Development of a chemical model of the Polar Regions

A. Kagawa and S. Hayashida

Faculty of Science, Nara Women's University, Nara, Japan

Abstract. The purpose of our study was to develop a chemical model to apply to polar ozone studies. We integrated a chemical model with photodissociation coeffi cients, PSC growing effects, and a trajectory tool. The numerical code used to calculate the mixing ratios of minor gas species was provided by ACD (Atmospheric Chemistry Division)/NCAR. We included sufficient species and chemical and photolysis reactions. The photodissociation coefficients for exceeding 90 degrees were calculated to apply the model to studies of the Polar Regions in winter and spring. A trajectory tool provided by EORC (Earth Obser vation Research Center)/ NASDA was used to calculate the trajectory from the ECMWF meteorological data. We also included PSC growth along with temperature change on trajectories assuming both supercooled ternary solution (STS) and nitric acid trihvdrate (NAT). Preliminary re sults from the model will be compared with satellite data.

Introduction

Since the first appearance of the Antarctic ozone hole in the early 1980s, the magnitude and extent of the ozone loss over Antarctica has grown each spring. Over the Arctic, a significant reduction in the ozone content was observed during late winter and early spring in six of the last nine years [*WMO*, 1998]. It is well recognized that heterogeneous reactions on polar stratospheric clouds (PSCs) play an important role in polar ozone depletion, because they con vert inactive chlorine from anthropogenic species to active chlorine that destroys ozone in the polar spring [e.g., *Solo mon*, 1990].

To estimate the chemical ozone loss in the Polar Re gions, *Becker et al.* [1998] compared box model calcula tions with the observed ozone loss determined from the 'Match' experiment for the 1991/92 Arctic winter. The Match experiment derives chemical ozone loss from a pair of balloon soundings that measure ozone in the same air parcel at different points on a trajectory [e.g., *Rex et al.*, 1997].

The aim of our study was to develop a chemical model to apply to polar ozone studies. We plan to integrate the chemical model with photodissociation coefficients, PSC growing effects, and a trajectory tool. Preliminary results from the model will be compared with satellite data.

Model Description

The numerical code used to calculate the mixing ratios of chemical species was provided by Lamarque and Walters, of the Atmospheric Chemistry Division (ACD), NCAR. The code uses RODAS and it is essentially the RungeKutta method [*Sandu et al.*, 1997]. We included 58 species, 50 photolysis reactions, and 112 gas phase reac tions. Heterogeneous reactions included in this model include:

$$N_2O_5 + H_2O = 2HNO_3 \text{ gamma} = 0.1$$
 (1)

$$CIONO_2 + HCl = Cl_2 + HNO_3$$
(2)

$$CIONO_2 + H_2O = HOC1 + HNO_3$$
(3)

$$HOC1 + HC1 = C1_2 + H_2O$$
(4)

The reaction rates of (2)-(4) are strongly dependent on temperature and therefore reactions (2)-(4) become important at low temperatures, as encountered in the polar winter. Reaction (1) is most important at warm mid-latitudes. Bromine reactions are included according to *Portmann et al.* [1996].

$$BrONO_2 + H_2O = HOBr + HNO_3$$
 (5)

$$HOBr + HCl = BrCl + H_2O$$
(6)

The chemical reaction and photolysis data are taken from *DeMore et al.* [1997]. We included recently updated key reactions in the stratosphere according to *Sander et al.* [2000]. Most of the initial values for chemical species were taken from the output of the 2-D Garcia-Solomon model [*Solomon et al.*, 1985], although some satellite data were also used.

Since polar ozone loss is sensitive to sunlight, the photodissociation coefficients were closely investigated to apply the model to studies of the Polar Regions in winter and spring. We calculate the air mass factor for exceeding 90 degrees according to *Brasseur and Solomon* [1984].

A trajectory tool provided by EORC (Earth Observation Research Center)/NASDA [*Mathuzono et al.*, 1998] was used to calculate the trajectory from the ECMWF meteoro logical data. We also included PSC growth along with temperature change on trajectories assuming both super cooled ternary solution (STS) [*Carslaw et al.*, 1995] and nitric acid trihydrate (NAT) [*Hanson and Mauersberger*, 1988].

Comparison with satellite data

We are going to present a preliminary comparison with satellite data obtained by ILAS (Improved Limb Atmos pheric Spectrometer). ILAS on board ADEOS (Ad

vanced Earth Observing Satellite) made intensive measure

ments of ozone-related species over the Arctic stratosphere in the winter of 1996/97 [*Sasano et al.*, 1999]. This winter was especially important because significant ozone loss was observed over the Arctic [e.g., *Newman et al.*, 1997].

Sasano et al. [2000] estimated the chemical ozone loss rate and the amounts from ILAS data using a technique similar to *Rex et al.* [1997]. This technique derives chemical ozone loss from analysis of a pair of ILAS ozone profiles that measured the same air parcel at different points, using a trajectory calculation. They found a maximum ozone loss rate of 84 ppbv/day on the 450 K potential temperature surface in February. This study demonstrated that satellite data with moderate altitude resolution can be used for the Match analysis.

We tried to estimate chemical ozone loss from ILAS observations using a similar technique to that of *Sasano et al.* [2000]. We used ECMWF meteorological data to calculate trajectories with better resolution and more fre quent measurements than the UKMO (United Kingdom Meteorological Office) data, which *Sasano et al.* [2000] used.

We tried to reproduce the chemical ozone loss in the winter of 1996/97 observed with ILAS. Preliminary re sults from the model will be compared with satellite data.

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