Present and Future of Modeling Global Environmental Change: Toward Integrated Modeling,
Eds., T. Matsuno and H. Kida, pp. 383–390.

Development of CCSR/NIES Nudging CTM and Ozone Simulation

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Abstract—Development of a new chemical transport model is described. The model has been developed based on CCSR/NIES AGCM. A nudging technique is used to assimilate the temperature and horizontal wind velocity data into the calculation values of the GCM. Photolysis rates of chemical species are directly calculated in the model by the two-stream approximation of the radiation transfer that is used for atmospheric heating rate calculations. Column amount distribution of ozone and the seasonal variation, and the distributions of HO_x, NO_x, ClO_x, and BrO_x in 1997 are simulated by the model with T10, T21, and T42 horizontal resolutions. It is shown that the T21 and T42 models simulate the global distributions of chemical species excellently.

INTRODUCTION

Chemical transport model is a powerful tool for studying the mechanisms of three-dimensional (3-D) distributions of chemical species in the atmosphere. Several 3-D chemical transport models have been developed and the developments are being continued for better understanding of global distribution of chemical constituents as well as the ozone depletion in the Antarctic and in the Arctic (e.g. Brassuer *et al.*, 1997; Lefevre *et al.*, 1998; Chipperfield, 1999). In order to develop a fully coupled, chemical-radiative-dynamical interactive model for prediction of future ozone layer, chemistry-radiation-coupled scheme must be incorporated into a GCM. The final goal of this study is to develop a 3-D chemical model that can be used both as a Chemical Transport Model constrained by meteorological data, and as a chemical-radiative-dynamical fully interactive GCM. Such model will enable us to check the chemical scheme and the advection scheme of the model by comparisons with observations. At the same time, a reliable prediction of future ozone in the chemical-radiative-dynamical interactive model will be possible. In this paper, development of a new CTM is described, then the calculated distributions and variations of several chemical species in 1997, when ILAS O_3, N_2O, and HNO_3 data were available, are shown and compared with the observations.

MODEL DESCRIPTION

A stratospheric nudging Chemical Transport Model has been developed in NIES based on CCSR/NIES AGCM (Center for Climate System Research, University of Tokyo/National Institute for Environmental Studies Atmospheric General Circulation Model), which has been developed by Numaguti (1993), Numaguti *et al*. (1995), and Numaguti *et al*. (1997). A detailed description of the dynamical, radiative, and chemical component of the privious version of our chemistry coupled GCM was given in Takigawa *et al*. (1999). The new nudging CTM was developed by incorporating a nudging module into the model and by replacing the chemical scheme with a more sophisticated one that has been developed in NIES and used in a 1-D coupled chemistry-radiation model (Akiyoshi, 2000).

The model includes BrO_x chemistry and heterogeneous reactions on NAT/ICE clouds in the stratosphere as well as the O_x, HO_x, NO_x, hydrocarbons, ClO_x gas phase chemical reactions for the stratosphere. The chemical species and the families predicted numerically in this model are O_x ($O(^1D) + O + O_3$), NO_x ($N + NO + NO_2 + NO_3$), ClO_x ($Cl + ClO + 2Cl_2O_2 + ClOO + OClO$), BrO_x ($Br + BrO$), CH_4, CO, N_2O, CCl_4, $CFCl_3$, CF_2Cl_2, CH_3CCl_3, CH_3Cl, $CClF_2CCl_2F$, $CHClF_2$, H_2O, HF, H_2O_2, HNO_3, HNO_4, N_2O_5, $ClONO_2$, HCl, HOCl, CF_2ClBr, CF_3Br, CF_2Br_2, $CHBr_3$, CH_3Br, HBr, HOBr, $BrONO_2$, Cl_2, Br_2, NO_y ($NO_x + HNO_3 + HNO_4 + 2N_2O_5 + ClONO_2 + BrONO_2$), Cl_y ($ClO_x + HCl + HOCl + ClONO_2 + BrCl + 2Cl_2$), and Br_y ($BrO_x + HBr + HOBr + BrONO_2 + BrCl + 2Br_2$). CH_3O_2, CH_3OOH, CH_2O, OClO, and BrCl were also predicted, but photochemical equilibrium concentrations were assumed during daytime. During nighttime, it was assumed that O_3 concentration was equal to O_x concentration, HO_2 concentration was equal to HO_x concentration, and the sum of NO_2 concentration and NO_3 concentration was equal to NO_x concentration. The nighttime chemical equilibrium concentration of NO_3 was calculated by using the equilibrium equation of Aliwell and Jones (1996). Nighttime chemical equilibrium was also assumed for ClO, Cl_2O_2, Br, and BrO.

Thirteen heterogeneous reactions were considered in the model. These reactions were tabulated in table 2 of Sessler *et al*. (1996). The code of a box model version of SLIMCAT model was used for the reactions. In this work, only NAT and ICE were considered as PSCs. The condensation process of H_2O and HNO_3 to generate PSCs was considered in the model stratosphere, which was defined as the region where the amount of water vapor mixing ratio was less than 6 ppmv.

Photolysis rates of chemical species were calculated directly from the outputs of the solar radiation fluxes in the model. The solar energy absorbed by all radiatively active chemical species, which was calculated by the convergence of solar radiation fluxes in an atmospheric layer, was distributed into the energy absorbed by each chemical species, weighted by absorption cross sections of chemical species (Akiyoshi, 2000).

The Schuman-Runge band photolysis processes of H_2O_2, N_2O, HNO_3, HNO_4, HCl, $ClONO_2$, CFCs were not included in the previous versions of our chemical 3-D models. The CCSR/NIES AGCM, which is the basic frame of the nudging CTM, does not include the ultraviolet radiation less than 200 nm, because the CCSR/NIES AGCM was originally a climate model, and the Schmann-Runge band effects on atmospheric energy budget in the troposphere is negligible. However, the effects cannot be neglected for photolysis process of chemical species in the stratosphere. Thus in the new version of the nudging CTM, the photolysis rates in the Schumann-Runge bands were calculated separately and added to the photolysis rates at wavelength more than 200 nm that was computed by the radiation code of the CCSR/NIES AGCM. The radiation flux parameterization in the Schumann-Runge bands by Minschwaner *et al.* (1993) was used.

The zonal wind velocity, the meridional wind velocity, and the temperature of ECMWF data were input at 0:00 UT every day, interpolated linearly with respect to the time step of the model, which is variable between 20 minutes and several minutes according to computation stability. Then the interpolated values were assimilated into the model with the nudging method,

$$\frac{dx}{dt} = -\frac{\left(x - x_{\mathrm{obs}}\right)}{\tau}, \quad x = u, v, T, \quad \tau = 1 \text{ day},$$

where u is zonal wind velocity, v is meridional wind velocity, and T is temperature, x is GCM values of u, v, and T, x_{obs} is the ECMWF data values (observation values), τ is the time scale of nudging. The time scale of 1 day was used for the calculation. Above 10 hPa, where no ECMWF data exist, monthly, zonal-mean CIRA temperature data were input into the model every month, and interpolated linearly with respect to the model time step, and nudged to the zonal-mean values of the model temperature. Thus vertical wind velocity was calculated in the model by the continuity equation.

RESULTS

The nudging processes greatly improved the temperature and wind distributions in the model compared with those calculated without it.

Temperature and zonal wind in the nudging CTM

Zonal-mean temperature difference between the ECMWF data and the nudging CTM was within 2 K below 10 hPa. The difference depends on the nudging time scale, and it was set to 1 day in this study. Figure 1 shows the monthly-mean zonal-mean temperature difference between the ECMWF data and the nudging CTM in March 1997. The nudging CTM temperature is –1.5 K cooler than the ECMWF data at the tropical tropopause, and this bias may affect the H_2O budget in the stratosphere.

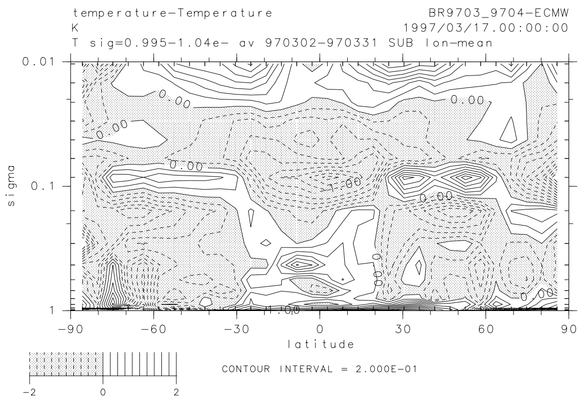


Fig. 1. Zonal-mean temperature difference between the ECMWF data and the nudging CTM in March 1997.

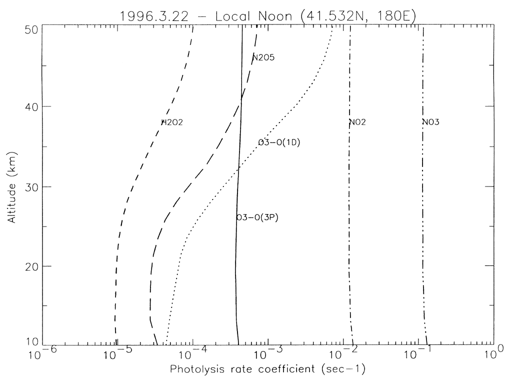


Fig. 2. Calculated vertical profiles of photolysis rates of O_3, H_2O_2, NO_2, NO_3, and N_2O_5 at 41.532N, 180E, at local noon.

Photolysis rate profiles

Photolysis rates of chemical species were calculated directly from the radiation flux convergence in each atmospheric layer of the model. The calculated profiles at local noon on March 22 are shown in Fig. 2. To verify the calculation, the profiles were compared with those of the JPL-97 profiles. The calculated photolysis rate profiles were very close to those of JPL-97, and this result shows that the photolysis calculations in the model were done successfully.

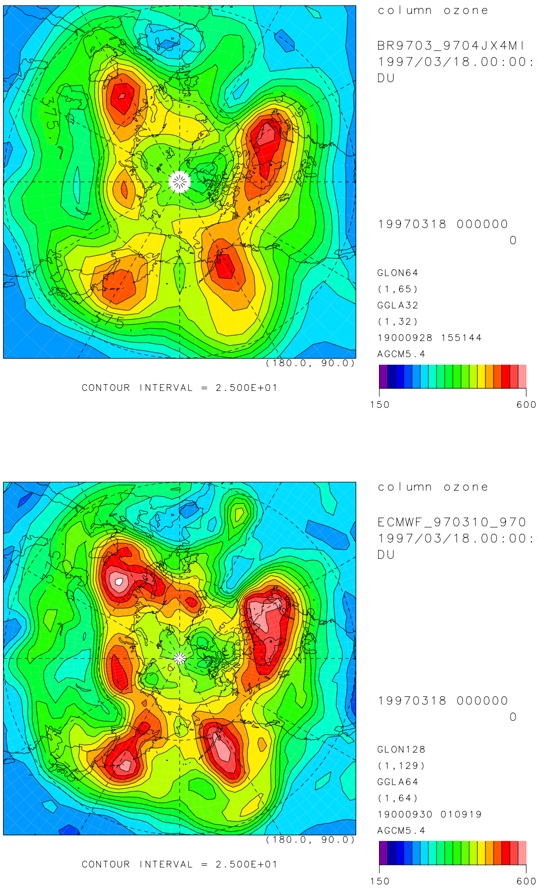
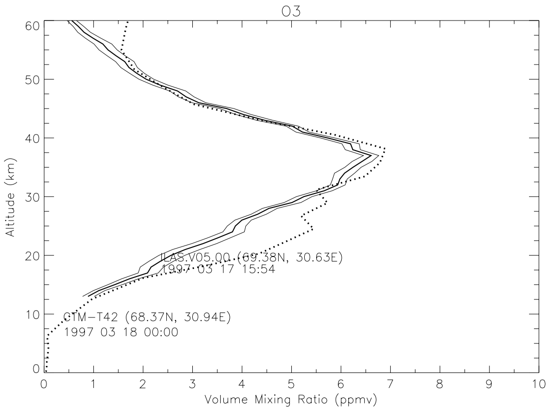
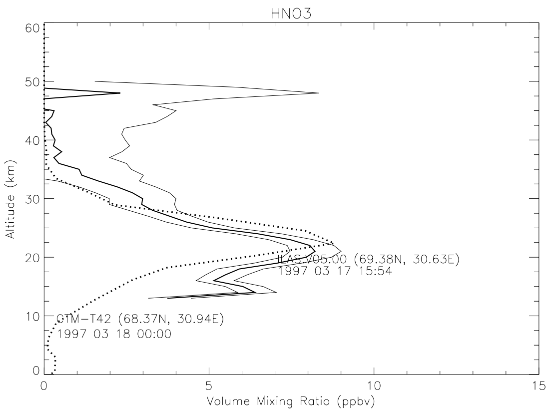


Fig. 3. Total ozone distribution in the Arctic at 0:00 UT on 18 March 1997 calculated by CCAR/NIES nudging CTM. By T21 model (upper) and by T42 model (lower).

Total ozone

Figure 3 shows the total ozone distribution in the Arctic region calculated by the T21 (5.6° × 5.6°) model and the T42 (2.8° × 2.8°) model at 0:00 UT. The distribution was simulated well, although the total ozone amount in the high latitudes is a little higher than the observation. The distributions had also been calculated by a low resolution T10 (11.2° × 11.2°) model, but the low resolution model was not capable to simulate the Arctic ozone distribution accurately. The improvement of the Arctic ozone distribution by using the T42 model instead of the T21 model was not substantial for the planetary scale distribution simulation. But the use of the T42 model may be necessary for comparisons of the vertical





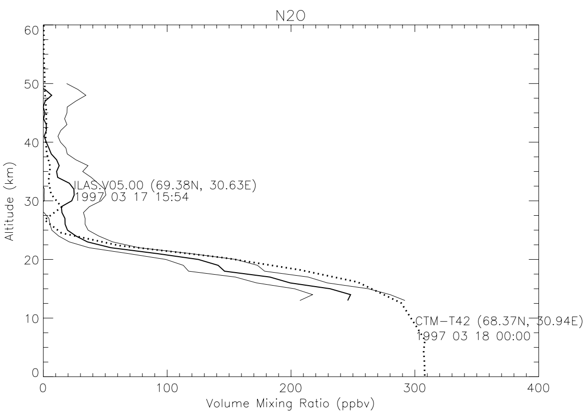


Fig. 4. (a) Comparison between nudging CTM O_3 profiles at 68.368N, 30.938E at 0:00 UT on 18 March 1997 (dotted line), and ILAS Ver. 5.00 O_3 profile at 69.38N, 30.63E at 15:54 on 17 March 1997 (solid line). (b) HNO_3. (c) N_2O.

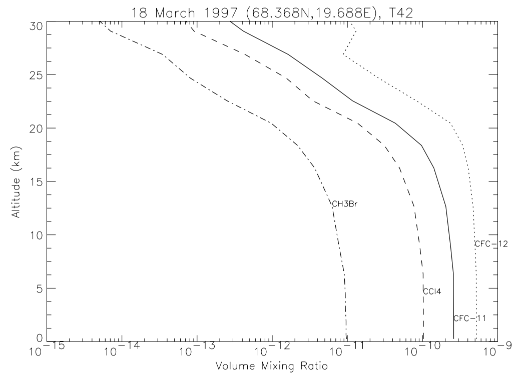


Fig. 5. Calculated profiles of CFCs and CH_3Br at 68.368N, 19.688E on 18 March 1997.

distribution and the time variation of chemical species at a location with the observation, because those at a location are considerably affected by the small scale distribution. At least horizontal T21 resolution is necessary for a realistic simulation of Arctic ozone distribution.

O_3, HNO_3, and N_2O vertical profiles—Comparison with ILAS observation

The vertical distribution of O_3 mixing ratio of the T42 model was compared with ILAS V05.00 data, which were analyzed by ILAS science team. The data point is inside the Arctic polar vortex near the vortex boundary on 18 March 1997. The calculated ozone amount is a little higher as shown by dashed line in Fig. 4(a). Figures 4(b) and (c) are the vertical distributions of HNO_3 and N_2O, respectively. The dashed lines show the calculated profiles. The HNO_3 profile was improved by including $H_2SO_4/HNO_3/H_2O$ ternary solution aerosols, and the N_2O profiles was improved by including Schumann-Runge band absorption effects into the model.

Water vapor in the stratosphere

Water vapor in the stratosphere of this model is supplied from the troposphere through the condensation process of water vapor due to the convection and oxidation of CH_4. The zonal mean meridional distribution of $H_2O + 2CH_4$. In the stratosphere was around 5.5 ppmv, a little smaller than the observation value of 6 ppmv.

CFC-11, CFC-12, CCl_4, and CH_3Br

The calculated profiles of CFCs and CH_3Br near the Kiruna station on 18 March 1997 are shown in Fig. 5. The profiles of CFC-11 and 12 are so close to the observation profiles obtained by the ILAS validation campaign.

CONCLUDING REMARKS

The nudging Chemical Transport Model simulated 3-D distributions and seasonal variations of chemical species, although there is small discrepancy between the calculations results and the observations in temperature, wind field, absolute amount of total ozone in the Arctic region. The calculations with a STS/ICE scheme are also going on, and the results and comparison with observations will be shown in the near future. Since it is easy to modify the model into a full-coupled chemistry GCM, the model will be used both as a CTM and as a chemical-radiative-dynamical full interactive GCM for atmospheric chemistry-transport studies and for prediction of the future ozone layer.

Acknowledgments—Computations were made on the NEC SX-4 in NIES. The GFD-DENNOU library 5.0.1 and the GTOOL 3.5 was used for Figs. 1 and 3.

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