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Modelling atmospheric chemistry with the new comprehensive module MECCA

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We present the multi-purpose atmospheric chemistry model MECCA (Module Efficiently Calculating the Chemistry of the Atmosphere). Owing to its versatility and modular structure, it can be used for tropospheric as well as stratospheric chemistry calculations. MECCA contains a comprehensive atmospheric reaction mechanism that currently includes: 1) the basic O_3, CH_4, HO_x, and NO_x chemistry, 2) non-methane hydrocarbon (NMHC) chemistry, 3) halogen (Cl, Br, I) chemistry, and 4) sulfur chemistry. Not only gas-phase chemistry but also aqueous-phase and heterogeneous reactions are considered. Arbitrary subsets of the comprehensive mechanism can be selected according to the research objectives, e.g. air pollution modelling. The program code resulting from the chemical mechanism can easily be used in any kind of model, from a simple box model to a sophisticated global general circulation model. The main features of MECCA are:

Chemical flexibility The chemical mechanism contains a large number of reactions from which the user can select a custom-designed subset. It is easy to adjust the mechanism, e.g. according to the latest kinetic insights.

Numerical flexibility The numerical integration is performed with the KPP software package. The user can choose between different solvers according to individual requirements of the stiff set of differential equations (efficiency, stability, accuracy, precision).

Modularity Due to its modular structure, the code can be easily coupled to other meteorological base models (e.g. box models, 1-dimensional column models, or 3-dimensional models).

Portability The Fortran95 code is written in a portable way to allow its use on different platforms (e.g. Linux, Unix).

Availability The code is freely available to the scientific community.