Product Specification Document

Long Range Transport of Tropospheric NO_2 As Simulated by FLEXPART

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1. PRODUCT DESCRIPTION

To better comprehend intercontinental transport, we use the Lagrangian particle dispersion model FLEXPART to simulate the outflow of air pollutants from North America towards Europe. Unlike trajectory models, which calculate the path of a single infinitesimally small air parcel, particle dispersion models compute the trajectories of a large number (millions) of parcels to describe transport as well as diffusion. FLEXPART also simulates dry and wet deposition and radioactive (or other) decay of tracers in the atmosphere.

Unlike Eulerian Chemistry Transport Models (CMTs), Lagrangian models do not suffer from numerical diffusion and have relatively fast computation times. A full description of the model (FLEXPARTv6.2) has been published in ACP (Stohl. et al., 2005). The model itself is freely available (along with additional information) on the following website: http://zardoz.nilu.no/~andreas/flextra+flexpart.html
Standard FLEXPART only allows a fixed decay half-life parameter. The atmospheric half-lifetime of NO_2 is typically set to 2 days. While this certainly overestimates the NO_2 lifetimes near the atmospheric boundary layer, it does describe the average lifetime of NO_2 at high altitudes (and thus cold temperatures). However due to the large overestimation of boundary layer NO_2, outflow features are often blotted out. To fix this we have updated FLEXPART. In stead of a fixed half life, we have included a temperature dependent half life:

NOx half life (s) = 55598*exp(-0.0668.3*T(°C))

The above values have been derived by running the IMAGES model during one year over the transatlantic domain. The IMAGES model (Muller and Stavrakou, Atmos. Chem. Phys., 2005) calculates the distribution of 68 chemical compounds in the global troposphere, including the Ox, HOx, NOx families, as well as CO, 16 precursor hydrocarbons and their degradation products. It has a resolution of 5 degrees in latitude and in longitude, with 40 levels in the vertical. Advection of chemical compounds is driven by monthly averaged winds obtained from ECMWF analyses. Boundary layer diffusion, deep convection and other cloud processes are parameterized based on daily ECMWF fields. The effective chemical lifetime of NO2 is determined by the main sinks of NOx, i.e. the OH+NO2 reaction and the hydrolysis of N2O5 at the surface of wet aerosols. The latter process is parameterized based on model-calculated sulfate distributions and reaction probabilities parameterized according to Evans and Jacob (GRL, 2005).
While the lifetime-temperature relationship can now be described by an exponential function, one needs to be aware that there is considerable variability in the data and that the above temperature dependence, while being a huge improvement over a constant lifetime, is still an approximation.

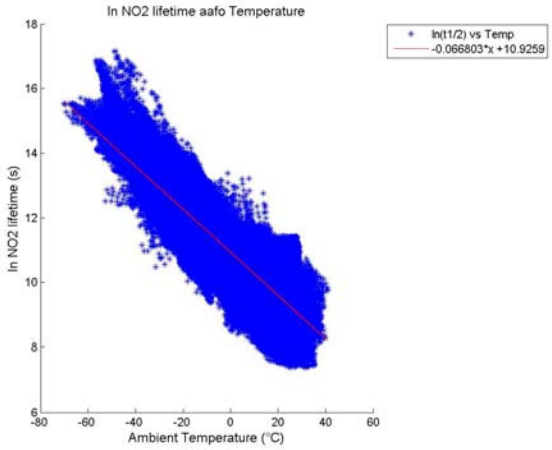

Fig 1: ln NO2 lifetime as a function of Temperature

Currently we use ECMWF 1°x1° 3hourly wind fields to drive the FLEXPART model. The NOx emission output has been taken from the EDGAR 3.2 Fast Track 2000 dataset (available at http://www.mnp.nl/edgar/).

We also simply assume that all NOx converts to NO_2. We used the 1°x1° emission grids within the 110°E to 50°E & 15°N to 65°N domain. Emission height is set to 250m. Output (3 hour average) is generated every 3 hours (at 00,03,06,09,12,15,18 and 21:00 UT). Only the results at 15:00 UT, which corresponds with the trans-Atlantic overpass-time of the OMI instrument, are plotted on the TEMIS website. All output however is stored in the daily hdf5 files.

All output is gridded on a 1°x1° grid with 10 vertical levels (1km each, up to 10km altitude above sea level). The output data file is available in hdf5 format and contains the 3-hourly full 3D-matrix output from FLEXPART (NOx concentration field, in ng/m3), the total columns (in molec/cm2) as a function of latitude and longitude and the highest NOx concentration (in molec/cm3) along each longitudinal band as a function of longitude and altitude. Note that the output matrix covers a slightly larger domain than that plotted on the TEMIS website. The lower-left corner coordinates of the output matrices are included as well.

2. KNOWN ARTEFACTS

Currently the FLEXPART output should be regarded only as a qualitative measure of NO_2 transport, not a quantitative one. One should be aware that we use annually averaged NOx emission fields, not a time-dependent emission climatology of NO_2. The lifetime of NO_2 is approximated by a simple algorithm since FLEXPART does not contain a chemical reaction scheme. Therefore these simulations are best used alongside independent observations (such as the retrieved OMI NO_2 product).

3. FUTURE IMPROVEMENTS

* Implement forecasting routines using either ECMWF or NCEP/GFS wind fields
* Implement better NOx emission climatology

4. REFERENCES

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