is called MIM2. It closely reproduces the results of the explicit isoprene mechanism of the Master Chemical Mechanism (MCM, http://mcm.leeds.ac.uk/MCM) by Saunders et al. (2003). The buffering capacity of MIM2 against changes in NO emissions is rather good and avoids the large biases for nitrogen oxides which are characteristic for MIM. Compared
10   to MCM, MIM2 computes small relative biases (<6%) for most intermediates and has already been used for global atmospheric simulations (Lelieveld et al., 2008; Butler et al., 2008). MIM2 is characterized by a low degree of species lumping. Thus, modifications are easy to implement and unlikely to introduce unintentional side effects on other parts of the mechanism (which can occur when changing
15   heavily parameterized schemes). This feature is particularly important since a poor knowledge of the low-NO_x isoprene oxidation has been linked to the large model bias for the HO_x measurements over a pristine tropical forest (Lelieveld et al., 2008). Recent theoretical and experimental advancements in isoprene oxidation chemistry may explain those discrepancies (Peeters et al., 2009, and others), and MIM2 is
20   suitable for an implementation of these results (e.g., Stavrakou et al., 2010).

The chemistry of propane (C_3H_8) and n-butane (C_4H_{10}) has been taken from the MCM and simplified. The OH-initiated oxidation of ethene is taken from Orlando et al. (1998), fully representing the temperature and NO_x dependence of the product distribution. Ozonolyis of ethene is taken from the MCM and simplified according to
25   the principles described by Taraborrelli et al. (2009).

Finally, the whole mechanism is now mass-conserving with respect to carbon, including CO and CO_2. It is thus suitable for assessments of CO production from biogenic sources and studying the carbon isotopic composition of trace gases.

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3.5 NH₃ chemistry

A mechanism for the chemical degradation of gaseous NH_3 has been added. Even though this sink is of minor importance for NH_3 (the chemical loss is only a few percent compared to deposition and heterogeneous chemistry), the degradation products contribute to the budgets of N_2O and NO_x. The reaction pathways towards either N_2O or NO depend on the concentrations of NO_2 and O_3: under low NO_x conditions (mixing ratios below $1 \, \text{nmol mol}^{-1}$), NH_3 acts as a source for NO_x, otherwise as a sink. The implemented reactions are taken from the condensed mechanism of Kohlmann and Poppe (1999).

3.6 Kinetic diagnostics and isotope chemistry

A tagging technique for the MECCA reaction mechanism has been implemented by Gromov et al. (2010). The new sub-submodel MECCA-TAG allows the explicit on-line calculation of the contributions of selected species to the budgets of other species of interest within a complex chemical mechanism. For example, one can estimate the contributions of methane and isoprene to the production of CO, as well as to the budgets of any associated intermediate like HCHO or CH_3O_2. In addition, tagging allows the direct calculation of the species' yields, e.g., number of molecules of CO produced per initially reacted methane or isoprene. MECCA-TAG substantially facilitates the analysis of the model results, considering the complex chemistry of isoprene oxidation in MECCA (MIM2, see Sect. 3.4).

An extended application of tagging is isotope chemistry modelling, which is now supported in MECCA. Isotope chemistry requires careful accounting for the isotopic composition transfer, specific isotope exchange reactions and kinetic isotope effects. MECCA-TAG offers a comfortable isotope chemistry parameterisation with all necessary input contained in one user-friendly configuration file (*.cfg). Only the list of species and isotopes of interest must be specified, without adding or changing any reactions: the parsing routines automatically process the equation (*.eqn) and

species (*.spc) files of the selected chemical mechanism and generate additional Fortran 90 code for CAABA/MECCA. The execution of the sub-submodel is controlled via a Fortran 90 namelist (*.nml). To date, we have implemented stable carbon (^{12}C/^{13}C) and oxygen (^{16}O/^{17}O/^{18}O) isotope configurations in MECCA that have been evaluated for CO and relevant species (Gromov et al., 2010). Isotope chemistry of other elements (e.g. H, S, N) is to be added in the future.

3.7 Further recent changes

To improve the up-to-dateness and the user-friedliness, and to facilitate the analysis of the model results, several minor changes have been applied to MECCA:

- Rate coefficients have been updated to recent recommendations and laboratory studies (Sander et al., 2006; Atkinson et al., 2004, 2006, 2007). A complete list of chemical reactions, rate coefficients, and references can be found in the file meccanism.pdf in the electronic supplement.

- During the generation of a new chemical mechanism, the user needs to answer several questions interactively about the selected reactions, the numerical solver, and other features. It is now possible to collect all answers in a batch file (*.bat) and then produce a new chemical mechanism non-interactively. Similarly, the new replacement files (*.rpl) allow easy switching between the standard mechanism and a mechanism modified for testing purposes. Both features are explained in more detail in the CAABA/MECCA user manual (see supplement).

- The kinetic preprocessor KPP, which performs the numerical integration of the chemical reaction mechanism, has been updated to version 2.1 by Sandu and Sander (2006), which provides more numerical integrators. To facilitate the installation and to ensure compatibility, the KPP software has been included into the MECCA distribution.

– The implementation of diagnostic tracers allows output of the reaction rates of selected reactions. Alternatively, output of *all* reaction rates can be switched on.

4 Summary

We have presented the current version of the versatile atmospheric chemistry box model CAABA/MECCA-3.0gmdd. Its chemical and numerical flexibility, its modularity, and its portability make it an ideal tool for many applications. The code is publicly available for atmospheric chemistry and climate research.

**Supplementary material related to this article is available online at:
http://www.geosci-model-dev-discuss.net/4/197/2011/
gmdd-4-197-2011-supplement.zip**.

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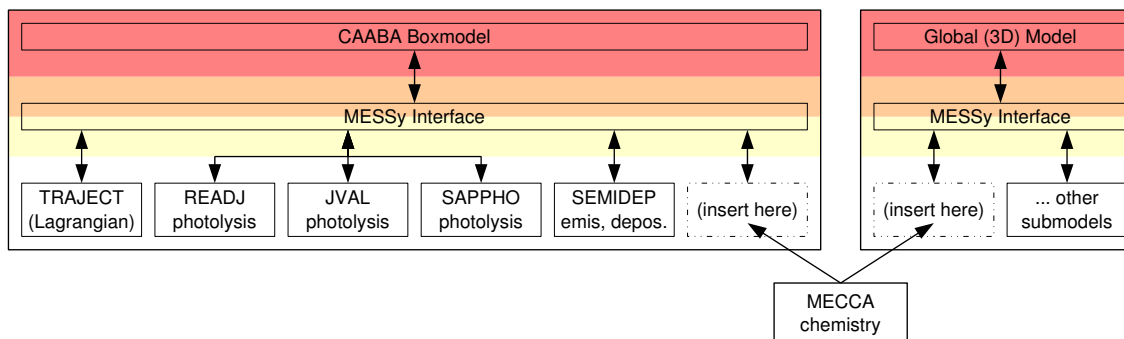
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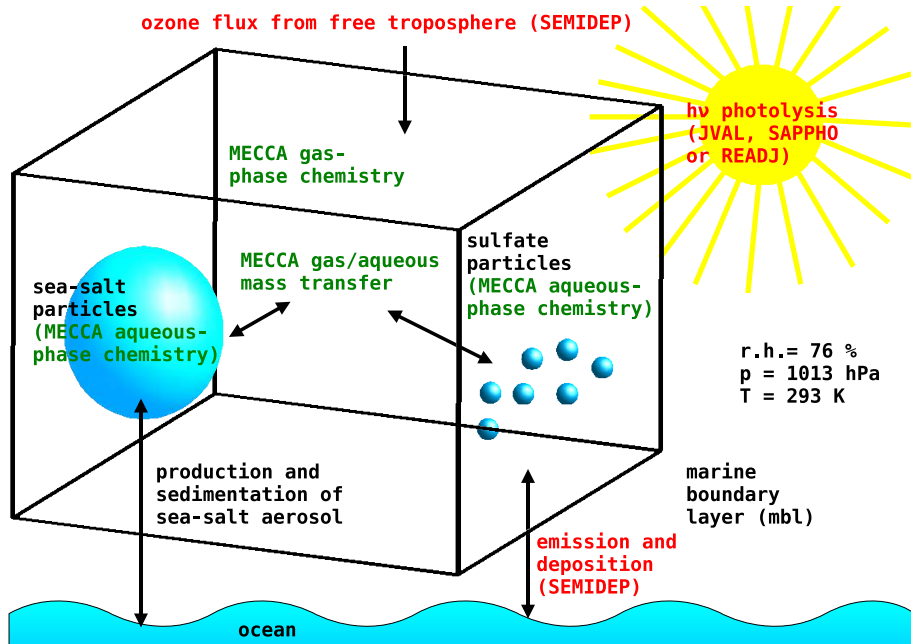
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Steffen, A., Douglas, T., Amyot, M., Ariya, P., Aspmo, K., Berg, T., Bottenheim, J., Brooks, S., Cobbett, F., Dastoor, A., Dommergue, A., Ebinghaus, R., Ferrari, C., Gardfeldt, K., Goodsite, M. E., Lean, D., Poulain, A. J., Scherz, C., Skov, H., Sommar, J., and Temme, C.: A synthesis of atmospheric mercury depletion event chemistry in the atmosphere and snow, Atmos. Chem. Phys., 8, 1445–1482, doi:10.5194/acp-8-1445-2008, 2008. 205

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Fig. 1. Left: the modular structure of the CAABA box model and its submodels, which are connected via the MESSy interface. Right: illustration showing that the MECCA chemistry submodel can also be plugged into a global (3-D) model, e.g., a general circulation model (GCM). Likewise, the photolysis submodel JVAL can also be plugged into a global model.

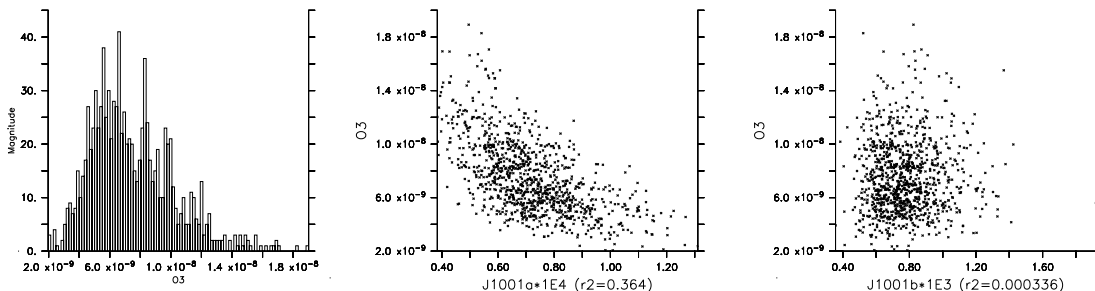**Fig. 2.** Illustration of the CAABA box model. MECCA chemistry is shown in green, and processes calculated by other submodels in red.
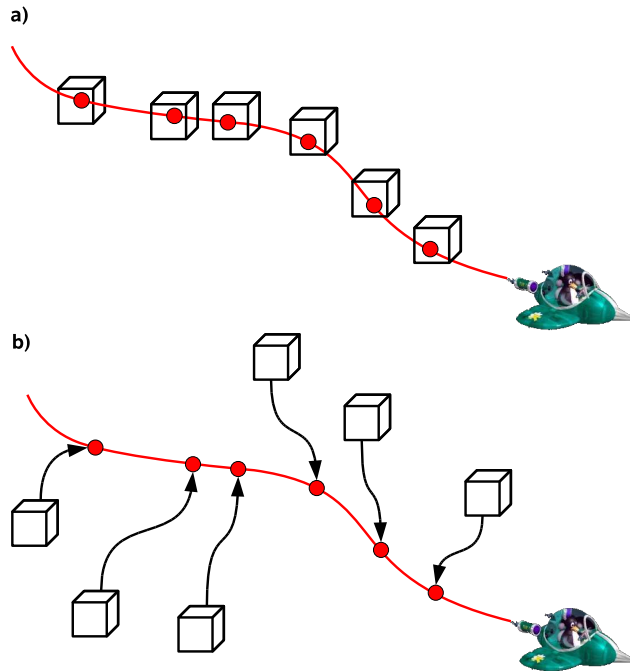
Fig. 3. A illustrative comparison of **(a)** the steady-state-mode, and **(b)** the trajectory mode of CAABA. The simulations start with conditions encountered at the boxes and they end at the red dots which represent the measured data sets.

Fig. 4. Example results of Monte-Carlo simulations. The first figure is a histogram showing the distribution of steady-state O_3 mixing ratios (mol mol^{-1}) in 1000 model runs. The other figures are scatter plots of O_3 against individual gas-phase photolysis rate coefficients (in s^{-1}). It can be seen that O_3 decreases with increasing values of J1001a ($O_3 + h\nu \rightarrow O(^1D)$). In contrast, its dependence on the photolysis rate J1001b ($O_3 + h\nu \rightarrow O(^3P)$) is statistically insignificant.