

This discussion paper is/has been under review for the journal Geoscientific Model Development (GMD). Please refer to the corresponding final paper in GMD if available.

# A fast stratospheric chemistry solver: the E4CHEM submodel for the atmospheric chemistry global circulation model EMAC

A. J. G. Baumgaertner<sup>1</sup>, P. Jöckel<sup>1,\*</sup>, B. Steil<sup>1</sup>, H. Tost<sup>1</sup>, and R. Sander<sup>1</sup>

<sup>1</sup>Max Planck Institute for Chemistry, 55020 Mainz, Germany

\* now at: Deutsches Zentrum für Luft-und Raumfahrt (DLR), Institut für Physik der Atmosphäre, Oberpfaffenhofen, 82234 Weßling, Germany

Received: 2 February 2010 – Accepted: 10 February 2010 – Published: 17 February 2010

Correspondence to: A. J. G. Baumgaertner (work@andreas-baumgaertner.net)

Published by Copernicus Publications on behalf of the European Geosciences Union.

**GMDD**

3, 181–200, 2010

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

## Abstract

The atmospheric chemistry general circulation model ECHAM5/MESSy (EMAC) and the atmospheric chemistry box model CAABA are extended by a computationally very efficient submodel for atmospheric chemistry, E4CHEM. It focuses on stratospheric chemistry but also includes background tropospheric chemistry. It is based on the chemistry of MAECHAM4-CHEM and is intended to serve as a simple and fast alternative to the flexible but also computationally more demanding submodel MECCA. In a model setup with E4CHEM, EMAC is now also suitable for simulations of longer time scales. The reaction mechanism contains basic  $O_3$ ,  $CH_4$ ,  $CO$ ,  $HO_x$ ,  $NO_x$  and  $ClO_x$  gas phase chemistry. In addition, E4CHEM includes optional fast routines for heterogeneous reactions on sulphate aerosols and polar stratospheric clouds (substituting the existing submodels PSC and HETCHEM), and scavenging (substituting the existing submodel SCAV). We describe the implementation of E4CHEM into the MESSy structure of CAABA and EMAC. For some species the steady state in the box model differs by up to 100% when compared to results from CAABA/MECCA due to different reaction rates. After an update of the reaction rates in E4CHEM the mixing ratios in both boxmodel and 3-D model simulations are in satisfactory agreement with the results from a simulation where MECCA with a similar chemistry scheme was employed. Finally, a comparison against a simulation with a more complex and already evaluated chemical mechanism is presented in order to discuss shortcomings associated with the simplification of the chemical mechanism.

## 1 Introduction

In an attempt to better understand atmospheric chemistry and the atmosphere as a whole, in the last decade atmospheric models have been extended by routines accounting for chemical reactions in the atmosphere. Today, a variety of implementations of algorithms which numerically solve the coupled differential equations that describe

**GMDD**

3, 181–200, 2010

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

the chemical reactions important in the atmosphere exist. Many chemistry climate models that include the stratosphere participate in the validation study CCMVal by the SPARC (Stratospheric Processes and their Role in Climate) project of WCRP. Such models and their performance have been reviewed and validated by e.g. Austin et al. (2003); Eyring et al. (2006, 2007); Austin et al. (2008); Austin et al. (2010).

The atmospheric chemistry general circulation model ECHAM5/MESSy (EMAC) already contains the very flexible chemistry module MECCA (Sander et al., 2005), which is also part of the boxmodel CAABA (Sander et al., 2010); the two models form a consistent model hierarchy (see also Riede et al., 2009). MECCA, which utilises the Kinetic PreProcessor (KPP, Sandu and Sander, 2006), is routinely used for simulations from the surface to the mesosphere (e.g. Jöckel et al., 2006). Here, we describe the implementation of a fast chemical submodel as a box model process for CAABA as well as for the 3-D model EMAC (Sect. 2) and compare the results with simulations using the existing submodels MECCA, PSC, and HETCHEM (Sect. 3). EMAC simulations with E4CHEM can be performed for many decades and are thus useful for climate simulations, where the feedback of radiatively active gases such as ozone is of particular interest.

## 2 Model description

The bases for the E4CHEM submodel were the chemical scheme and solver contained in the CHEM subroutine of ECHAM3/4-CHEM, introduced by Steil et al. (1998). In the ECHAM3/4 implementations the subroutine CHEM has been used extensively, results are for example presented by Hein et al. (2001), Steil et al. (2003), Manzini et al. (2003), Lemmen et al. (2006), Dameris et al. (2005), and Grewe (2007). The solver has been described in detail by Steil et al. (1998), therefore we will only summarize the employed technique here.

The chemistry module focuses on stratospheric ozone chemistry but also includes tropospheric background  $\text{NO}_x$ - $\text{HO}_x$ - $\text{CH}_4$ - $\text{CO}$ - $\text{O}_3$  chemistry. In addition to the gas phase

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



chemistry, E4CHEM also accounts for heterogeneous chemistry on polar stratospheric clouds and sulfate aerosol and contains its own PSC-scheme. It considers 110 photochemical reactions of 38 species:  $\text{N}_2\text{O}$ ,  $\text{CH}_4$ ,  $\text{H}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{CH}_3\text{O}_2\text{H}$ ,  $\text{HCHO}$ ,  $\text{CH}_3\text{O}_2$ ,  $\text{CH}_3\text{O}$ ,  $\text{HO}_x$  ( $= \text{H} + \text{OH} + \text{HO}_2$ ),  $\text{H}_2\text{O}_2$ ,  $\text{NO}_x$  ( $= \text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3 + \text{HNO}_4 + 2 \cdot \text{N}_2\text{O}_5$ ),  $\text{HNO}_3$ ,  $\text{HCl}$ ,  $\text{ClONO}_2$ ,  $\text{CFC11}$ ,  $\text{CFC12}$ ,  $\text{CH}_3\text{Cl}$ ,  $\text{CH}_3\text{CCl}_3$ ,  $\text{CCl}_4$ ,  $\text{ClO}_x$  ( $= \text{Cl} + \text{ClO} + \text{HOCl} + 2 \cdot \text{Cl}_2\text{O}_2 + 2 \cdot \text{Cl}_2$ ),  $\text{O}_x$  ( $= \text{O}_3 + \text{O}(^3\text{P}) + \text{O}(^1\text{D})$ ), type I PSC(NAT), and type II PSC(ice). The results of the experimental study of Hanson and Mauersberger (1988) are applied to determine when PSCs are thermodynamically possible, based on the simulated temperature and the mixing ratios of  $\text{HNO}_3$  and  $\text{H}_2\text{O}$ . It is assumed that ice forms on large NAT particles. The sedimentation velocity of NAT and ice is considered to be identical if ice is present, otherwise sedimentation is neglected. The stokes velocity of ice particles is calculated every timestep according to the changing radius due to condensation or evaporation of water vapour. This scheme may underestimate denitrification in the Arctic but is well suitable for the Antarctic lower stratosphere where ice particles occur frequently. In general, the numerical methods used to integrate the chemical system are semi-implicit, positive definite and mass conserving. The numerics are based on an advanced family concept. The prognostic equations are integrated using a semi-analytic exponential approach or Eulerian backward. There are three major changes compared to the standard family approach. Firstly, not only the steady state approach is used to partition the families, but depending on the lifetime of the species also the Eulerian backward and the Exponential method. Secondly, to partly overcome the process splitting problem in the family approach (i.e. the fixed order in integrating the families which can cause instabilities if a too strong coupling between families exists), a combined “super-family” for nitrate and chlorine containing species has been introduced to account for the strong coupling, especially in the case of heterogeneous chemistry on PSCs. Lastly, the definition of families for transport and chemistry does not necessarily coincide, e.g. chlorine nitrate ( $\text{ClONO}_2$ ) is transported separately but included in the  $\text{NO}_x$ - $\text{ClO}_x$  - super-family. To further improve the numerical efficiency, E4CHEM has a special reduced nighttime chemistry. The numerics of E4CHEM pro-

## GMDD

3, 181–200, 2010

### A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

vides two considerable advantages. The accuracy of the integration shows just a weak dependence on the length of the timestep. This allows decoupling of the chemistry timestep from the timestep of the hosting model, i.e. E4CHEM can easily be called at a multiple of the GCM-timestep (a feature that has not been applied for the simulations of the this paper). This makes E4CHEM attractive for the use in high resolution models with short time steps. Essentially, the cost for the chemistry integration itself can be neglected and just the additional overhead caused by the transport of species remains. Furthermore, the numerics of E4CHEM provide a well defined, good-natured error behaviour. The chosen numerical methods ensure that in the case of a numerical error the system moves towards chemical steady-state. This stability characteristic is especially favourable in long-term integrations.

While a comparison with state of the art chemistry modules requires an update of the employed reaction rates, an evaluation against published results that employed the CHEM subroutine is only possible with the original rates. Therefore, the new reaction rates were implemented as an alternative that can be selected at compile time. The new reaction rates were taken to be the same as in MECCA, see Sander et al. (2010) for references to the individual reaction rate studies. Some differences to the MECCA mechanism in the hydrocarbon chemistry remain, so a perfect agreement cannot be expected. Note also that the photolysis rates, in EMAC and CAABA calculated by the submodel JVAL (based on Landgraf and Crutzen, 1998), so there will be differences to the results of previous studies with CHEM even if the original reaction rates are used.

In order to comply with the MESSy standard (Jöckel et al., 2005), the code was completely converted from FORTRAN77 to Fortran 90/95. As required by MESSy, the solver is located in the submodel core layer and called from the submodel interface layers, currently either an ECHAM5 interface, or a CAABA box model interface.

## 2.1 Implementation in the boxmodel CAABA

CAABA (Sander et al., 2010) is an atmospheric chemistry box model which uses MESSy to couple the individual processes. E4CHEM was integrated as an alternative

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



solver in CAABA, where it can replace the gas phase chemistry submodel MECCA. Like MECCA, it uses JVAL to obtain photolysis rates.

## 2.2 Implementation in the 3-D model EMAC

In the 3-D model EMAC, E4CHEM can be used as an alternative to MECCA, similar to the integration into CAABA. Note that CAABA and EMAC use identical submodel core layer files, only the interface layer differs. The interface of E4CHEM to the basemodel ECHAM5 in EMAC is very similar to the respective interface of MECCA. It contains:

- the call to the initialisation subroutines, such as the precalculation of temperature dependent reaction rates and the stratospheric sulphuric acid aerosol surface areas;
- the coupling to other submodels. In the standard setting the photolysis rates are taken from the submodel JVAL, the tropopause height is taken from the submodel TROPOP. If E4CHEM is also used for scavenging calculations, then it couples also to CLOUD, CVTRANS, and CONVECT;
- the coupling to the MESSy submodel TRACER (Jöckel et al., 2008), which is used to create and manage the tracers. This also allows to easily define tracer families (via the corresponding namelist) for advection;
- the call to the solver subroutine CHEM which resides in the core layer.

The submodels PSC and HETCHEM, needed for EMAC simulations with MECCA, can be switched off if E4CHEM is used, since E4CHEM already contains heterogeneous chemistry on sulphate aerosols and polar stratospheric clouds.

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)



[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

### 3 Model evaluation

#### 3.1 E4CHEM in the box model CAABA

The box model version of the solver and chemistry of E4CHEM has been evaluated by comparison to the quasi-exact scheme of FACSIMILE in Steil (1997) and we restrict the evaluation here to a comparison with MECCA.

The here applied MECCA mechanism, which is equivalent to the E4CHEM chemistry, contains the reactions labelled for the stratosphere, however, bromine, iodine and mercury containing reactions have to be excluded (thus the selection string is (St && !Br && !I && !Hg)).

Figure 1 depicts selected box model results from simulations with CAABA employing MECCA (black lines) and E4CHEM using the original (red) and updated (green) reaction rates. The simulations were performed for mid-latitude (45° N) summer (1 July–8 July), at 10 hPa. The chemistry was initialised using the results from a 3-D simulation with EMAC. A time step of 20 min was selected.

There is a good agreement for NO, NO<sub>2</sub>, N<sub>2</sub>O<sub>5</sub>, HNO<sub>3</sub>, OH, HO<sub>2</sub>, HCHO and ozone in all simulations. However, large discrepancies are found for HNO<sub>4</sub>, H<sub>2</sub>O<sub>2</sub>, and H between the E4CHEM simulation with the original reaction rates and the other two simulations. For CH<sub>3</sub>OOH the difference between MECCA and E4CHEM with new reaction rates is smaller by 50% when compared to E4CHEM with the old reaction rates, but still amounts to approximately 20%. This is likely due to the differences between E4CHEM and MECCA in the hydrocarbon mechanism as mentioned above. The supplement at (<http://www.geosci-model-dev-discuss.net/3/181/2010/gmdd-3-181-2010-supplement.zip>) contains a comparison for all chemical species contained in E4CHEM.

The CPU time consumed by the CAABA simulations with E4CHEM or MECCA switched on was measured on an IBM Power6 architecture using simulation lengths of 30 days. The E4CHEM simulations need approximately 35% less CPU time than the MECCA simulation with the equivalent chemistry setup. Note that a significant part

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



of the performance increase in the chemistry is concealed by the JVAL submodel as well as other parts of CAABA (e.g. output routines) which also require a significant amount of CPU time.

### 3.2 E4CHEM in the EMAC 3-D model

5 As mentioned above, the chemical scheme of E4CHEM has been tested and used extensively in chemistry climate models. In order to evaluate E4CHEM in the EMAC model system, we compare three simulations, the first using E4CHEM, the other two using MECCA. The differences between the simulations are summarised in Table 1. All simulations were carried out for the year 1998 with a spectral truncation of T42,  
10 corresponding to a horizontal resolution of approximately  $2.8^\circ$  by  $2.8^\circ$ , and 90 layers in the vertical (L90MA) reaching up to 0.01 hPa. Other submodels that were switched on in all simulations are CLOUD (cloud routines), CONVECT (convection parametrisation, see Tost et al., 2006b), CVTRANS (convective tracer transport), DRYDEP (dry deposition, see Kerkweg et al., 2006a), H<sub>2</sub>O (consistent feedback of the chemical tracer  
15 water vapour with specific humidity of the base model), JVAL (based on Landgraf and Crutzen, 1998), LNOX (a lightning NOX parametrisation, see Tost et al., 2007), OFFLEM (offline emission of trace gases, see Kerkweg et al., 2006b), ONLEM (online calculated emission of trace gases, see Kerkweg et al., 2006b), QBO (assimilation of QBO zonal wind observations), RAD4ALL (radiation code), SCAV (scavenging  
20 parametrisation by Tost et al., 2006a), TNUDGE (Newtonian relaxation of long-lived trace gases at the surface), and TROPOP (diagnostics submodel). In the simulations with MECCA the submodels HETCHEM and PSC were switched on additionally. Note that all simulations were nudged to observed meteorology (ECMWF analysis data).

25 A side by side comparison of all species contained in the E4CHEM chemical scheme is contained in the supplement at <http://www.geosci-model-dev-discuss.net/3/181/2010/gmdd-3-181-2010-supplement.zip> and we present only a few examples here. Figure 2 depicts ozone mixing ratios for the zonal average at  $30^\circ$  S– $50^\circ$  S. In general, there is good agreement between all simulations. The ozone maximum is

---

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

---

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



located at about 33 km, but is larger by approximately  $0.5 \mu\text{mol/mol}$  in the S-E4CHEM simulation from January to February. Above an altitude of 0.15 hPa S-E4CHEM ozone is lower by about  $0.5 \mu\text{mol/mol}$ .

For  $\text{NO}_x$ , depicted in Fig. 3, a similarly good agreement is obtained. The variation with time and altitude is captured well by S-E4CHEM, with differences only in the mesosphere.

Zonal mean total column ozone is compared as a function of latitude, averaged over the entire year 1998, in Fig. 4. S-E4CHEM (black), S-MECCA(E4CHEM) (red) and S-MECCA(EVAL). Differences are generally less than 2%, only at high latitudes differences are greater with simulation S-MECCA(EVAL) showing the smallest ozone columns. Since the S-MECCA(EVAL) chemical mechanism also incorporates bromine-containing substances, polar ozone loss is stronger in this simulation. Differences in polar ozone between the simulations S-E4CHEM and S-MECCA(E4CHEM) are likely due to the differences in the polar stratospheric cloud schemes, as well as in the aerosol surface area assumptions.

Finally, we compare polar winter ozone loss which is an important atmospheric phenomenon. Minimum total ozone is a commonly used quantity for the diagnostic of the ability of chemistry climate models to reproduce the ozonehole. During the Southern Hemisphere winter 1998, TOMS satellite observations of total column ozone showed a minimum of approximately 100 DU (WMO, 2006). The minimum ozone as a function of time is shown in Fig. 5 for all three simulations. It is evident that there is a strong correlation in minimum ozone between the three simulations due to the very similar dynamics, which is due to the nudging to observed meteorology. Only in September and October minimum ozone in the simulation S-MECCA(EVAL) is significantly lower than in the other two simulations, which, as already mentioned above, is most likely due to the fact that S-MECCA(EVAL) also contains ozone-destroying bromine chemistry.

The computational resource demand of the E4CHEM submodel in comparison to the ECHAM5 basemodel is small. Note that other submodels, but especially the advection routine which has to consider a larger number of species, contribute to a moderate rise

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)



[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

in resource demands compared to the hosting basemodel. On parallel architectures, load imbalancing is also much reduced compared to other chemical solvers.

## 4 Conclusions

The fast chemical scheme E4CHEM has been implemented as a MESSy submodel. For stratospheric and tropospheric background chemistry applications it serves as an alternative to the flexible MECCA submodel. The main advantage is its low computational resource demand compared to MECCA, making it useful for simulations of long timescales. However, including additional species or reactions is complicated and constitutes a major disadvantage.

The E4CHEM submodel has been evaluated in the box model CAABA and the 3-D model EMAC by comparing the results to simulations with MECCA (plus the submodels for heterogeneous chemistry). For the box model, it was shown that the agreement improves clearly if updated reaction rates are used in E4CHEM. Only for some hydrocarbon species significant differences remain, which are due to differences in the hydrocarbon mechanisms. For the most important chemical species such as ozone, water vapour, and nitrogen compounds no disconcerting differences to the simulations with MECCA were found. Due to the very successful use of the chemistry subroutines of E4CHEM in previous implementations in chemistry climate models, we can conclude that the EMAC implementation will be useful for many applications.

An existing extension of CHEM that provides a chemical budget analysis will also be implemented in E4CHEM. It is planned to extend the chemical mechanism by bromine containing species, in order to better represent the ozone depletion related to these compounds. Further, NMHC (non-methane hydrocarbon) chemistry will be included for a better representation of the troposphere, and the sulphur cycle will be completed in order to realistically simulate volcanic eruptions.

*Acknowledgements.* This work was funded by the TIES project within the DFG SPP 1176 CAWSES. The Ferret program (<http://www.ferret.noaa.gov>) from NOAA's Pacific Marine

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)



[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



Environmental Laboratory was used for creating some of the graphics in this paper. Thanks go to all MESSy developers and users for their support. The model simulations were performed on the POWER-6 computer at the Max Planck Computer Centre in Garching, RZG.

- 5 The service charges for this open access publication have been covered by the Max Planck Society.

## References

- Scientific Assessment of Ozone Depletion: Tech. rep., World Meteorological Organization, 2006. 189
- 10 Austin, J., Shindell, D., Beagley, S. R., Brühl, C., Dameris, M., Manzini, E., Nagashima, T., Newman, P., Pawson, S., Pitari, G., Rozanov, E., Schnadt, C., and Shepherd, T. G.: Uncertainties and assessments of chemistry-climate models of the stratosphere, *Atmos. Chem. Phys.*, 3, 1–27, 2003, <http://www.atmos-chem-phys.net/3/1/2003/>. 183
- 15 Austin, J., Tourpali, K., Rozanov, E., Akiyoshi, H., Bekki, S., Bodeker, G., Brühl, C., Butchart, N., Chipperfield, M., Deushi, M., Fomichev, V. I., Giorgetta, M. A., Gray, L., Kodera, K., Lott, F., Manzini, E., Marsh, D., Matthes, K., Nagashima, T., Shibata, K., Stolarski, R. S., Struthers, H., and Tian, W.: Coupled chemistry climate model simulations of the solar cycle in ozone and temperature, *J. Geophys. Res.*, 113, D11306, doi:10.1029/2007JD009391, 2008. 183
- 20 Austin, J., Struthers, H., Scinocca, J., Plummer, D., Akiyoshi, H., Baumgaertner, A. J. G., Bekki, S., Bodeker, G. E., Braesicke, P., Bruehl, C., Butchart, N., Chipperfield, M., Cugnet, D., Dameris, M., Dhomse, S., Frith, S., Garny, H., Gettelman, A., Hardiman, S., Jöckel, P., Kinnison, D., Lamarque, J. F., Marchand, M., Michou, M., Morgenstern, O., Nakamura, T., Nielsen, J. E., Pitari, G., Pyle, J., Shepherd, T. G., Shibata, K., Smale, D., Stolarski, R., Teysse, H., and Yamashita, Y.: Chemistry climate model simulations of the Antarctic ozone hole, *J. Geophys. Res.*, submitted, 2010. 183
- 25 Dameris, M., Grewe, V., Ponater, M., Deckert, R., Eyring, V., Mager, F., Matthes, S., Schnadt, C., Stenke, A., Steil, B., Brhl, C., and Giorgetta, M. A.: Long-term changes and variability in a transient simulation with a chemistry-climate model employing realistic forcing, *Atmos.*

**GMDD**

3, 181–200, 2010

---

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Chem. Phys., 5, 2121–2145, 2005,

<http://www.atmos-chem-phys.net/5/2121/2005/>. 183

Eyring, V., Butchart, N., Waugh, D. W., Akiyoshi, H., Austin, J., Bekki, S., Bodeker, G. E., Boville, B. A., Brühl, C., Chipperfield, M. P., Cordero, E., Dameris, M., Deushi, M., Fioletov, V. E., Frith, S. M., Garcia, R. R., Gettelman, A., Giorgetta, M. A., Grewe, V., Jourdain, L., Kinnison, D. E., Mancini, E., Manzini, E., Marchand, M., Marsh, D. R., Nagashima, T., Newman, P. A., Nielsen, J. E., Pawson, S., Pitari, G., Plummer, D. A., Rozanov, E., Schraner, M., Shepherd, T. G., Shibata, K., Stolarski, R. S., Struthers, H., Tian, W., and Yoshiki, M.: Assessment of temperature, trace species, and ozone in chemistry-climate model simulations of the recent past, *J. Geophys. Res.*, 111, D22308, doi:10.1029/2006JD007327, 2006. 183

Eyring, V., Waugh, D. W., Bodeker, G. E., Cordero, E., Akiyoshi, H., Austin, J., Beagley, S. R., Boville, B. A., Braesicke, P., Brühl, C., Butchart, N., Chipperfield, M. P., Dameris, M., Deckert, R., Deushi, M., Frith, S. M., Garcia, R. R., Gettelman, A., Giorgetta, M. A., Kinnison, D. E., Mancini, E., Manzini, E., Marsh, D. R., Matthes, S., Nagashima, T., Newman, P. A., Nielsen, J. E., Pawson, S., Pitari, G., Plummer, D. A., Rozanov, E., Schraner, M., Scinocca, J. F., Semeniuk, K., Shepherd, T. G., Shibata, K., Steil, B., Stolarski, R. S., Tian, W., and Yoshiki, M.: Multimodel projections of stratospheric ozone in the 21st century, *J. Geophys. Res.*, 112, D16303, doi:10.1029/2006JD008332, 2007. 183

Grewe, V.: Impact of climate variability on tropospheric ozone, *Sci. Total Environ.*, 374, 167–181, 2007. 183

Hanson, D. and Mauersberger, K.: Laboratory studies of the nitric acid trihydrate – Implications for the south polar stratosphere, *Geophys. Res. Lett.*, 15, 855–858, doi:10.1029/GL015i008p00855, 1988. 184

Hein, R., Dameris, M., Schnadt, C., Land, C., Grewe, V., Köhler, I., Ponater, M., Sausen, R., B. Steil, B., Landgraf, J., and Brühl, C.: Results of an interactively coupled atmospheric chemistry general circulation model: Comparison with observations, *Ann. Geophys.*, 19, 435–457, 2001,

<http://www.ann-geophys.net/19/435/2001/>. 183

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, 2005,

<http://www.atmos-chem-phys.net/5/433/2005/>. 185

Jöckel, P., Tost, H., Pozzer, A., Brühl, C., Buchholz, J., Ganzeveld, L., Hoor, P., Kerk-

**GMDD**

3, 181–200, 2010

---

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

weg, A., Lawrence, M. G., Sander, R., Steil, B., Stiller, G., Tanarhte, M., Taraborrelli, D., van Aardenne, J., and Lelieveld, J.: The atmospheric chemistry general circulation model ECHAM5/MESSy1: consistent simulation of ozone from the surface to the mesosphere, *Atmos. Chem. Phys.*, 6, 5067–5104, 2006,

<http://www.atmos-chem-phys.net/6/5067/2006/>. 183, 195

Jöckel, P., Kerkweg, A., Buchholz-Dietsch, J., Tost, H., Sander, R., and Pozzer, A.: Technical Note: Coupling of chemical processes with the Modular Earth Submodel System (MESSy) submodel TRACER, *Atmos. Chem. Phys.*, 8, 1677–1687, 2008, <http://www.atmos-chem-phys.net/8/1677/2008/>. 186

Kerkweg, A., Buchholz, J., Ganzeveld, L., Pozzer, A., Tost, H., and Jöckel, P.: Technical Note: An implementation of the dry removal processes DRY DEPosition and SEDimentation in the Modular Earth Submodel System (MESSy), *Atmos. Chem. Phys.*, 6, 4617–4632, 2006a. 188

Kerkweg, A., Sander, R., Tost, H., and Jöckel, P.: Technical note: Implementation of prescribed (OFFLEM), calculated (ONLEM), and pseudo-emissions (TNUDGE) of chemical species in the Modular Earth Submodel System (MESSy), *Atmos. Chem. Phys.*, 6, 3603–3609, 2006b. 188

Landgraf, J. and Crutzen, P. J.: An Efficient Method for Online Calculations of Photolysis and Heating Rates., *J. Atmos. Sci.*, 55, 863–878, doi:10.1175/1520-0469(1998)055, 1998. 185, 188

Lemmen, C., Dameris, M., Müller, R., and Riese, M.: Chemical ozone loss in a chemistry-climate model from 1960 to 1999, *Geophys. Res. Lett.*, 33, L15820, doi:10.1029/2006GL026939, 2006. 183

Manzini, E., Steil, B., Brühl, C., Giorgetta, M. A., and Krüger, K.: A new interactive chemistry-climate model: 2. Sensitivity of the middle atmosphere to ozone depletion and increase in greenhouse gases and implications for recent stratospheric cooling, *J. Geophys. Res.*, 108(D14), 4429, doi:10.1029/2002JD002977, 2003. 183

Riede, H., Jöckel, P., and Sander, R.: Quantifying atmospheric transport, chemistry, and mixing using a new trajectory-box model and a global atmospheric-chemistry GCM, *Geosci. Model Dev.*, 2, 267–280, 2009. 183

Sander, R., Kerkweg, A., Jöckel, P., and Lelieveld, J.: Technical note: The new comprehensive atmospheric chemistry module MECCA, *Atmos. Chem. Phys.*, 5, 445–450, 2005, <http://www.atmos-chem-phys.net/5/445/2005/>. 183

Sander, R., Baumgaertner, A. J. G., Gromov, S., Harder, H., Jöckel, P., Kerkweg, A., Ku-

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

- bistin, D., Riede, H., Taraborrelli, D., and Tost, H.: The atmospheric chemistry box model CAABA/MECCA-3.0, Geosci. Model Dev., in preparation, 2010. 183, 185
- Sandu, A. and Sander, R.: Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, Atmos. Chem. Phys., 6, 187–195, 2006, <http://www.atmos-chem-phys.net/6/187/2006/>. 183
- Steil, B.: Modellierung der Chemie der Strato- und Troposphäre mit einem drei-dimensionalen Zirkulationsmodell, Ph.D. thesis, Institut für Meteorologie, Universität Hamburg, 1997. 187
- 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, <http://www.ann-geophys.net/16/205/1998/>. 183
- Steil, B., Brühl, C., Manzini, E., Crutzen, P. J., Lelieveld, J., Rasch, P. J., Roeckner, E., and Krüger, K.: A new interactive chemistry-climate model: 1. Present-day climatology and inter-annual variability of the middle atmosphere using the model and 9 years of HALOE/UARS data, J. Geophys. Res., 108(D9), 4290, doi:10.1029/2002JD002971, 2003. 183
- Tost, H., Jöckel, P., Kerkweg, A., Sander, R., and Lelieveld, J.: Technical note: A new comprehensive SCAVenging submodel for global atmospheric chemistry modelling, Atmos. Chem. Phys., 6, 565–574, 2006a. 188, 195
- Tost, H., Jöckel, P., and Lelieveld, J.: Influence of different convection parameterisations in a GCM, Atmos. Chem. Phys., 6, 5475–5493, 2006b. 188
- Tost, H., Jöckel, P., and Lelieveld, J.: Lightning and convection parameterisations – uncertainties in global modelling, Atmos. Chem. Phys., 7, 4553–4568, 2007, <http://www.atmos-chem-phys.net/7/4553/2007/>. 188

**GMDD**

3, 181–200, 2010

---

**A fast stratospheric  
chemistry solver in  
EMAC**

A. J. G. Baumgaertner et  
al.

---

[Title Page](#)

[Abstract](#)

[Introduction](#)

[Conclusions](#)

[References](#)

[Tables](#)

[Figures](#)

[⏪](#)

[⏩](#)

[◀](#)

[▶](#)

[Back](#)

[Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.

**Table 1.** Overview of the performed EMAC simulations.

Simulation	S-E4CHEM	S-MECCA(E4CHEM)	S-MECCA(EVAL)
Chemistry submodel	E4CHEM	MECCA, selected mechanism similar to E4CHEM	MECCA, mechanism from evaluation study
Tracer families for transport	NO <sub>x</sub> , ClO <sub>x</sub> , O <sub>x</sub> , HNO <sub>3</sub> + NAT	NO <sub>x</sub> , ClO <sub>x</sub> , O <sub>x</sub>	NO <sub>x</sub> , ClO <sub>x</sub> , BrO <sub>x</sub>
Scavenging see Tost et al. (2006a)	simplified scavenging (effective Henry's law (pH 5))	simplified scavenging (effective Henry's law (pH 5))	detailed algorithm, as in evaluation study by Jöckel et al. (2006)
Heterogenous chemistry and polar stratospheric clouds	accounted for in E4CHEM core	submodels HETCHEM and PSC	submodels HETCHEM and PSC

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

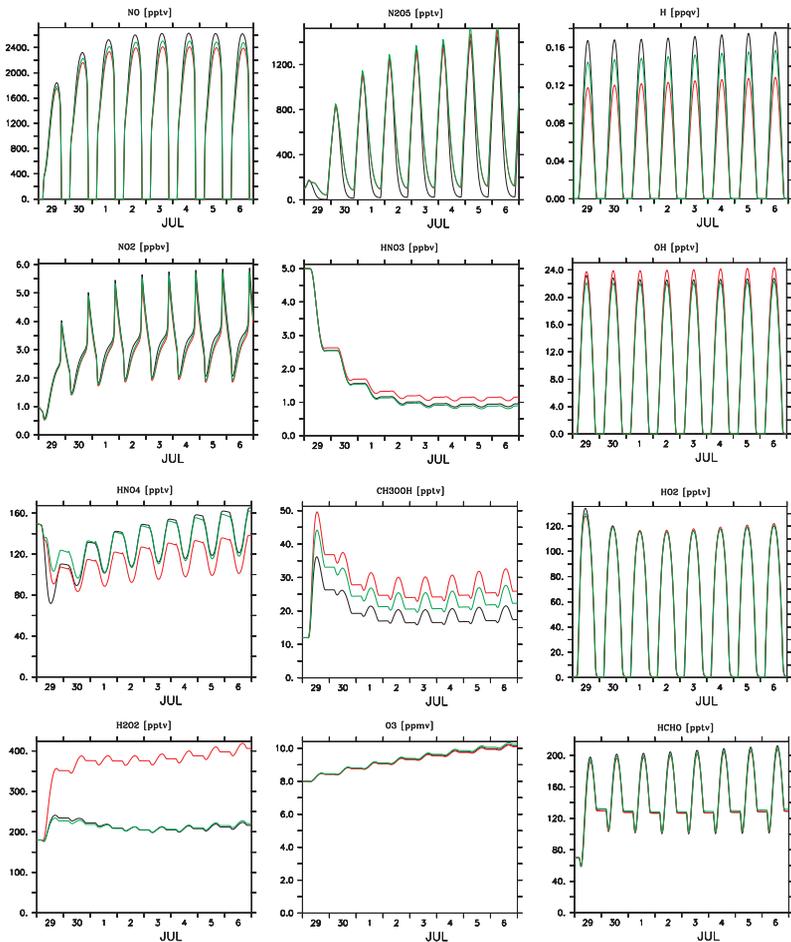
Back

Close

Full Screen / Esc

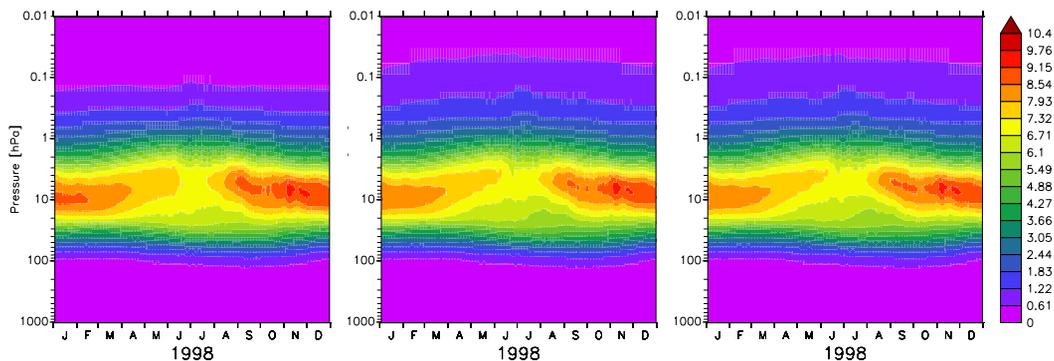
Printer-friendly Version

Interactive Discussion

**A fast stratospheric  
chemistry solver in  
EMAC**A. J. G. Baumgaertner et  
al.

**Fig. 1.** CAABA box model simulation results with MECCA (black), E4CHEM with original rates (red), and E4CHEM with updated rates (green) for selected species.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

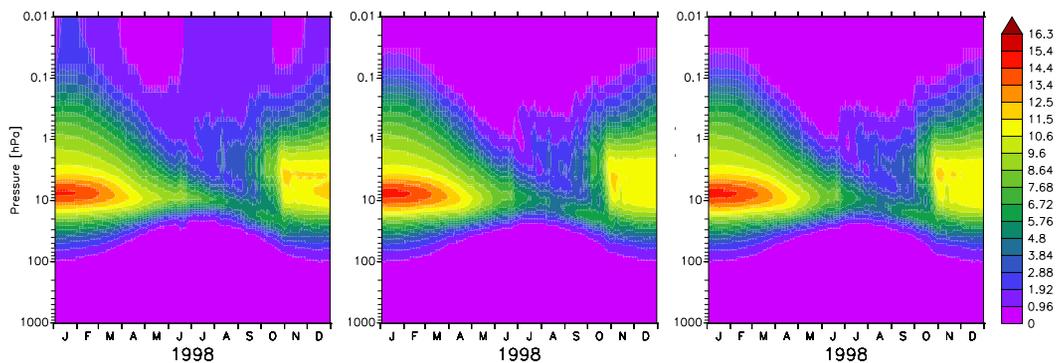
**A fast stratospheric  
chemistry solver in  
EMAC**A. J. G. Baumgaertner et  
al.

**Fig. 2.** EMAC ozone ( $\mu\text{mol/mol}$ ) from simulations with S-E4CHEM (left), S-MECCA(E4CHEM) (middle) and S-MECCA(EVAL) (right) for the zonal average at  $30^\circ\text{S}$ – $50^\circ\text{S}$ .

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

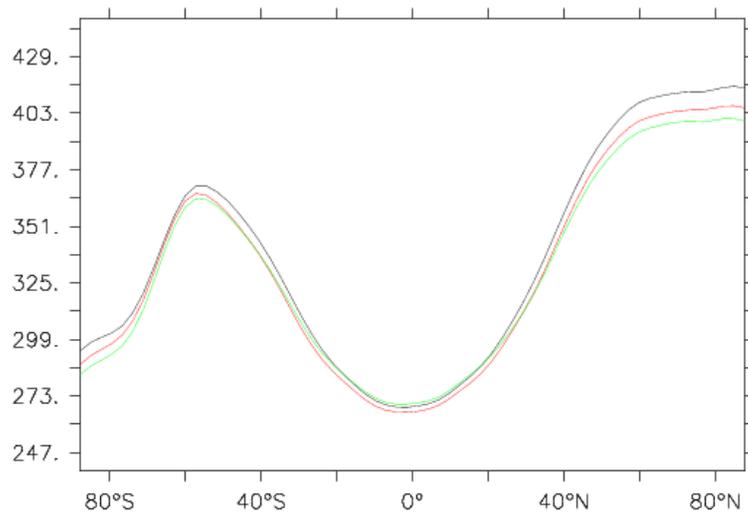
## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.



**Fig. 3.** Same as Fig. 2 but for  $\text{NO}_x$  (nmol/mol) for the zonal average at  $60^\circ\text{S}$ – $90^\circ\text{S}$ .

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

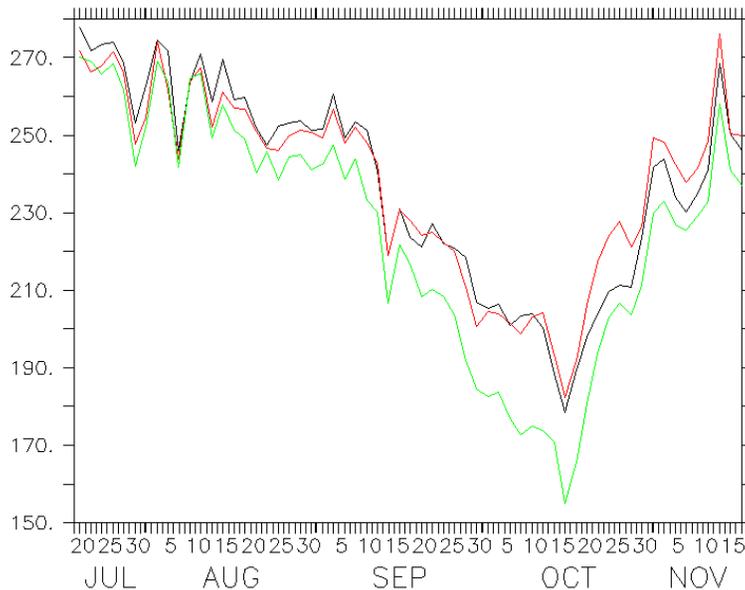
**A fast stratospheric  
chemistry solver in  
EMAC**A. J. G. Baumgaertner et  
al.

**Fig. 4.** Zonal and time average (January–December 1998) of total column ozone (DU) for S-E4CHEM (black), S-MECCA(E4CHEM) (red) and S-MECCA(EVAL) (green).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

## A fast stratospheric chemistry solver in EMAC

A. J. G. Baumgaertner et al.



**Fig. 5.** Minimum total column ozone (DU) for S-E4CHEM (black), S-MECCA(E4CHEM) (red) and S-MECCA(EVAL) (green).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)