

Validation of trajectory calculations – interim report for the ECMWF special project spdetraj

Nicole SPICHTINGER, Richard DAMOAH

Lehrstuhl für Bioklimatologie und Immissionsforschung,
Technische Universität München,
Am Hochanger 13, D-85354 Freising-Weihenstephan, Germany

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1 Introduction

Trajectory and particle-dispersion models are important tools for describing air mass motions and are often used to establish source-receptor relationships in the atmosphere. However, the accuracy of such calculations is limited by various factors such as numerical truncation, interpolation methods, the treatment of vertical velocity and possible errors in the underlying wind fields [Stohl, 1998]. It is therefore vital to assess the impact of these potential error factors on trajectory accuracy for concrete atmospheric situations. Using comprehensive wind-field data available from the ECMWF, it is the continued aim of this special project to employ various three-dimensional trajectory computation methods and particle dispersion techniques to assess accuracy, both intrinsically and between different models.

In parallel with this on-going assessment we continued our investigation of the lifetime of NO₂ by comparing FLEXPART simulations with satellite data. We extended the study with SCIAMACHY data and now can estimate the lifetime of NO₂ at selected point sources with high emissions.

Additionally, ECMWF windfield data were used to simulate a lightning event in the Gulf of Mexico in August 2000. During this event GOME detected lightning NO₂ for the first time.

We further used ECMWF windfield data for modeling a „pyro-convection“ event over Alaska in June 2004.

2 Models

FLEXTRA [<http://zardoz.nilu.no/~andreas/flextra+flexpart.html>] is a Lagrangian model for calculating accurately 3D trajectories based on high-density meteorological data, either forwards or backwards in time, with several user options to change trajectory types and initial configuration. FLEXTRA has been used to make the first detections of intercontinental transport of ozone [Stohl and Trickl, 1999] and of Canadian forest fire emissions over Europe [Forster et al., 2001] and was used for the first global airstream climatology [Stohl, 2001] and a 15-year climatology of warm conveyor belts [Eckhardt et al., 2004]. It was furthermore used recently in combination with a microphysical model to study freezing mechanisms of cirrus clouds [Haag et al., 2003].

FLEXPART [<http://zardoz.nilu.no/~andreas/flextra+flexpart.html>] is a Lagrangian particle dispersion model which calculates the fully 3D transport and dispersion of non-reactive

tracers, driven by high resolution meteorological data, providing highly accurate simulations of transport processes in the atmosphere. FLEXPART has been validated with measurement data from large-scale tracer experiments [Stohl et al., 1998], during case-studies of stratospheric intrusions [Zanis et al., 2003] and performs well in comparison with other similar models [Meloan et al., 2003]. It has been used for studying the intercontinental transport of ozone [Stohl and Trickl, 1999], the advection of Canadian forest fire emissions to Europe [Forster et al., 2001, Spichtinger et al., 2001], hemispheric transport of forest fire emissions [Spichtinger et al., 2004, Damoah et al., 2004], the dispersion of aircraft emissions in the stratosphere [Forster et al., 2003], and has been used for inverse modelling in order to determine the source regions of North American pollution plumes measured over Europe [Stohl et al., 2003], for example. FLEXPART has also been used to calculate a climatology of stratosphere-troposphere exchange (STE) processes, based on the ECMWF 15-year re-analysis dataset (ERA-15) [James et al., 2003a,b]. Recently a new version with a revised convection scheme is to be downloaded at the above webpage.

3 NO_x lifetime

To tie up to the last report, the lifetime estimation using GOME and SCIAMACHY data was continued. The comparison of spatial patterns in satellite measurements and FLEXPART model runs was investigated for different lifetimes. For some point sources, NO_x lifetimes of about 6 hours were derived. We investigated the possibility of estimating the lifetime of NO_x in more detail by additionally including SCIAMACHY data. As an example, Fig. 1 shows the point source Riad, where we derived a lifetime of approximately 4 days from SCIAMACHY data compared to FLEXPART model runs. Our future prospects concerning this topic are to focus on SCIAMACHY data and run FLEXPART with 0.5*0.5° ECMWF windfields to get better resolved results.

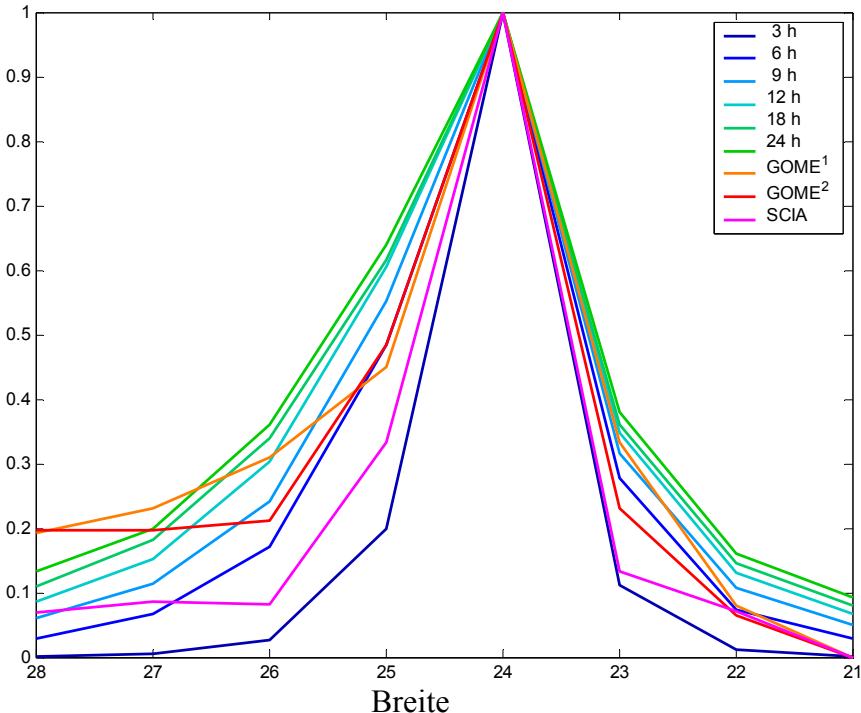


Fig. 1: Cross-section of NO_2 column densities (standardised) through Riad from FLEXPART (blue-green different lifetimes, yearly average 1997), GOME (1: 1997; 2: 1996-2001) and SCIAMACHY (2003). The relative high GOME-values at higher latitudes come from interferences with other sources by reason of low spatial resolution. SCIAMACHY-data give a lifetime of lower than 6h.

4 NO_x production from lightning

Nitrogen oxides ($\text{NO}_x = \text{NO} + \text{NO}_2$) play an important role in atmospheric chemistry. In the troposphere, they drive catalytic ozone production. Furthermore, NO_x controls OH concentration and thus the atmosphere's oxidizing capacity. In total, about 50 Tg [N] of nitrogen oxides are released annually, half of due to fossil fuel combustion [Lee et al., 1997]. Lightning produced NO_x (hereafter named LNO_x) is estimated to contribute about 5 Tg[N]/year [Lee et al., 1997]. However, the best estimates of recently published studies still vary between 0.9 and 12.2 Tg[N]/year [Nesbitt et al., 2000; Price et al., 1997], and the given uncertainties typically are one order of magnitude. Thus lightning is the least known source of nitrogen oxides. Furthermore, in contrast to other sources, LNO_x is directly released in the upper troposphere where the lifetime of NO_x is of the order of some days (e.g. [Jaeglé et al., 1998]), i.e. several times longer than for the boundary layer (~hours). Hence LNO_x has a higher efficiency for catalytic ozone production. For the correct assessment of NO_x inventories - a prerequisite for reliable model calculations of atmospheric chemistry - better knowledge on LNO_x is essential.

An unique event of GOME capturing LNO_x just produced was found on 30 August 2000 over the Gulf of Mexico. A sequence of about ten GOME pixels detects high NO_2 TVCDs that by far exceed normal levels over ocean (Fig. 2a). Fig. 2b depicts the flashes detected by the NLDN (national lightning detection network) before the ERS-2 overpass, i.e. 16:49 UTC, illustrating the spatial coincidence with the increased NO_2 TVCDs. For better comparison, the GOME pixel grid is overlaid. To illustrate also the temporal coincidence, Fig. 2c displays the time of the latest flash occurrence. More than half of the detected flashes occurred less than 3 hours before ERS-2 overpass. Black dots indicate flashes with less than 5 minutes time difference. Cloud data (Fig. 2c/2d) reveals that the enhanced NO_2 TVCDs are observed for a cloudy scene of a height of about 10 km.

This particular event is unprecedented as the lightning activity coincides perfectly with the GOME measurement both in space (the area affected by lightning fits in the eastern GOME subpixels) and in time (most flashes have occurred during the last 2 hours). The lightning event took place over sea and remote from polluted regions. The possible impact of anthropogenic emissions from the US being transported over the Gulf of Mexico and lifted up within the thunderstorm is estimated with FLEXPART calculations to be below $0.2 \cdot 10^{15}$ molec/cm². The observed enhanced NO_2 TVCDs are thus unambiguously due to LNO_x . As far as we know, such a clear and direct detection of LNO_x from satellite has never been reported before. This study will be published in Beirle et al. [2005].

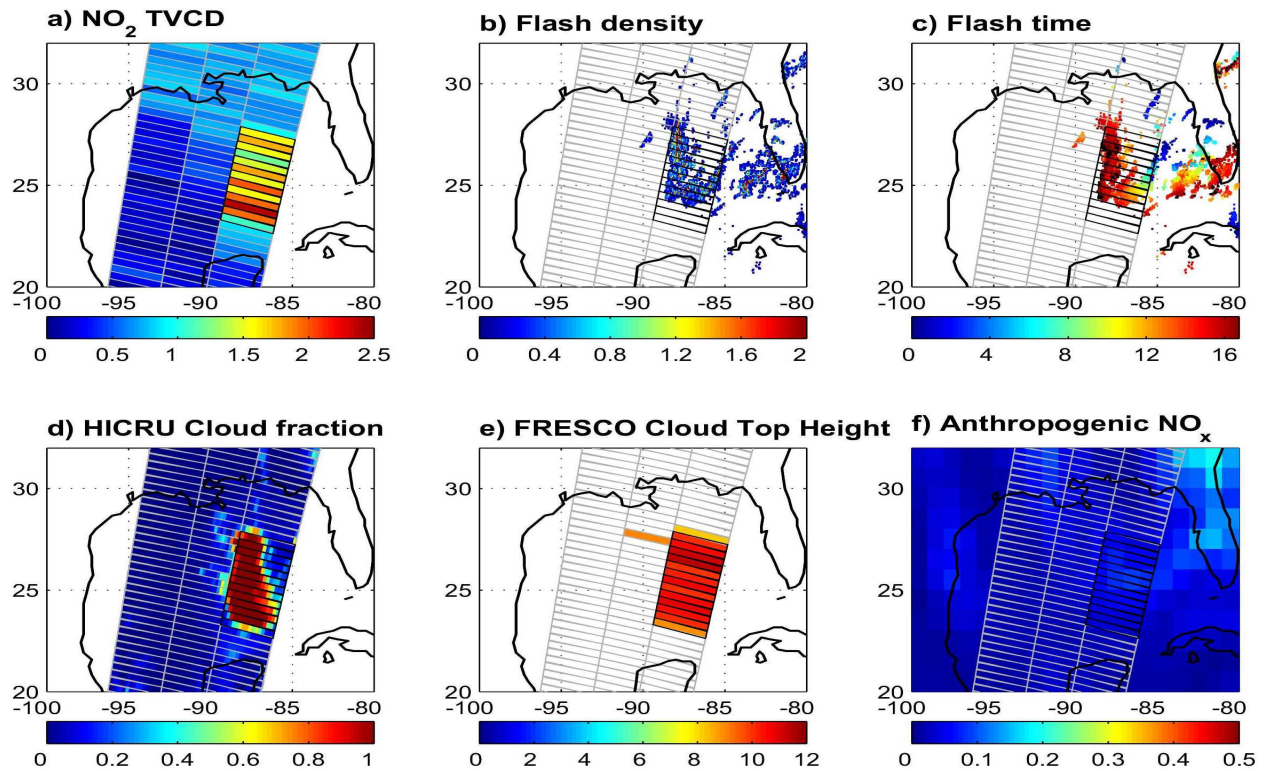


Fig.2: (a) GOME NO_2 TVCD (10^{15} molec/ cm^2) (stratospheric AMF). (b) lightning detection of NLDN (flashes/ km^2) underlying GOME pixels. (c) time (UTC) of lightning detection. (d) cloud cover from GOME (HICRU). (e) Cloud top heights from spectral GOME measurements (FRESCO). (f) anthropogenic NO_x above 8500m (10^{15} molec/ cm^2) calculated with FLEXPART assuming a lifetime of 24 h.

5 Pyroconvection

Summer 2004 saw severe forest fires in Alaska and the Yukon Territory that were mostly triggered by lightning strikes. The area burned ($>2.7 \times 10^6$ ha) in the year 2004 was the highest on record to date in Alaska. Pollutant emissions from the fires lead to violation of federal standards for air quality in Fairbanks.

We studied deep convection events that occurred in the burning regions at the end of June 2004. The convection was likely enhanced by strong forest fire activity (so-called pyroconvection) and fire emissions penetrated into the lower stratosphere, up to about 3 km above the tropopause. Emissions from the fires did not only perturb the UT/LS locally, but also regionally. POAM data at the approximate location of Edmonton (53.5° N, 113.5° W) show that the UT/LS aerosol extinction was enhanced by a factor of 4 relative to unperturbed conditions. Simulations with FLEXPART, setup with the new subgrid-scale deep convective transport scheme, showed transport of forest fire emissions into the stratosphere, in qualitatively good agreement with the enhancements seen in satellite data (Fig 3a,b,c,d). A corresponding simulation with the deep convection scheme turned off did not result in such deep transport (Fig. 3e,f). This study will be published in Damoah et al. [2005].

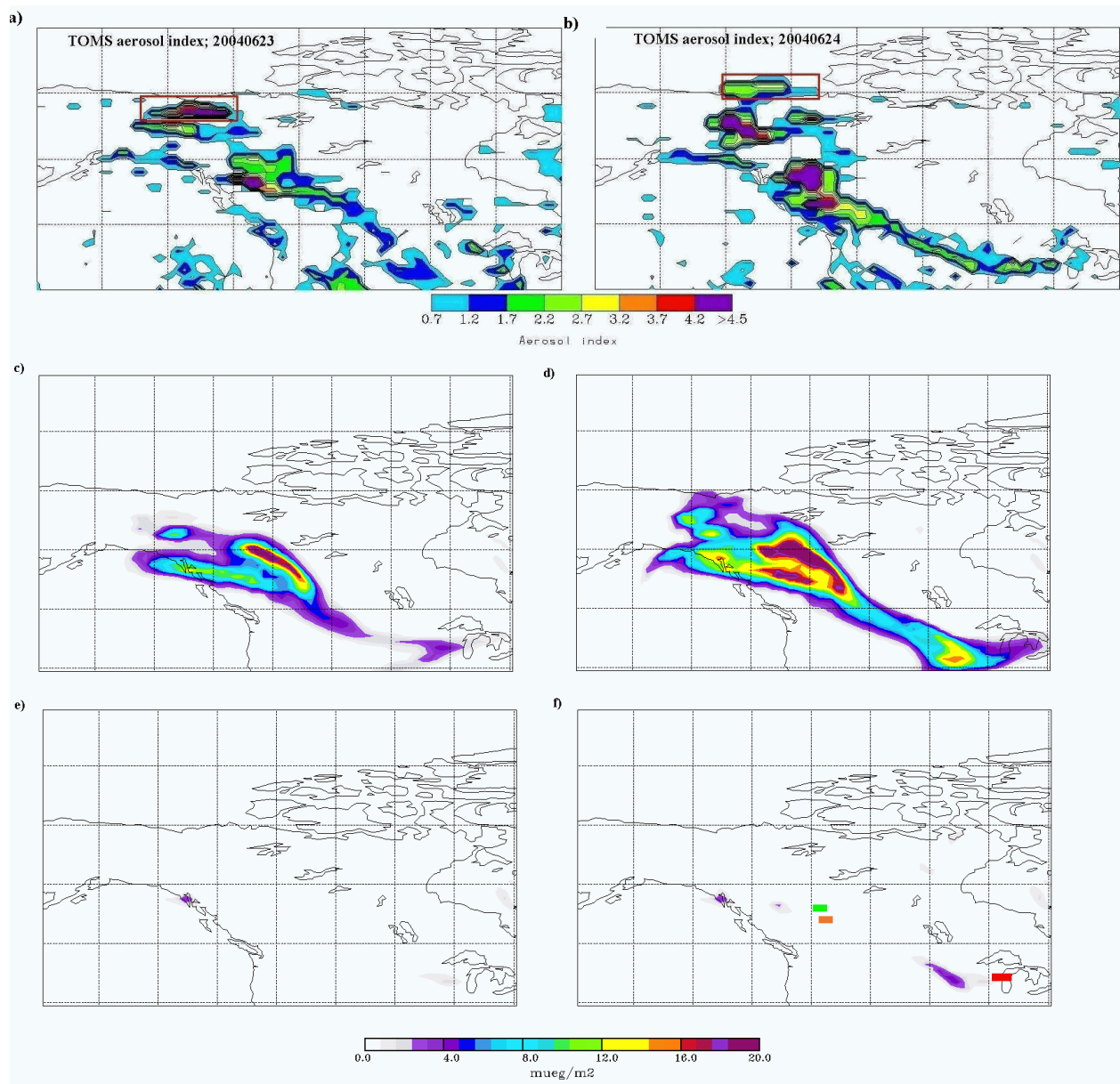


Fig. 3: TOMS aerosol index over North America on (a) 23 and (b) 24 June, 2004. FLEXPART 9-15 km CO tracer columns over North America with convection turned on, at (c) 23 June 03 UTC, (d) 24 June 03 UTC. (e) and (f) Same as c) and d), respectively, but with convection turned off.

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