A CHEMISTRY MODEL FOR USE IN COMPREHENSIVE CLIMATE MODELS

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Abstract. A complex chemistry model for use in 3D-modelling has been developed from the chemistry code of the Mainz 2D-Model to describe the major aspects of stratospheric homogeneous and heterogeneous chemistry and by including the methane and carbon monoxide oxidation chain, also of tropospheric chemistry. The routine has been coupled to the HAMBURG GCM, ECHAM. Results of an one year integration are presented.

Introduction

Because of the principal difficulties of 2D models in describing the transport especially in the lower stratosphere, a chemical module for ECHAM has been developed. Two general problems which arise in implementing a chemistry module in a GCM should be mentioned.

The rates for heterogeneous processes depend very sensitively on the temperature and water vapour concentration, which governs the formation of PSC particles and the activation of chlorine on the sulfate aerosol. It is well known (Boer et al., 1991, Roeckner et al., 1992) that a common deficiency of GCM's is a cold bias in the polar upper troposphere and lower stratosphere, which is nearly independent of season, hemisphere, model physics or horizontal resolution and possibly caused by an insufficient vertical resolution of the stratosphere.

A goal should be to prognose height dependent changes in the radiation budget due to the change in various greenhouse gase. So the chemically calculated changes have to feed back to the radiation transfer code of the GCM. In doing so one expects stability problems, well known from coupling GCM's with ocean models, due to the non linearity of the two models.

Model Description

The chemistry module encompasses the following prognostic chemical species, families and aerosols:

H_2O, CH_4, N_2O, HNO_3, HCl, H_2O_2, CO, CH_3O_2H,
type I PSC's ($NAT : HNO_3.3H_2O$), type II (ice) PSC's,

$$
\begin{aligned}
ClOX &= Cl + ClO + ClOH + ClNO_3 + 2 \cdot Cl_2O_2 + 2 \cdot Cl_2, \\
NOX &= N + NO + NO_2 + NO_3 + HNO_4 + ClNO_3 + 2 \cdot N_2O_5, \\
OX &= O_3 + O(^3P) + O(^1D) + ClO + ClOH + 2 \cdot ClNO_3 + 2 \cdot Cl_2O_2 + \\
&\quad NO_2 + HNO_3 + HNO_4 + 2 \cdot NO_3 + 3 \cdot N_2O_5 \cdot
\end{aligned}
$$

Intermediate products of the methane oxidation, such as CH_2O, CH_3O_2, CH_3O and the HOX-family : $H + OH + HO_2$ are computed from diagnostic equations. For type I

PSC's the model mixing ratios of HNO_3 and H_2O and temperatures are used with the expression of Hanson and Mauersberger (1988) to predict when they are thermodynamically possible. For type II PSC's the equilibrium pressure of water vapour over ice is determined to decide if they can exist. For NAT and ICE an unimodular distribution is assumed with prescribed number densities $n_{NAT} = 1cm^{-3}$ and $n_{ICE} = 0.1cm^{-3}$. The sedimentation of NAT and ICE particles is included to describe the denitrification in the Antarctic stratosphere. It is assumed that ICE particles are nucleating on the biggest NAT particles, so that NAT is removed by the sedimentation of ICE. The stratospheric sulfuric acid aerosol droplet distribution is described according WMO 1991 statistic. The model includes an option for the use of a flux-correction for the temperatures used by the chemistry with data from an ECMWF-climatology.

The photolysis-routine of the Mainz 2D-Model (Brühl, 1989) has been coupled with ECHAM. Photolysis rates are calculated every three days for the full diurnal cycle and 8 longitude sections considering the ECHAM clouds, albedo, temperature and pressure.

The model is running with initial data from the 2D-model. The background destribution of the most important source gases for chlorine radicals: $F11$, $F12$, CCl_4, CH_3Cl, CH_3CCl_3 are also taken from the 2D-model to limit the CPU-Time requirements. Sources and sinks of various gases in the troposhere are parameterized using experience from 3D-model MOGUNTIA and a scheme developed by G.J. Roelofs and J. Feichter.

Results and Discussion

The simulation presented here is done with a prelimenary version of ECHAM IV, T21, with a horizontal resolution of 5.6° and 19 layers up to 10 hPa (DKRZ 1992, Roeckner). The temperature correction scheme for the chemistry is not used.

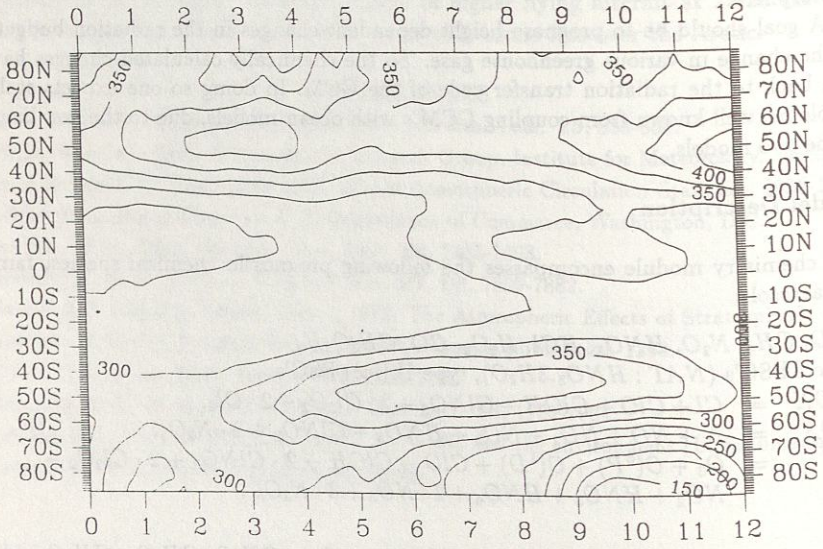

Fig. 1 Variation of total ozone, [*Dob.*], with latitude and season for the first year of integration.

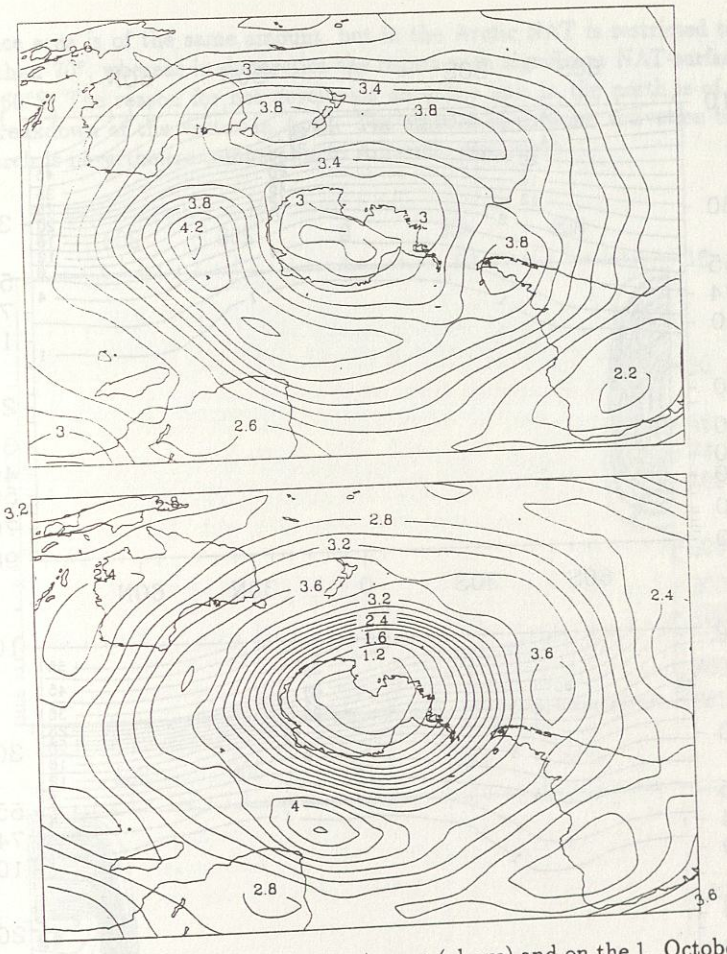

Fig. 2 Ozone, [*ppmv*], in 55 hPa on the 1. August (above) and on the 1. October (below).

To get a general impression of the mean state of the model the global total ozone distribution versus latitude and time is shown in Fig.1. The development of an ozone hole during the Antarctic spring can clearly be seen. It starts to develop in the mid of August, reaches the maximal ozone depletion in October and November, with values below 150 [*Dob.*] in latitudes higher than 80°. The ozone columns begin to recover in December. The stereographic projection in Fig.2 gives an impression of the vortex and the ozone depletion inside the vortex by comparing the ozone volume mixing ratio at 55 hPa. Fig.1 also shows two problems of the model in describing ozone, which may be caused by the coarse vertical resolution of the stratosphere and cold bias in the lower stratosphere. The ozone columns In the northern hemisphere and in the tropics are about 30[*Dob.*] units to high and the natural minima seem to be shifted. This is most pronounced in the northern hemisphere, where the minimum for middle latitudes occure in August and September and not in September and October.

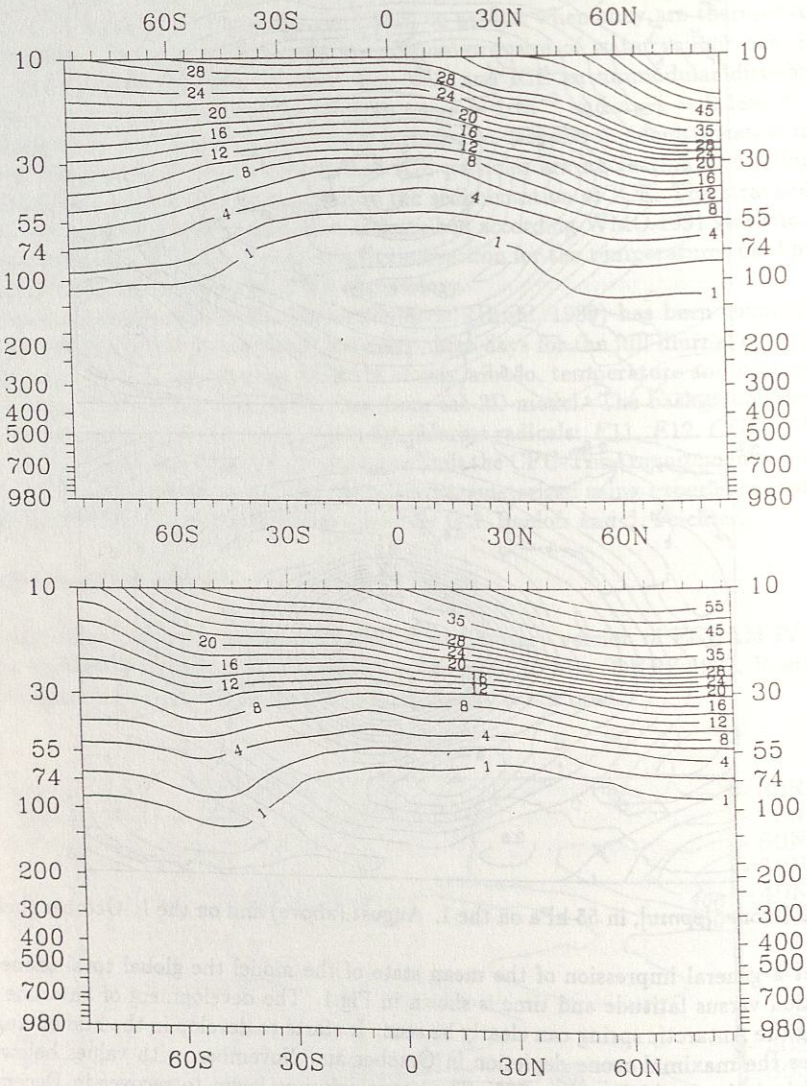

Fig. 3 $NOY = NOX + HNO_3 + NAT$, [*ppbv*], April-mean (above), August-mean (below).

From Fig. 3 the effect of dinitrification during the Antarctic winter on the total NOY can be seen. Dinitrification takes place between 60°S - 90°S and reaches south of 70°S values of 50 - 70%. A control run without sedimentation (not presented on this conference) shows that the dinitrification causes an additional ozone loss of about 30[*Dob.*]. A comparison of NAT-surfaces (Fig.4) between Arctic and Antarctic indicates that the values

of surface area is of the same amount, but in the Arctic NAT is restricted to latitudes higher than 70°, whereas in Antarctica the region with significant NAT-surfaces reaches almost 60°S. The reason for not developing an ozone hole in the north is of course the rapid breakdown of the vortex in April. The amount of chlorine activation in February and March is nevertheless comparable to Antarctic conditions.

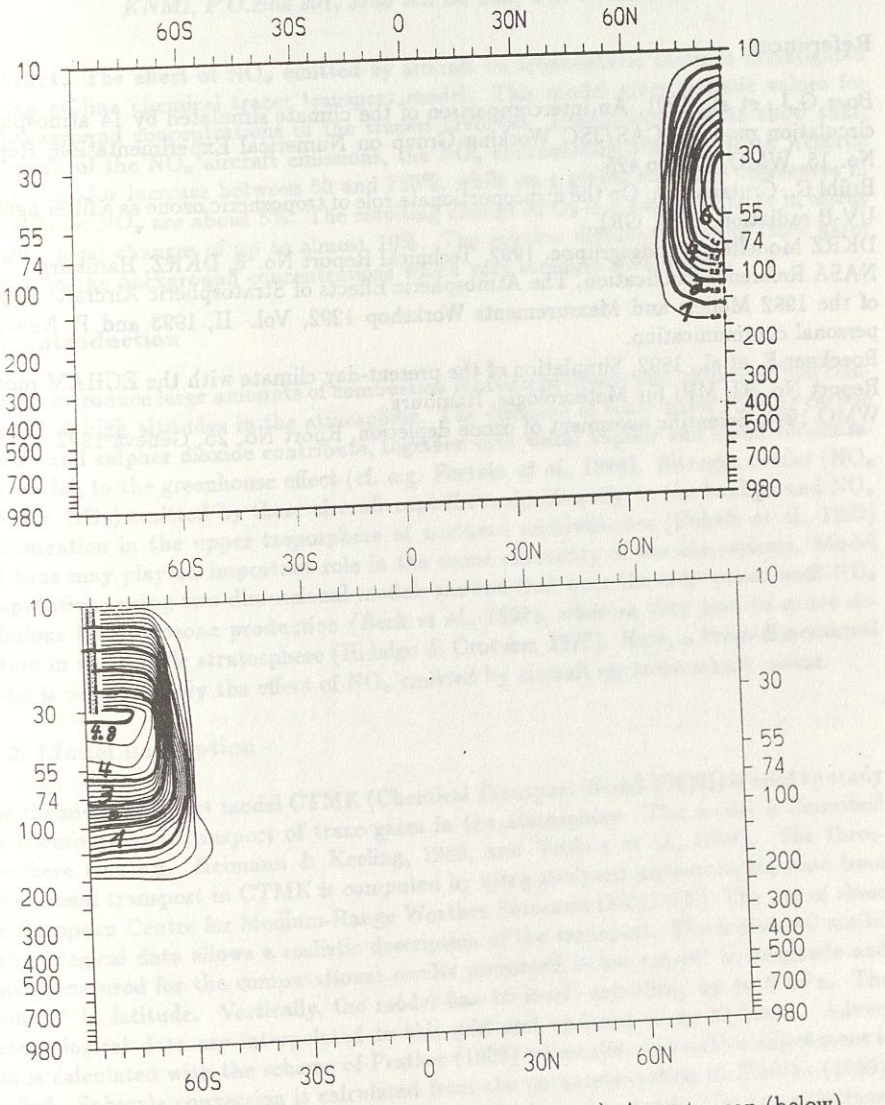

Fig. 4 NAT-Surfaces, $[10^{-8} cm^2/cm^3]$, March-mean (above), August-mean (below).

Finally we can say that beside of the deficiencies of the model, coarse vertical resolution of the stratosphere, cold bias in the lower stratosphere and upper troposphere, some main features are represented remarkably well and the model seems to have the potential to be a good tool to investigate the complex impact of aircraft emissions.

References

Boer G.J., et al., 1991, An intercomparison of the climate simulated by 14 atmospheric circulation models. CAS/JSC Working Group on Numerical Experimentation, Report No. 15, WMO/TD-No.425.

Brühl C., Crutzen P.J., On the disproportionate role of troposheric ozone as a filter against UV-B radiation, 1989, GRL.

DKRZ Modellbetreuungsgruppe, 1992, Technical Report No. 6, DKRZ, Hamburg.

NASA Reference Publication, The Atmospheric Effects of Stratospheric Aircraft: Report of the 1992 Models and Measurements Workshop 1292, Vol. II, 1993 and P. Newman personal communication.

Roeckner E. et al., 1992, Simulation of the present-day climate with the ECHAM model. Report No. 93, MPI für Meteorologie, Hamburg.

WMO 1991, Scientific assesment of ozone depletion, Rport No. 25, Geneva 1992