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PHOTOCHEMICAL TRAJECTORY MODELLING STUDIES
OF THE 1987 ANTARCTIC SPRING VORTEX

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Simulations of Antarctic ozone photochemistry performed using a photochemical model integrated along air parcel trajectories are described. This type of model has a major advantage at high latitudes of being able to simulate correctly the complex interaction between photolysis and temperature fields, which, because of the polar night cannot be represented accurately in a zonally averaged framework. Isentropic air parcel trajectories were computed using Meteorological Office global model analyses and forecast fields from positions along the ER2 flight paths during the Airborne Antarctic Ozone Experiment in Austral Spring 1987. A photochemical model is integrated along these trajectories using the aircraft observations to initialise constituent concentrations. The model was adapted from Austin et al. (1987a) and includes additional reactions of the ClO dimer and also bromine reactions, which are thought to play a significant role in Antarctica (McElroy et al., 1986; Molina and Molina, 1987). The model also includes heterogeneous reactions (Solomon et al., 1986) which are invoked when the air parcel passes through a polar stratospheric cloud (PSC). The existence of a PSC is determined throughout the course of the model integration from the parcel temperature and the saturated vapour pressure of water over an assumed H₂O/HNO₃ mixture (Toon et al., 1986). The air parcel temperature is used to determine the saturated vapour pressure of HNO₃ over the same mixture. Mixing ratios which exceed saturation result in condensation of the excess in the model and hence lead to a reduction of the amount of gas phase NO_x available for chemical reaction.

In the paper, modelled and observed constituent concentrations outside and within the chemically perturbed region of the vortex are compared. Figure 1 shows examples of 6 day trajectories starting on 4 Sept 1987, at latitudes 58S and 72S. The arrows denote the date at 0GMT and the crosses indicate the locations of PSCs encountered along the trajectory. Note that only the more poleward air parcel experienced a PSC in the model. Figures 2 and 3 show selected species from the chemical model for the two trajectories as functions of time. The integrations have identical initialisations, for comparison purposes, and correspond to species concentrations measured in the chemically perturbed region of the vortex. Results from the more poleward trajectory show that in the model, the heterogeneous reactions cause the ClO concentration to become elevated to levels comparable to that observed within the chemically perturbed region from the ER2, and to produce a substantial O₃ depletion of over 1% per day largely through the ClO dimer destruction cycle. However, for the trajectory starting at 58S (nominally outside the chemically perturbed region) the O₃ concentration levels off after only 4 days of integration, despite the initial conditions being favourable for O₃ depletion.

Further integrations over 80 day trajectories from 1 Aug 1987 are presented in which the net O₃ destroying potential of the perturbed

chemical region is assessed for different conditions. The importance of the level of denitrification and of the frequency of PSCs in determining the net O₃ depletion is emphasised. Results indicate that given suitable initial partitioning of the chlorine species, ClO concentrations can increase during the model integration as observed throughout the AAOE. The extent to which this is consistent with other (column) observations is assessed.

References:

- Austin et al. Q.J.R.M.S 113, 361-392, 1987.
McElroy et al. Nature 321, 759-762, 1986.
Molina and Molina J.Phys.Chem 91, 433-436, 1987.
Solomon et al. Nature 321, 755-758, 1986.
Toon et al. Geophys.Res.Lett., 13, 1284-1287, 1987.

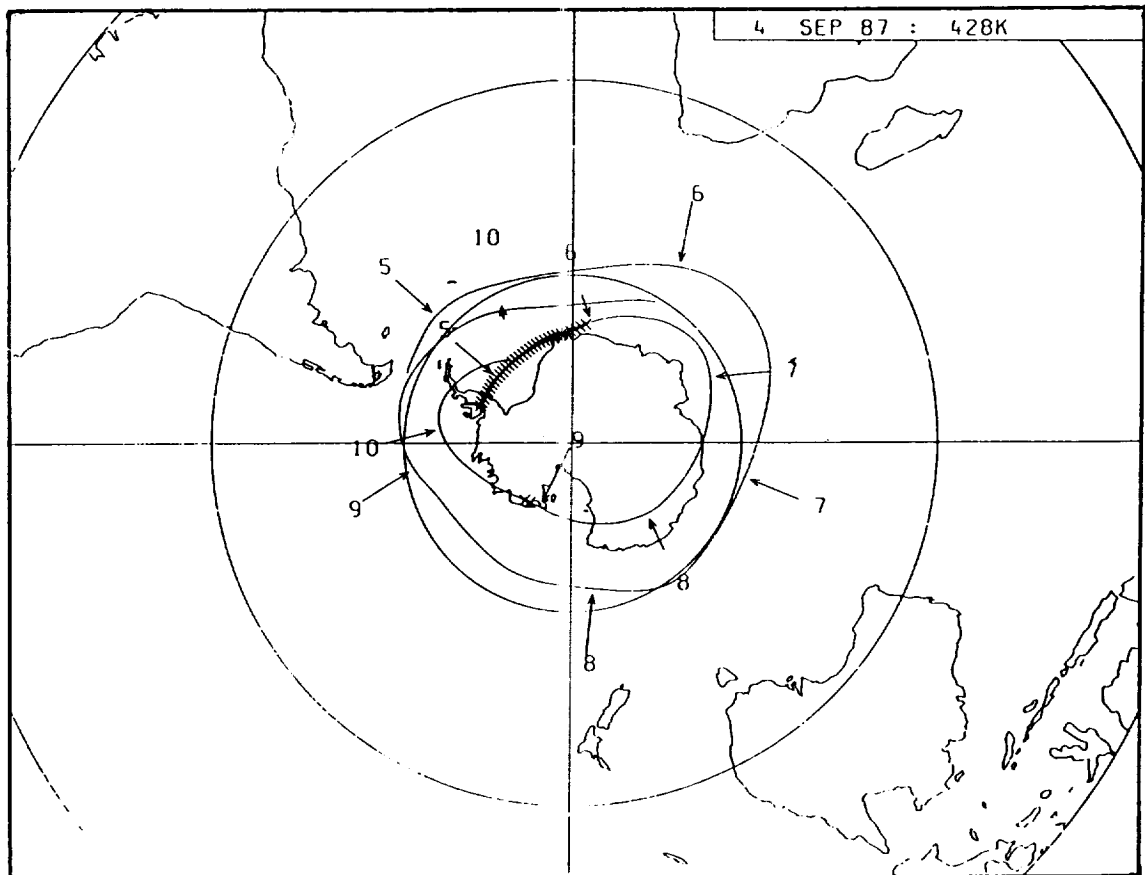


Figure 1 6 day isentropic trajectories calculated from UK Meteorological Office global model analyses initialised on 4 Sept. 1987.. Regions of the trajectories in PSCs are denoted by crosses.

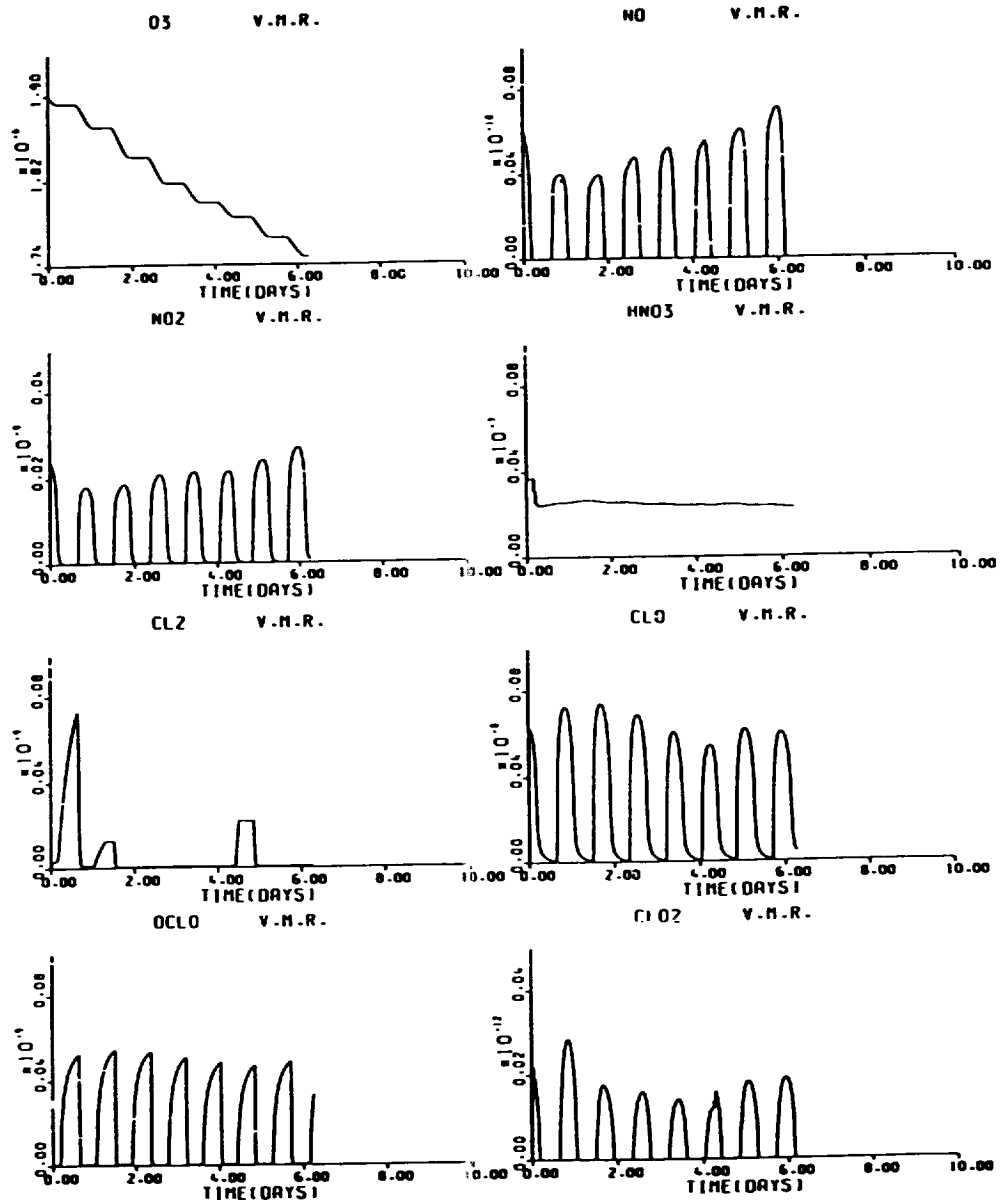


Figure 2 Calculated time variation of selected chemicals from the model run initialised at 72S (inside the chemically perturbed region).

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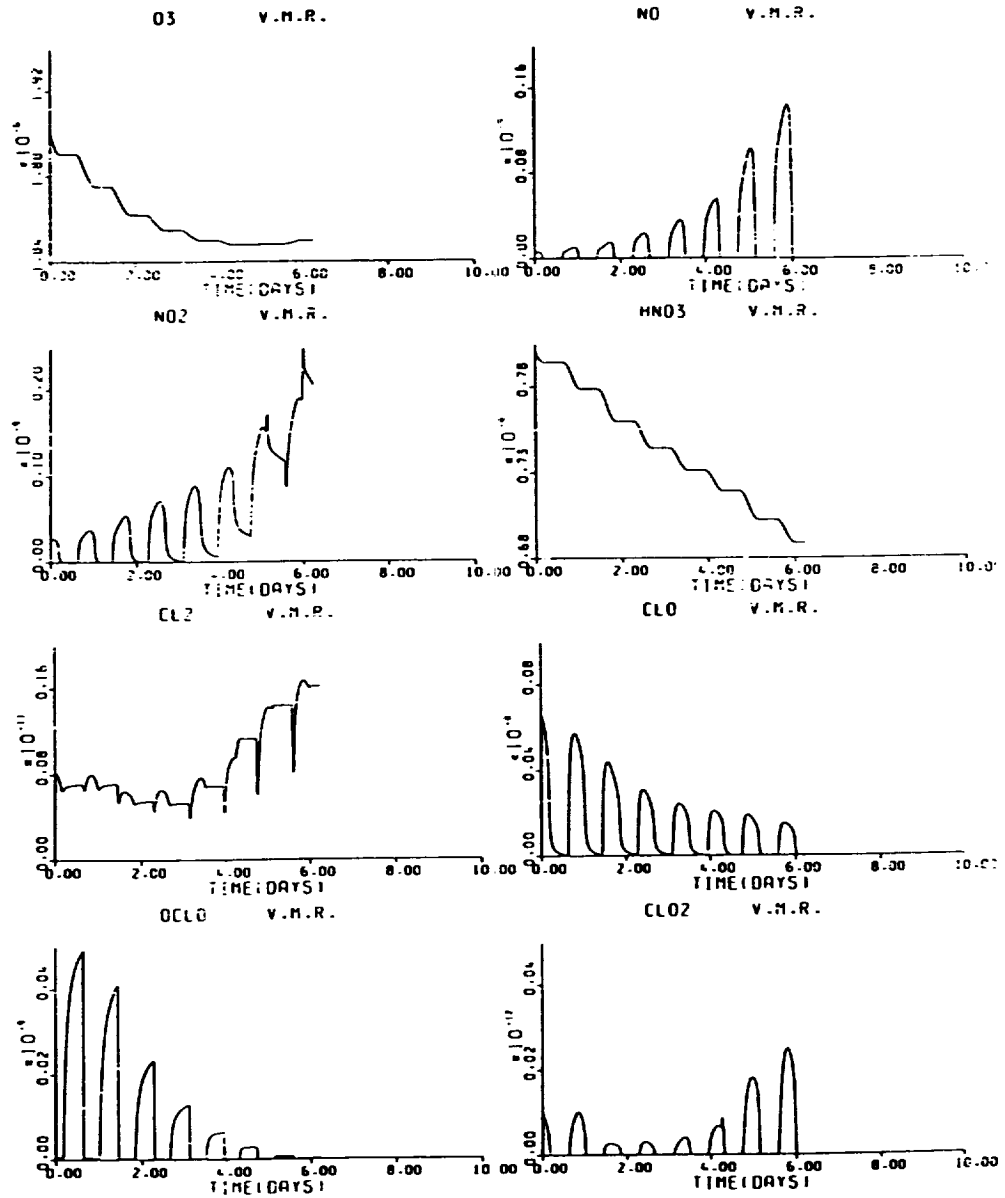


Figure 3 Calculated time variation of selected chemicals from the model run initialised at 58S (outside the chemically perturbed region).