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GLOBAL THREE-DIMENSIONAL CONSTITUENT FIELDS DERIVED FROM PROFILE DATA

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Abstract. The success of 3D simulations of stratospheric constituent variability depends critically on the initialization of the constituent fields within the global model. We describe a technique for generating global 3D fields from vertical constituent profiles. The technique uses potential vorticity (q) and potential temperature (θ) to map the profiles onto the global domain. The profiles used here are obtained from a 2D model calculation that reproduces the relationship between θ, q, N_2O and O_3 observed during the Airborne Arctic Stratospheric Expedition (AASE). The method is verified by comparison with satellite data, aircraft data and model simulations.

Introduction

The Arctic winter is characterized by successive planetary wave events which cause latitudinal and longitudinal stretching of the polar vortex. Compared to the Antarctic, the Arctic shows many more intrusions of middle latitude air to high latitudes with corresponding movement of polar air to lower latitudes. The Rossby wave activity that dominates the northern hemisphere winter circulation is a fundamentally three-dimensional (3D) process.

The measurements of constituent concentrations, pressure, temperature and wind made during the Airborne Arctic Stratospheric Expedition (AASE) characterize the chemical and meteorological state of the north polar region near Stavanger, Norway (59° N, 5° 38" E) during January and February, 1989. This effort uses a 3D model described by Rood et al. [1989] to place the AASE measurements in a global context, and to assess the hemispheric impact of heterogeneous processes within the polar vortex.

Computational constraints limit both the number and duration of 3D calculations. Typically, during the initial period of integration, a 3D model exhibits high variance as fields come into dynamical adjustment. Reducing the initial variance minimizes integration time between initialization and realistic representation of observed variability. Previous model experiments show that 2-3 weeks of integration are needed for constituent fields to develop mature horizontal structure from zonal mean initial conditions. However, using 3D fields from the Limb Infrared Monitor of the Stratosphere (LIMS) the adjustment to the initial fields is significantly reduced.

For AASE there are no 3D data suitable for model initialization in the lower stratosphere. The use of zonal mean data would severely compromise the utility of the 3D model in AASE applications. Therefore, a technique was developed to produce 3D constituent fields that are chemically self-consistent and spatially consistent with wind fields by mapping constituent profiles onto 3D fields. Here, a 2D model [Douglass et al., 1989] is used to provide the profiles to maximize chemical self-consistency and to initialize constituents for which no measurements are available.

The next section presents a short discussion of theory and a description of the technique. This is followed by a validation of results by comparison of the generated fields for ozone with LIMS measurements, Total Ozone Mapping Spectrometer (TOMS) measurements, and AASE measurements. Finally, the model characteristics are highlighted, and model integrations are used to demonstrate the utility of the initialization.

Theory and Method

Schoeberl et al. [1989] have discussed the representation of Airborne Antarctic Ozone Experiment (AAOE) data in potential temperature (θ) - potential vorticity (q) space. Using this representation, they developed an algorithm to reconstruct constituent distributions outside of the ER-2 flight path area. The technique here is based on the consistent, strong relationship between constituents, θ, and q discussed in Schoeberl et al. [1989].

This technique assumes that q is a dynamical tracer, and therefore, transport of q is correlated with transport of constituents. The discussion here is limited to constituents with lifetimes of at least several days so that photochemical processes can be neglected. Initialization techniques for molecules with short lifetimes require explicit consideration of chemical terms [Kaye and Rood, 1989].

While the technique is generally applicable for long lived constituents and families, O_3 is used here as an example. Characteristic O_3 profiles are selected for three latitude bands: the tropics (5° N - 25° N), middle latitudes (35° N - 55° N), and polar vortex (75° N - 85° N). The profiles are fit to polynomial functions of θ; separate functions are defined above and below the ozone mixing ratio peak. Tropospheric ozone is derived from the lowest stratospheric model level, in proportion to the 2D model.

The absolute vorticity (Z = Earth's vorticity + curl of the velocity field), used as a surrogate for potential vorticity, is calculated using winds from the data assimilation [see Rood et al., 1989]. In the stratosphere, where vertical scales are long, the same value of Z can be used to partition the globe at all altitudes. This assumption may

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break down during stratospheric warmings. Values of Z were selected to characterize the vortex, middle latitudes, and tropical air. Contour ranges for each regime were chosen by averaging Z at 30 mb for 10 days in January 1979 during which the polar vortex was undisturbed (Figure 1). These contour ranges are used with the vorticity field on any given day to determine the horizontal structure.

In constructing fields, for each point P(θ,Z) the appropriate θ functions to calculate the O_3 concentration are selected based on the value of Z. For values of Z which are outside the shaded regions given in Figure 1, constituent concentrations for the particular θ are linearly interpolated from the two appropriate functions.

The characteristic ozone profiles could be measured or modeled profiles. Although measured profiles might provide a more accurate representation, for this application ozone profiles are taken from 2D model calculations. This choice ensures chemical consistency among species if several must be initialized simultaneously, and provides a means of initializing species for which insufficient measurements are available (e.g., HCl, HF).

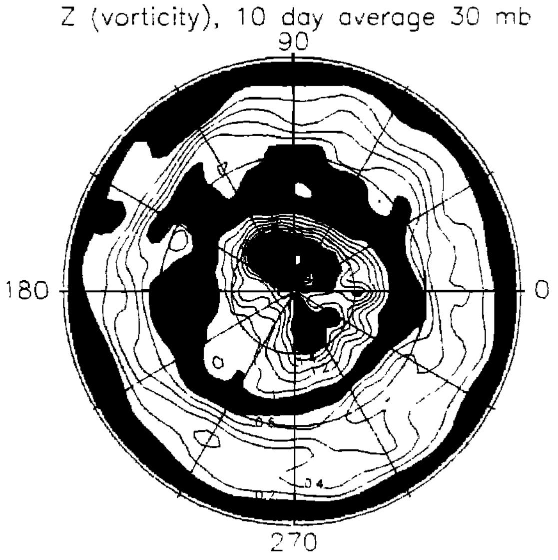

Fig. 1. Average absolute vorticity x $10^4 \mathrm{sec}^{-1}$) for the first 10 days of 1979. Shaded areas represent polar air (Z > 1.6), middle latitude air (0.7 < Z < 1.0) and tropical air (Z < 0.2). Constituent values in intermediate areas are calculated by linear interpolation.

The latitude and time dependence of the zonal mean total ozone produced by the 2D model approximates that of observations [Jackman et al., 1989]. However, the high latitude lower stratospheric values of species such as N_2O and O_3, produced by the 2D model do not agree with the values measured inside the polar vortex during AASE. We have found that it is possible to alter the 2D transport to produce polar values for N_2O and O_3 that are in approximate agreement with measurements for vortex air. Model results used here have reduced horizontal diffusion at 65° N between 13 and 25 km. Calculated N_2O values in this altitude range are substantially smaller than for the base model. Although the ozone mixing ratio peak is broadened and appears at a slightly lower altitude, the total calculated ozone is reasonable because the peak value is reduced by about 1 part per million. The calculated N_2O and O_3 are broadly consistent with the AASE measurements, as shown by the reconstruction technique of Lait et al. [1989].

It is also possible to produce low values of N_2O by increasing the high latitude downward motion. However, this brings the ozone mixing ratio peak to a lower altitude, and produces unreasonably high values of total ozone.

The cases shown here are all derived for northern hemisphere winter; the tropics and southern hemisphere would compare better with data if the same effort were expended. To represent the southern hemisphere properly, profiles as functions of θ are needed in additional latitude bands.

Results

Validation

The derived O_3 fields are validated by comparison with LIMS ozone data, given in Figure 2 Jan. 26 at 30 mb.

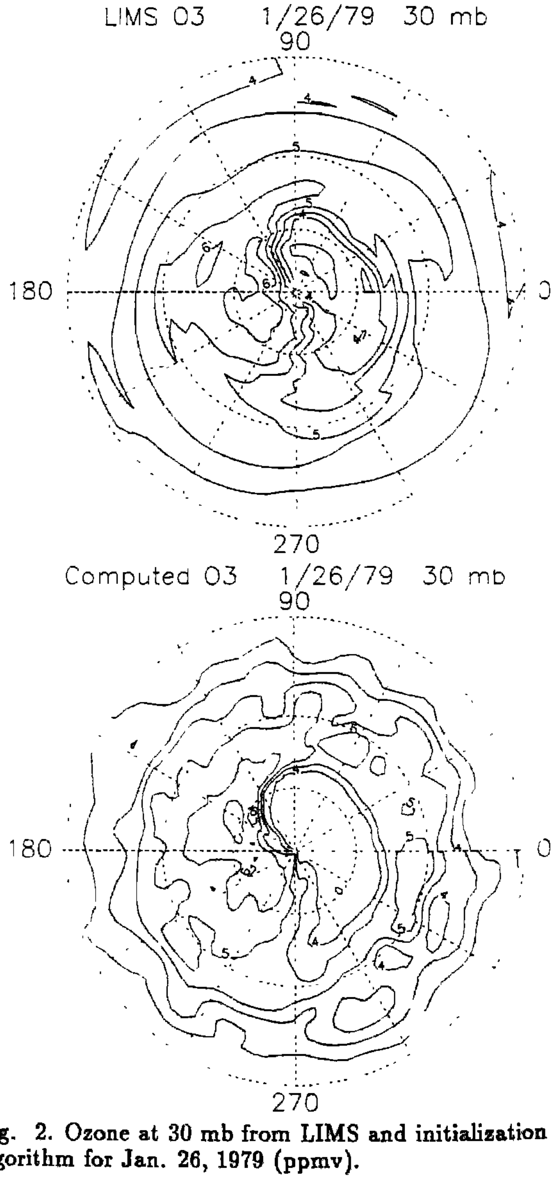

Fig. 2. Ozone at 30 mb from LIMS and initialization algorithm for Jan. 26, 1979 (ppmv).

The vortex on this date is highly disturbed, in contrast to the conditions for which the horizontal partitioning was derived (see Figure 1). In the Aleutian anticyclone, there are irregular areas of 6 ppmv in both fields. The 4 and 4.5 ppmv contours indicate the distinct vortex that is stretched out to middle latitudes during the warming. Note the sharp gradient present in the calculated and measured fields in the narrow region near 120 ° E poleward of 50° N which separates the vortex from the anticyclone. Good agreement is found at all levels up to and including 10 mb, and the calculated total ozone represents both the location and the magnitude of the major features of the TOMS measured field. Agreement between the derived fields and the satellite fields confirms the validity of this method.

AASE

Model calculations for the AASE are needed for January and February, 1989. The model was initialized on Dec. 28, 1988. Figure 3 shows the initial calculated total ozone compared with the TOMS total ozone. This column measurement is the only constituent measurement with nearly global daily coverage for this time period, and therefore, is the best validation field available.

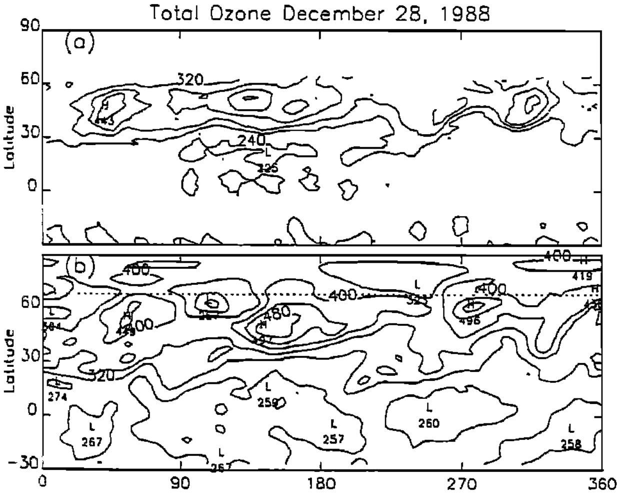

Fig. 3. Total ozone from TOMS and initialization algorithm for Dec. 28, 1988. The dashed line is the northernmost latitude seen by the TOMS instrument (DU)

The initial condition correctly locates the four highs seen between 40° and 60° N in the TOMS data. The magnitude of the high near 50° E is accurately captured. The low between this high and the high near 140° E is much more distinct in the initialization field, and the center of the high is displaced. It is difficult to compare to the high at 260° E because of missing TOMS data, but the structure of this high and the high near 330° E are captured. Although the calculated total ozone is somewhat higher than the TOMS values, it generally lies within 10 % of the observations.

North of the terminator there are no TOMS data. Sonde data from the Ozone Data Center in Toronto compares well with the initial condition, suggesting that the ozone gradient north of the terminator has been properly represented.

There are two significant sources of error which may affect these comparisons. First, the TOMS data are taken at much higher resolution than the model grid, and geographically small local maxima and minima can be measured. Second, total ozone from the initialization is sensitive to the representation of the tropopause. The model vertical resolution (approximately 3.5 km) does not adequately resolve the tropopause, so significant errors in the total ozone might be expected. The initialization successfully captures the geometry of the TOMS fields and in most cases the magnitude with 10 per cent. The apparent high bias between the calculated and measured fields for the Dec. 1988 comparison is not observed in the Jan. 1979 comparison.

Figure 4 shows N_2O and O_3 derived for Dec. 28 and data from the ER-2 flight of Jan. 3. The ER-2 data are typical of the three flights in early January. The spread of the N_2O is smaller in the initialization than in the data. The ozone spread is closer to observations. The spread in both fields is indicative of the 2D model fields. The 2D model could be modified to produce an N_2O spread that is more consistent with the data. However, such modifications adversely affect the comparison of ozone with both AASE and TOMS measurements.

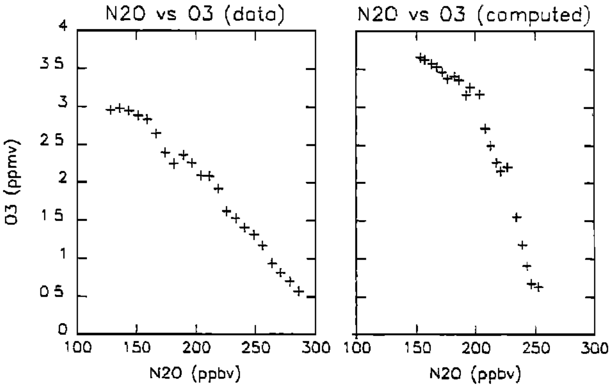

Fig. 4. These plots show averaged values of O_3 in bins of N_2O. a) Initialization algorithm for Dec. 28, 1988 (gaps are due to model resolution, b) AASE data for Jan. 3, 1989.

The basic features of the AASE data are represented by these initial fields. Low N_2O and high O_3 are confined to the polar vortex. There is a distinct jump in the constituent fields as the vortex edge is traversed, indicating the separation of polar and middle latitude air. This separation is present in HCl, HF, and N_2O and is the fundamental signal of the AASE data that constrains the procedure.

Model Integrations

A stringent test of the initialization is the quality of the model simulations. The initial fields are used in the 3D transport and chemistry model that uses winds from a data assimilation procedure [Rood et al., 1989; Kaye et al., 1989a, 1989b]. The model maintains constituent gradients at the vortex edge, and simulates lower stratospheric transport accurately for at least two months. For these experiments a single constituent is transported with specified chemical production and loss coefficient.

Figure 5 shows time series from the TOMS data and the model at the model grid point closest to Stavanger and a grid point at the same latitude but at 185° E(Aleutian anticyclone). At both points the model variability is highly correlated with the TOMS data throughout the integration. The correlation coefficient for the smoothed data is 0.86 at Stavanger and 0.79 in the Aleutian anticyclone.

The time series trace each other within a few days of initialization. In the Stavanger series there is a slight period of adjustment. On Dec. 28 Stavanger is in a region with strong local gradients; therefore, initial transients are expected. Weak gradients are present in the Aleutian anticyclone, the transience is smaller, and the integration does well from the beginning. The high quality of the integrations suggests that the initialization technique provides a realistic constituent representation [Kaye et al., 1989b].

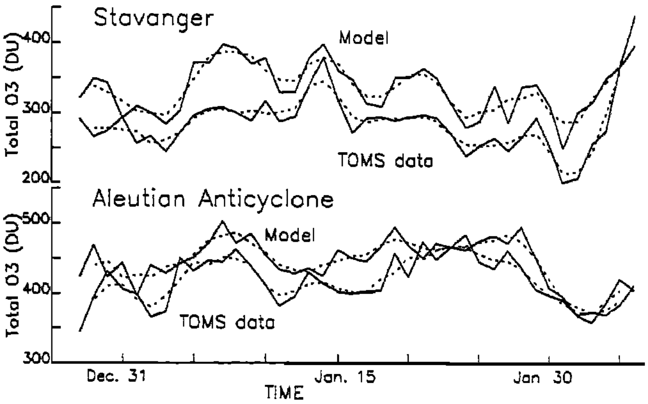

Fig. 5. Times series of TOMS and model ozone from 12/28/88 through 2/5-89 at Stavanger and at 180 °E (DU). Correlation coefficients: Stavanger, 0.77, 0.82 (smooth); 180 °E , 0.63, 0.78 (smooth).

Summary and Conclusions

Results show that by consideration of instantaneous dynamical conditions, realistic global fields can be generated from a limited set of profile measurements. Profile data are needed from at least 3 latitude bands in each hemisphere. Calculations in the tropics are complicated by the difficulties of computing vorticity and the weakening of the relation between vorticity and θ.

The algorithm presented here, used to provide initial conditions, could be used for other applications such as extrapolation of geographically sparse profile data to a global base. Such extrapolations could help determine if a ground based monitoring network represents global conditions.

The initial fields generated by the outlined procedure have been used in 3D simulations of constituent variability during AASE. These simulations have been found to represent local variability during AASE accurately [Kaye et al., 1989b]. Comparison with TOMS data, which provides the only current measure of global constituent variability, indicates that the model accurately captures variability throughout the winter hemisphere. Therefore the model provides a physically and chemically consistent tool to extrapolate the local variability observed in AASE to the hemispheric scale. These are the first experiments to our knowledge to simulate local variability accurately for such long time periods in a 3D model.

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