Anhang 2

Supplement to the

Final Report on the Project TRACHT-MODEL

Transport, Chemistry and Distribution of Trace Gases in the Tropopause Region: Model

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Content

1 Introduction

The troposphere and the stratosphere form an interactive system in which dynamics and transport in the tropopause region play a crucial role. The project TRACHT (Transport, CHemistry and Composition in the Tropopause Region) of the German Program on Atmospheric Research AFO2000 has been aiming at a contribution to a comprehensive investigation of the tropopause region by employing high-resolution global remote sensing data of the uppermost troposphere and lower stratosphere (UTLS), a global and a meso-scale chemistry transport model. The high spatial resolution of the remote sensing data made it possible to resolve meso-scale features of tracer distributions in much greater detail than before. Such features were chosen as the main focus of the project.

Recent studies (e. g. Ebel et al. 1996, Beekmann et al. 1997, Kowol-Santen et al. 2000) have shown that the meso-scale component of cross-tropopause tracer fluxes is highly variable and considerably depends on the dynamical processes controlling meso-scale transport. Regarding air mass exchange between the stratosphere and troposphere, estimates of global or hemispheric efficiency of these processes may therefore significantly deviate from global estimates based on planetary scale circulation features (Holton et al. 1995, Grewe and Dameris 1996). Furthermore, the vertical extension of meso-scale features forced from below into the lowermost stratosphere needs to be explored in more detail since this aspect is rather relevant for the understanding of chemical transformation of reactive species transported into this region.

The space-born remote sensing data employed in this study have been provided by the CRISTA-2 experiment (CRISTA: CRyogenic Infrared Spectrometers and Telescopes for the Atmosphere; Offermann et al., 1999). During the flight of the instrument from 8 to 16 August 1997 several peculiar meso-scale features showed up in the observations of minor constituents in the UTLS. Two of the most prominent and intriguing events, namely a blocking and an intrusion of dry subtropical and midlatitudinal air into a tropical region with strong convective activity (Fig. 1) have been chosen for comprehensive analysis of their impact on the tracer distribution in the tropopause region. The treatment of the latter case was also motivated by the availability of extraordinarily well resolved remote sensing data from CRISTA-2.

2 Model and Data

2.1 The EURAD Model

The model that has been used to conduct detailed simulations of meso-scale features is the EURAD system (EURopean Air pollution Dispersion model). It has been designed for the simulation of air pollution in the boundary layer and free troposphere. It consists of a meteorological (MM5, Grell et al., 1994), chemistry-transport (CTM2, based on RADM) and emission (EEM) module (for references see Ebel et al., 1997). Aiming at the treatment of UTLS conditions it has been extended up to 10 hPa.

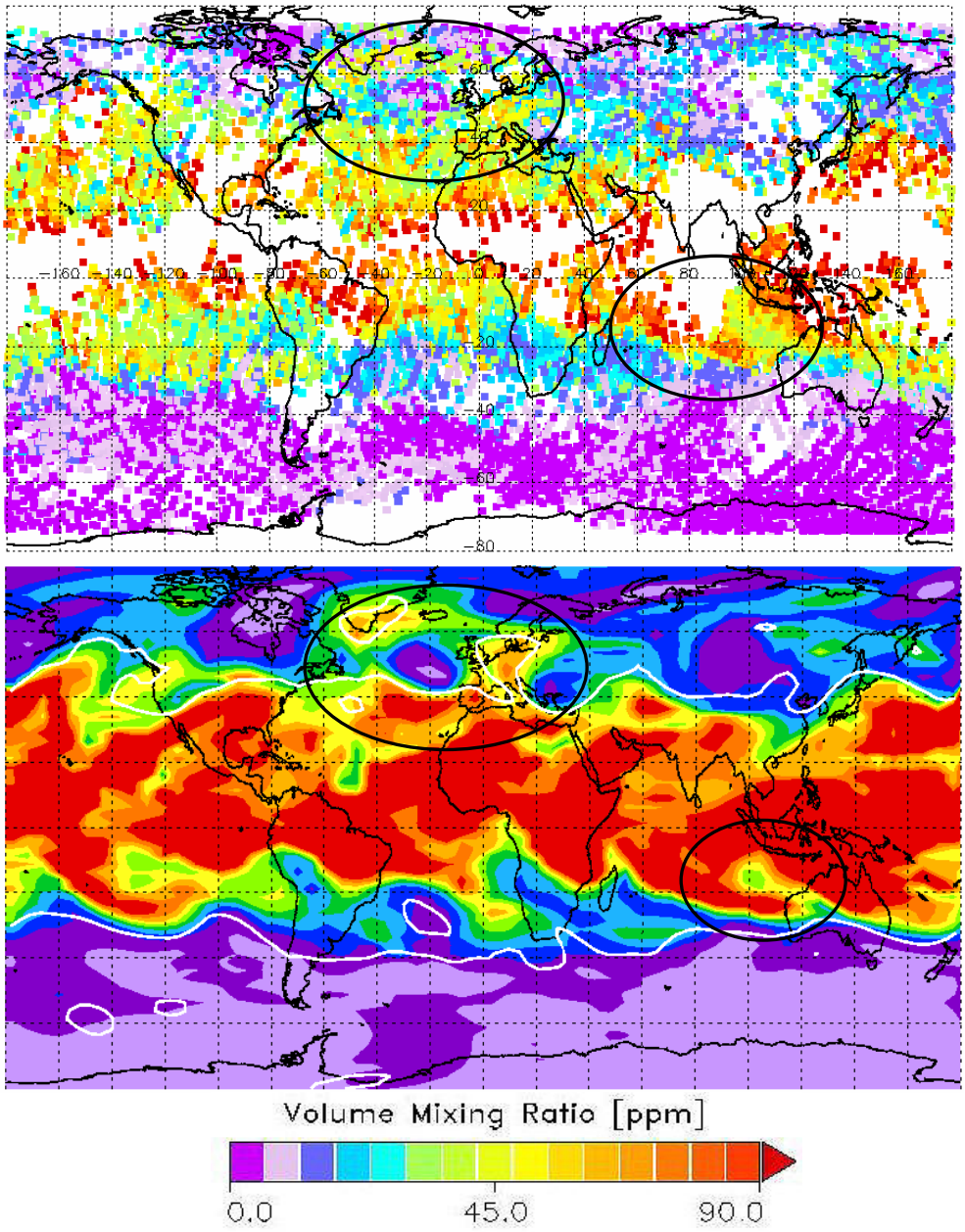

Figure 1.1: Global water vapour distribution as observed with CRISTA-2. Left panel: Mixing ratios (ppmV) at the 215-hPa constant pressure surface from CRISTA-2 measurements compiled for the episode 8 – 15 August 1997. Right panel: H_2O mixing ratios (ppmV) at 215 hPa on 12 Aug. 1997, 00 UTC, from CRISTA-2 observations assimilated with the ROSE model. The intersection between the 215-hPa constant pressure and the 2.5 PVU constant potential vorticity surface is indicated by a white line. The latter surface indicates the tropopause outside the tropics. The meso-scale features analysed in this study are encircled.

Grid

Different vertical grid resolutions have been tested within the project. The EURAD model uses the terrain following σ-coordinate system, according to:

(1) $$\sigma = \frac{p - p_{top}}{P_{surface} - p_{top}}$$

with p = pressure on the specific model layer, p_{top} = pressure at upper boundary of the model, $p_{surface}$ = surface pressure

For the model applications a 29 layer version and a 50 layer version were used. The layer thickness is a few hundred meters in the upper troposphere and increases with height. Above 100 hPa the vertical resolution is rather coarse. Applications for the middle stratosphere would need a better resolution in this height range.

The horizontal resolution of the model is 54 km for the regional applications and 100 km for the hemispheric scale.

Meteorological Model

All meteorological simulations within TRACHT-Model were performed with the mesoscale model MM5 (Grell et al., 1994) Although non-hydrostatic simulations were done for comparison, most of the calculations were performed in the hydrostatic mode – which is sufficient for the selected grid resolutions.

Sensitivity studies have been done for the forecast mode of the model to provide a free development meso-scale dynamical structures, which is optimal for flux calculations and the FDDA (four dimensional data assimilation or "nudging") mode of the model for comparison.
A mixed phase explicit scheme and the Grell type cumulus parameterization are used for the moisture physics. Cloud effects are included in the radiation calculation. The Blackadar scheme is used as boundary layer parameterization.

Chemistry Transport Model

The EURAD chemistry transport model version 3 (CTM3) is used for the chemistry transport calculations (Hass et al. 1993; Ebel et al., 1997). It uses the 4th order Bott advection (horizontally and vertically) and a boundary layer scheme based on scaling regimes. The cloud scheme is based on Walcek and Taylor. It has been modified with respect to the application of water vapour parameters provided to the CTM by MM5 (Roeben, 1999). Within CTM3 a number of chemical mechanisms are available (RADM, RACM, MADE, CHEST). In addition, a tracer version of the model (TTM) without chemical transformations has been implemented.

2.2 Input Data

Meteorological Data

Two analysis data sets have been used as input for the meteorological simulations. One of them contains ECMWF analyses with 1.68° x 1.68° resolution and 14 pressure levels up to 10 hPa

and is available every 6th hour. The other one is taken from the NCAR/NCEP 40-year re-analysis (NNRP, Kalnay et al., 1996). It is stored on a 2.5° x 2.5° grid and has a somewhat higher vertical resolution than the ECMWF data set and has the same temporal resolution. Humidity data are available only up to 300 hPa from NNRP analyses.

Both data proved to be suitable for TRACHT simulations. Temperature deviations were small, e.g. less than 1K over the TRACHT domain with a correlation coefficient around 0.99 (Fig. 2.1). There is a slight positive bias of ECMWF temperatures compared to those from NNRP. The temperature difference for the region of the cut-off low is larger then the bias. There, the ECMWF temperature exceeds NNRP up to about 3 K (Fig. 2.2, centre part).

There is a lot more scatter in the in the differences of the data for water vapour from ECMWF and NNRP (Fig. 2.3) At 300 hPa there is a high bias of NNRP over ECMWF (Fig. 2.4) for August 12. But the differences are variable in height and date. In general the correlation coefficient is lower than 0.8. For the region of the cut-off low region the average water vapour concentration is 238 ppmV for NNRP and 218 ppmV for ECMWF (Fig. 2.4). The distribution of the NNRP data is smoother. These mixing ratio differences should be kept in mind when regional numerical simulations of moisture initialised with the mentioned analyses are validated.

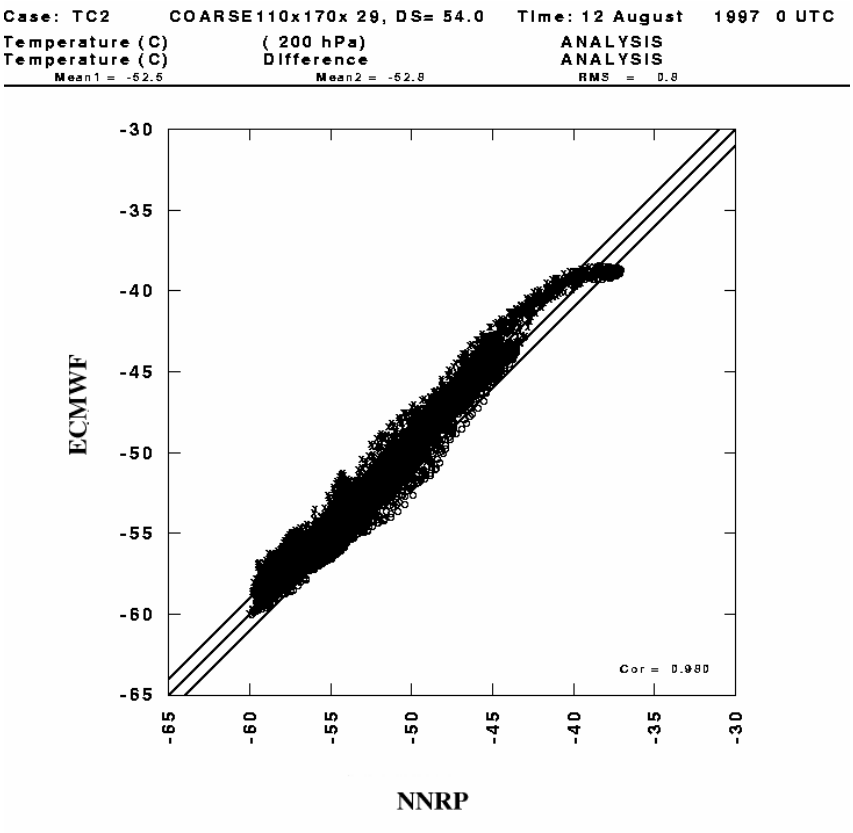

Figure 2.1: Comparison ECMWF-analysis vs. NNRP-data. Temperature at 200 hPa, 12 August, 0 UTC over the TRACHT-Atlantic domain. Vertical axis: ECMWF (field1), horizontal NNRP (field2).

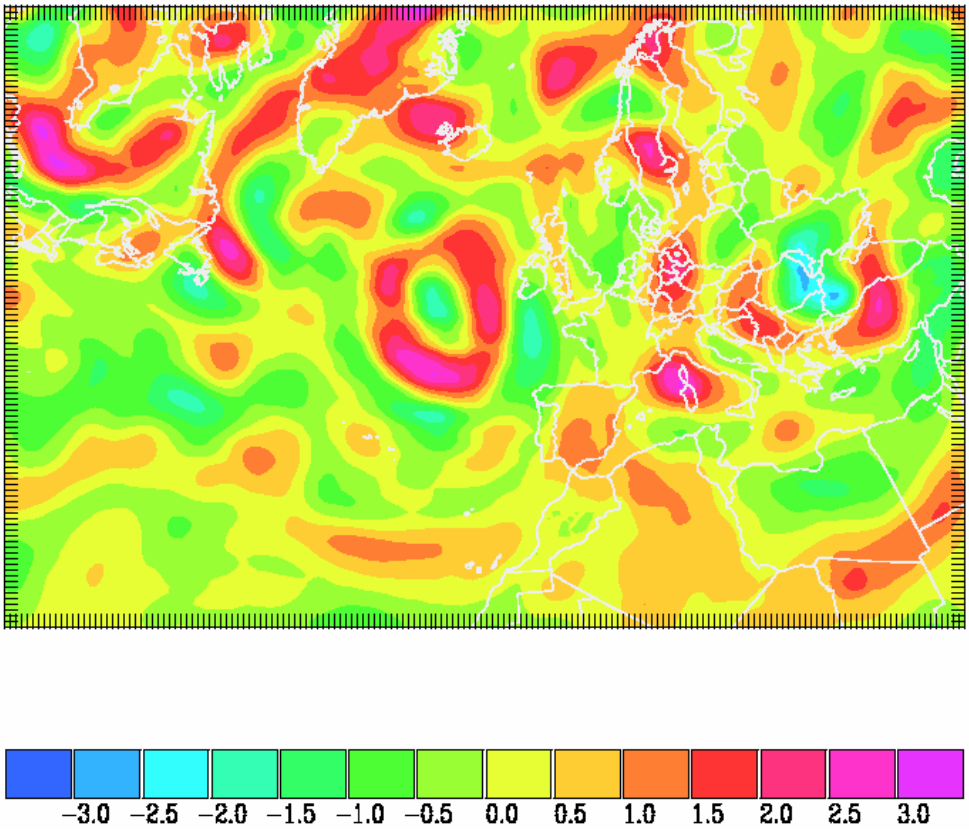

Figure 2.2: Temperature difference (in K), ECMWF-NNRP at 200 hPa for August 12, 00 UTC

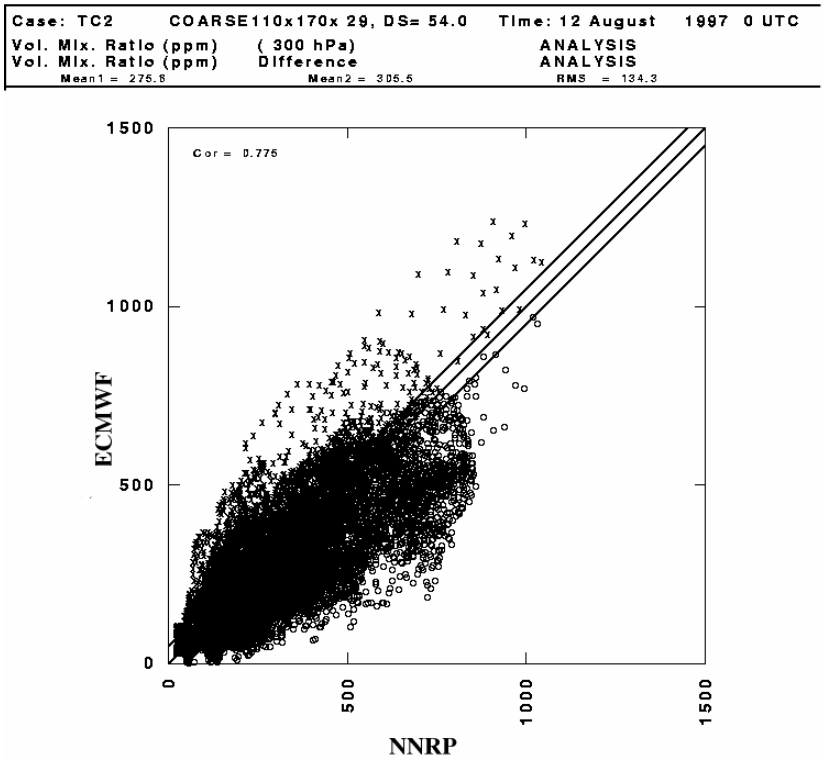

Figure 2.3: Scatter diagram H2O [ppmV] at 300 hPa – complete TRACHT-Atlantic domain - for 12 August 1997, 0UTC. Vertical axis ECMWF, horizontal axis NNRP.

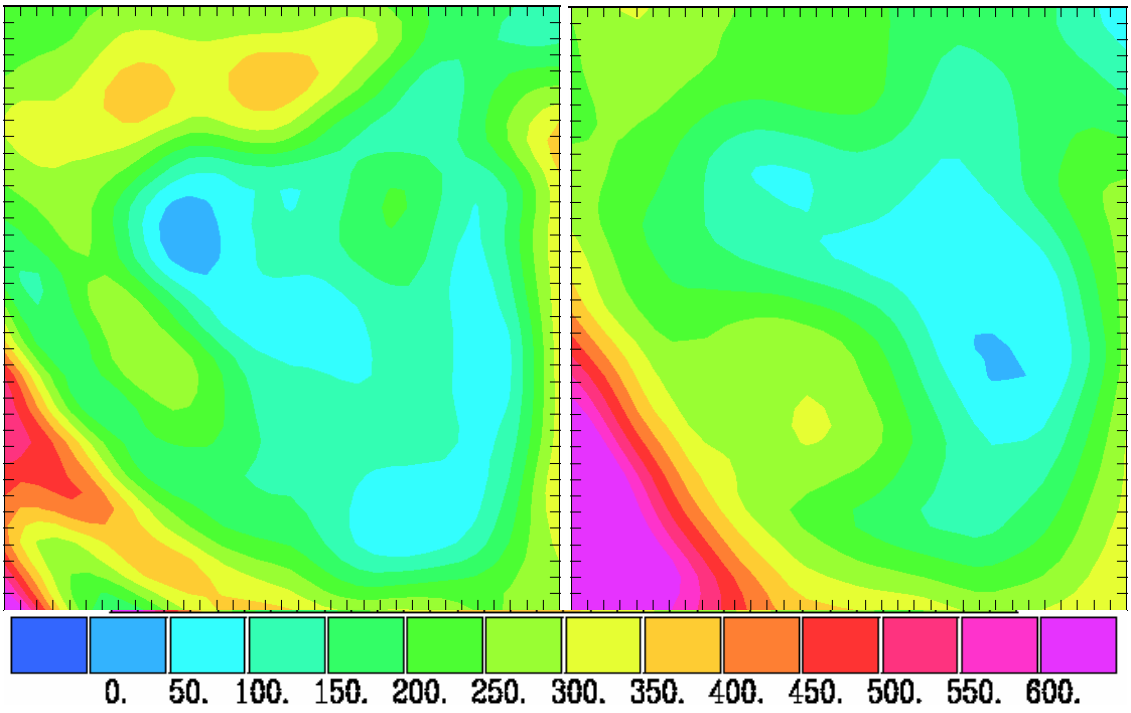

Figure 2.4: H_2O [ppmV] at 300 hPa in the region of the cut-off low on 12 August, 0 UTC. Left side: ECMWF; right side NNRP.

Emissions

The EDGAR3.2 global emission inventory is used as emission data. A description can be found in Olivier et al. (2001/2002) For Europe also the EMEP inventory has been tested. Although EDGAR-data have a coarse resolution (1° x 1°) compared to EMEP (50 km x 50 km) both inventories lead to comparable near surface trace gas concentrations.

The NCAR Rose data

A global data set from the chemistry transport model NCAR-ROSE (see report of TRACHT-DATA for details) has been provided by the University Wuppertal. The data set included meteorological parameters and the concentrations of chemical species: water vapour, ozone and CFC11. The data are available on 10 levels between 316 hPa and 10 hPa. The data of the lowermost four (at 316 hPa, 215 hPa, 146 hPa and 100 hPa) has mainly been used for regional modelling in the TRACHT project.

2.3 Model Development and Adjustment

For the applications within TRACHT the EURAD system had to be modified in several ways. The numerical efficiency had to be increased to enable large scale, high-resolution simulations. The higher efficiency has been achieved by reformulating the code for better parallelization and memory utilization.

A tracer version of the EURAD chemistry transport module has been developed to study the dynamical effects of passive tracers without chemical transformation in an efficient way.
Next, modifications had to be made to enable simulations outside Europe (topography, land use data, photolysis rates, etc.). There were hemispheric scale application and for the first time applications of the EURAD model to the equatorial region and for domains within the southern hemisphere.

Interfaces to introduce global scale data into the EURAD model had to be developed. There are two different interfaces:

- The water vapour data was included in the REGRID pre-processor of the MM5 modelling system. This has been done to account for the cloud physics treatment of the meteorological model MM5.
- The other chemical species - provided by the ROSE model - have linearly been interpolated on horizontal surfaces to the specific EURAD model grid. The vertical interpolation is executed within the EURAD-CTM to account for the actual profiles of the relevant meteorological parameters.

A specific problem has been posed by the height range below 316 hPa, were no NCAR-ROSE data is available. For water vapour there is a small overlap with the NNRP data – which have humidity fields up to 300 hPa. The transition between the two data sets depends on the vertical distance of the EURAD model level from the next available data level. Sensitivity studies have been performed to study the effects of the transition. In general the NNRP humidity fields have higher concentrations than NCAR-ROSE. This seems to be more realistic in regions with high humidity - like cloud regions and fronts. On the other hand, the comparison with the observations (see report TRACHT-DATA) demonstrates clearly that the MM5 simulations based on ECMWF or NNRP humidity provide much too high concentrations regions with stratospheric influence. Within these regions NCAR-ROSE driven simulations give better results. No fully satisfactory solution to this problem could be provided until now.

For the other chemical tracers other solutions had to be found. For CFC11 the available climatological data suggests a rather uniform distribution with only very small concentration variations for this trace gas in the troposphere. Therefore, a constant value - which is consistent with climatological data and CRISTA - has been assumed for the troposphere as initial and boundary value.
For the other species climatological values have been used as initial and boundary values were no actual information was available. The data were taken from different measurement campaigns (see for instance Emmons et al., 2000, and references there in).
For some species – especially ozone – correlations were used. The method has widely been used (See Ebel et al., 1997). The height dependence of the correlation factor has been chosen according to Ravetta et al. (1999) and adjusted to ozone sonde observations carried out at Hohenpeissenberg.