

Supplemental Information

Exploring sources of biogenic secondary organic aerosol compounds using chemical analysis and the FLEXPART model

Johan Martinsson^{1,2}, Guillaume Monteil³, Moa K. Sporre⁴, Anne Maria Kaldal Hansen⁵, Adam Kristensson¹, Kristina Eriksson Stenström¹, Erik Swietlicki¹, Marianne Glasius⁵

¹Division of Nuclear Physics, Lund University, Box 118, SE-22100, Lund, Sweden

²Centre for Environmental and Climate Research, Lund University, Ecology Building, SE-22362, Lund, Sweden

³Department of Physical Geography, Lund University, Lund, Box 118, SE-22100, Lund, Sweden

⁴Department of Geosciences, University of Oslo, Postboks 1022, Blindern, 0315, Oslo, Norway

⁵Department of Chemistry and iNANO, Aarhus University, Langelandsgade 140, DK-8000, Aarhus, Denmark

Correspondence to: Johan Martinsson (johan.martinsson@nuclear.lu.se)

FLEXPART configuration

The footprints were computed using the FLEXPART 10.0 model, with a modified output routine. Here we provide an overview of the FLEXPART configuration files, and we briefly describe the way footprints are computed.

Footprints computation

In the standard FLEXPART code, with the settings “iout = 1”, a 4D (space and time) domain is defined in the “OUTGRID” configuration file, and a gridded output is generated, representing the sensitivity of the observation to each grid point. That sensitivity is defined as the sum of the residence time of all the FLEXPART “particles” in the grid box.

The spatial coordinates of the output grid are given in degrees, for the lat/lon coordinates, and meters, for the vertical coordinates. The latter can be problematic, in particular close to the surface, since the height of the boundary layer can vary significantly between day and night. In our modified setup, the vertical component of the output grid is defined as a fraction of the boundary layer. The surface layer is defined as the layer between the surface and $0.5H_{bl}$ with H_{bl} the boundary layer height at the particle time and position (calculated at each time step, for each particle, within the “advance” subroutine in FLEXPART 10.0).

Besides this modification of the footprint computation, our FLEXPART setup is standard and our results should be reproducible using the following COMMAND and SPECIES configuration files:

COMMAND file

```
&COMMAND
LDIRECT= -1,
IBDATE= 20120608,
IBTIME= 000000,
IEDATE= 20120726,
IETIME= 000000,
LOUTSTEP= 3600
LOUTAVER= 3600
LOUTSAMPLE= 900
ITSPLIT= 999999999
LSYNCTIME= 150
CTL= 6.0000000
IFINE= 4
IOUT= 1
IPOUT= 0
LSUBGRID= 1
LCONVECTION= 1
LAGESPECTRA= 0
IPIN= 0
IOUTPUTFOREACHRELEASE= 0
IFLUX= 0
MDOMAINFILL= 0
IND_SOURCE= 1
IND_RECEPTOR= 1
MQUASILAG= 0
NESTED_OUTPUT= 0
LIMIT_COND= 0
SURF_ONLY= 0
```

```
CBLFLAG= 0
OHFIELDS_PATH= undefined
/
```

SPECIES file (SPECIES_025: AERO-TRACER)

```
*****
*
*      Input file for the Lagrangian particle dispersion model FLEXPART   *
*      Definition file of chemical species/radionuclides                 *
*      This file is on the format required by version 10 (05/2015)      *
*****
AERO-TRACER      Tracer name
-999.9           Species half life
1.0             Below-cloud scavenging (gases and particles) - A
1.0             Below-cloud scavenging (gases and particles)- B
0.9             In-cloud scavenging (gases and particles) - Ai
0.1             In-cloud scavenging (gases and particles) - Bi
-9.9            Dry deposition (gases) - D
                Dry deposition (gases) - Henrys const.
                Dry deposition (gases) - f0 (reactivity)
1.4E+03         Dry deposition (particles) - rho
2.5E-07         Dry deposition (particles) - dquer
1.25           Dry deposition (particles) - dsig
-9.99          Alternative: dry deposition velocity
 29.00         molweight
-9.99E-09      OH Reaction rate - C [cm^3/molecule/sec]
-9.9           OH reaction rate - D [K]
-9.9           OH Reaction rate - N (no unit)
-9             number of associated species (neg. none)
-99.99        KOA - organic matter air partitioning
```

Detailed description of the nine surface categories with largest air mass exposure

The surface categories used in the analysis were derived from the CORINE database. The CORINE database supplies high resolution maps that consist of 44 different surface categories. For easier interpretation we selected nine surface categories with the largest mean air mass exposure. A tenth category named “Other” contained the remaining 34 surface categories. Here we present a summarizing description of the primary nine surface categories used in the analysis, all information are retrieved from the CORINE website.¹

- **Pastures**

Dense grass cover, of floral composition, dominated by Graminaceae, not under a rotation system. Mainly for grazing, but the folder may be harvested mechanically. Includes areas with hedges (bocage).

- **Discontinuous urban fabric**

Most of the land is covered by structures. Buildings, roads and artificially surfaced areas are associated with vegetated areas and bare soil, which occupy discontinuous but significant surfaces. Discontinuous urban fabric comprises residential areas around the edge of urban district centers, and certain urban districts in rural areas. These districts consists of blocks of flats, individual houses, gardens, streets and parks, each of these elements having a surface

area of less than 25 ha. Buildings, roads and artificially surfaced areas cover between 50-80% of the total surface area of the unit.

- **Non-irrigated arable land**

Cereals, legumes, fodder crops, root crops, and fallow land. Includes flowers and trees. Nurseries, cultivation and vegetables, whether open field or under plastic or glass (includes market gardening). Includes aromatic, medicinal and culinary plants. Does not include permanent pasture.

- **Sparsely vegetated areas**

Includes steppes, tundra and badlands. Scattered high-altitude vegetation.

- **Broad leaved forest**

Vegetation formation composed of principally trees, including shrub and bushes, where broad leaved species predominate.

- **Lakes and ponds – Originally called “Water bodies”**

Natural or artificial stretches of water.

- **Moors and heath – Originally called “Moors and heathland”**

Vegetation with low and closer cover, dominated by bushes, shrubs and herbaceous plants (heather, briars, broom, gorse, labumum, etc.)

- **Coniferous forest**

Vegetation formation composed of principally trees, including shrub and bushes, where coniferous species predominate.

- **Sea and ocean**

Zones seaward of the lowest tide limit. This category was modified in this study by addition of the remaining open sea.

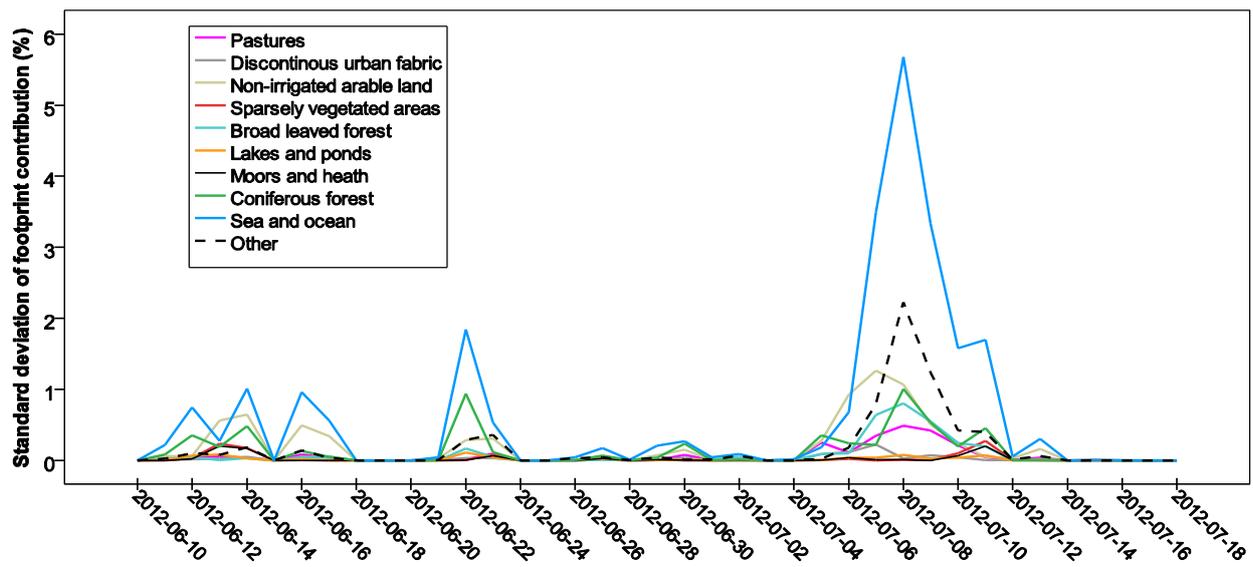


Figure S1. Standard deviation in absolute percentage points for each surface category. Footprints and associated uncertainties are based on 3, 5 and 7 back trajectory exposure.

1. EEA List of Corine Reports. <http://www.eea.europa.eu/publications/COR0-part2/page001.html>