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Evaluating the Long-range Transport of Persistent Organic Pollutants – Computation and Analysis of Air Mass Backward Trajectories

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Abstract

Persistent organic pollutants (POPs) are present in all environmental compartments. Most of them are products of human activities, however a small part of some POPs is of natural origin. They are lipophylic and therefore accumulate in organisms. A problem is also the fact that some of their metabolites and products of degradation processes are of a more dangerous character than the original pollutant. POPs are subject to long-range transport, mainly in the atmosphere.

We can use mathematical models to describe the movement of POPs and other pollutants inside of single environmental compartments and between them. In case of the atmosphere it is possible to use dispersion models which evaluate the transport, dispersion and transformation of pollutans from the known source. We can also use different types of receptor models to describe the situation at a receptor (sampling) site. Receptor models can be used if there is only an uncomplete or inaccurate inventory of sources available or the existence of unknown sources is supposed. Both models are very often based on the analysis of forward or backward air mass trajectories.

A trajectory is the path of an imaginary air parcel as it is acted on by winds. There exist different ways of computation but all of them require meteorological data computed or measured regularly during the whole time of considered air mass transport. The accuracy of a computed trajectory depends on the spatial and temporal resolution of meteorological observations, errors in data measurement and analysis and simplifying assumptions. Also, the longer a trajectory is, the less accurate it is.

Air mass trajectories used in our study were calculated using the HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) model developed by the Air Resources Laboratory of the American NOAA (National Oceanic and Atmospheric Administration) which is available free of charge on their READY website.

Backward trajectories were calculated to examine the situation at the regional background observatory Košetice (Pelhřimov district, Czech Republic) which is a part of EMEP (Co-operative Programme for Monitoring and Evaluation of the Long-Range Transmission of Air Pollutants in Europe). The study focused on 16 according to EPA prior polycyclic aromatic hydrocarbons (PAHs), seven polychlorinated bifenyls (PCBs), four isomers of hexachlorocyclohexane (HCH), dichlorodiphenyl trichloroethane (DDT) and two metabolites, hexachlorobenzene (HCB) and pentachlorobenzene (PeCB).

There exist various ways of evaluating backward trajectories. To examine the direction from which the most polluted air masses arrived it is possible to use the EMEP „sector“ method. These results can be supported by determining countries over which territories these air masses traveled. Other simple methods include the residence time analysis, identification of subsets of trajectories associated to air masses of a specific air quality or statistics methods.

The last three mentioned methods require gridding the considered area into regular cells and evaluating the abundance of trajectory endpoints within them. Here the geographic information system (GIS) comes into use together with the ArcGIS 8 computer programme and its special modules for data processing. The results can be presented in form of tables, graphs and also maps showing areas over which polluted air masses traveled and which have led with

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some probability to increased pollutant concentrations measured at the receptor site. It is useful to compare the results with already existing knowledge on industrial or agricultural areas too.

Data from the observatory Košetice for the years 1999 to 2001 were already evaluated by the EMEP method – we found the western sector to be dominant for more polluted air masses and this is in agreement with general meteorological conditions for the Czech Republic too. Also the states were previously roughly evaluated and except our neighbouring countries also France was more abundant.

The analysis of air mass trajectories helps to reveal connections between the meteorological activity and measured ambient air quality parameters. Evaluating backward trajectories also helps to identify pollutant sources and/or areas which is the first step when developing effective pollutant control strategies. Revealing air mass transport patterns for a background station like Košetice is also useful for the characterization of atmospheric long-range transport for a whole region.

1. Receptor models

Receptor models are based on the principle of chemical balance and the analysis is done using a large data set of chemical characteristics of samples from the receptor area. The advantage of receptor models is that their results are based on interpreting real measured data. Generally it is possible to describe a receptor model as a contribution of a number of independent sources to the presence of all chemical substances in the sample (Miller/Friedlander/Hidy 1972, 165).

From the receptor model point of view it is possible to divide pollutant sources into three categories: known source (location, composition and emission rates), known source tracers and unknown source. Table 1 lists different receptor models. Note that the models used to identify unknown sources are based on the analysis of backward air mass trajectories while models for source apportionment or the identification of source types require some information about the sources and do not use trajectories.

Receptor model	**Backward trajectories?**	**Known source?**	**Output information**	**Literature**
Potential Source Contribution Function (PSCF)	Yes	No	Potential source areas	Hopke/Li/Cizek/ Landsberger 1995, 69
Concentration Weighted Trajectory (CWT)	Yes	No	Potential source areas	Hsu/Holsen/ Hopke 2003, 545
Residence Time Weighted Concentration (RTWC)	Yes	No	Potential source areas	Stohl 1996, 579
EMEP "Sector" method	Yes	No	Direction of source areas	EMEP 2005, 2004
Cluster Analysis	Yes	No	Direction of source areas	Brankov/Rao/Porter 1998, 1525
Factor Analysis/ Principal Component Analysis	No	Source tracers – yes Source location – no	Source types	Bzdusek/Christensen/ Li/Zou 2004, 97
Chemical Mass Balance (CMB)	No	Yes	Source apportionment	Lawrimore/Aneja 1997, 2751

Tab 1: Selected receptor models and their basic characteristics

2. Calculation of trajectories

Air mass backward trajectories for the Košetice observatory were calculated using the HYSPLIT model which computes forward and backward trajectories (Draxler/Rolph 2003). It is available on the READY website of the NOAA (Rolph 2003). The input information was as following:

a) isobaric trajectories (this dynamic computation approach uses pressure fields)
b) 96 hours length (covers the interest area and is not too long)
c) 18 UTC starting time (18 p.m. is the middle of the sampling interval)
d) 500 m starting height (approximately corresponds to the pressure level of 925 hPa which is the representative height for tropospheric air flow)
e) geographical coordinates for Košetice

The basic computation output are the coordinates for trajectory points marking the position of the air mass in regular hourly intervals. Output files for each trajectory had to be transformed into the dbf format to be applicable for ArcView.

3. Potential source contribution function

The PSCF method is a simple and useful receptor model based on backward trajectory analysis. It calculates the number of points of trajectories *i* in grid cells *j* which cover the whole area of interest. The computation formula is described by Hopke/Li/Cizek/Landsberger (1995, 69):

$$PSCF_{ij} = m_{ij} / n_{ij}$$

where n_{ij} is computed for all trajectories and m_{ij} only for those belonging to "contaminated" samples. Cells with a high PSCF value indicate areas with possible high contribution to the pollutant concentration at the receptor site.

A disadvantage of PSCF is the impossibility of determining uncertainties for the PSCF values but this can be done by applying the bootstrapping method to trajectory sets. In the study of Hopke/Li/Cizek/Landsberger (1995, 69) it also led to a better localization of sources. PSCF allows distinguishing between moderate and major sources by changing the definition of "contaminated" samples.

4. ArcView 8.2

For the application of the PSCF model GIS come into use. We have the ArcView 8.2 programme. The first layer is represented by a map of Europe over which a grid of 0,5° × 0,5° cells is layed (a special Point Grid Wizard script is used). The cell size can vary according to the size of the trajectory set.

The next step is using the dbf files for adding trajectory points X and Y coordinates as next layers. This is done for the whole trajectory set. They are connected with the grid by the Spatial Join function and a join output layer for all trajectories is created by adding data from attribute tables of each trajectory. The sum of points in each grid cell is computed. The density of points over the map of Europe can be showed by using the Properties - Symbology function. The whole process is repeated for trajectories belonging to "contaminated" samples. Finally for each cell the sum of points of "contaminated" trajectories is divided by the sum of points of all trajectories. The Properties – Symbology function is then used to draw a map showing potential source areas.

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