MODELLING OF POLYCYCLIC AROMATIC HYDROCARBONS FROM SELECTED POINT AND AREA SOURCES IN CENTRAL EUROPE

Christos Efstathiou [1], Jana Matejovičová [1,2], Gerhard Lammel [1,3], Jana Krajčovičová [2], Martin Kremler [2]

[1] Research Centre for Toxic Compounds in the Environment, Masaryk University, Kamenice 5 - A29, 625 00 Brno, Czech Republic
[2] Slovak Hydrometeorological Institute, Jeséniova 17, 833 15 Bratislava, Slovakia
[3] Max Planck Institute for Chemistry, Hahn-Meitner-Weg 1, 55128 Mainz, Germany

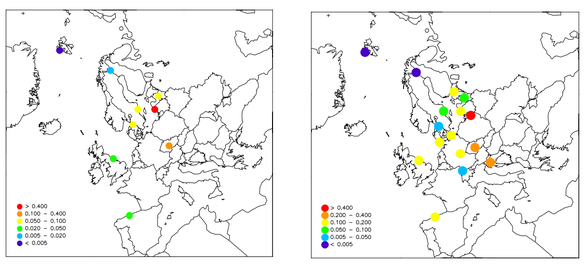
Motivation

Mean annual concentrations of benzo(a)pyrene (B(a)P) frequently exceed the target value 1 ng m^{-3} at air quality measurement stations across Europe. Air quality modelling can bring additional information on the spatial distribution and the main sources of B(a)P, regional transport and processes, which influence its atmospheric levels. This study consists of two parts – simulations of B(a)P concentrations on the regional and local scales and their linkage with existing monitoring networks.

Introduction

Atmospheric levels of polycyclic aromatic hydrocarbons (PAH) were established in the local and regional scales with a combination of modelling approaches and tools. The spatial distribution of benzo(a)pyrene B(a)P was modelled for a domain covering Europe using a modified version of the Community Multi-scale Air Quality (CMAQ) modelling system linked with the Weather Research and Forecast (WRF) model. In addition, the Lagrangian model CALPUFF was used to study the significance of point and area sources for B(a)P levels on the local scale.

Measurement Networks



In the framework of the EMEP measurement programme there were 9 sites measuring POPs in two atmospheric phases (gas and particulate) in 2006 and 16 such sites measuring POPs in 2008.

Figure 1: Mean annual concentration of benzo(a)pyrene (ng m^{-3}) at EMEP stations in 2006 (left) and 2008 (right). *Source: Aas & Breivik 2008, 2010.*

REGIONAL STUDY
- space distributin of B(a)P concentrations

Models used

The Community Multi-scale Air Quality (CMAQ) modelling system was used to simulate air pollution in the regional scale. The computational design involves the preparation of meteorological inputs with the Weather Research and Forecasting (WRF) model for a gridded domain that covers Europe. A detailed emission inventory was created using the SMOKE-EU emissions model developed by the Institute for Coastal Research of Helmholtz Centre Geesthacht (Bieser et al. 2011).

This work demonstrates the initial steps towards modelling of the processes that determine the concentrations of POPs in the atmosphere.

Meteorological input data

Preliminary daily runs of WRF 3.2.1 have been completed with GFS data (spatial resolution 0.5° x 0.5°). Computational domain: 450 x 370 grid cells, spatial resolution 12 km x 12 km, 36 vertical levels.
Set up of WRF 3.2.1: WSM 3-class simple ice scheme, radiation long wave scheme 'rrtm'; radiation short wave scheme ' Dudhia ', near-surface Monin-Obukhov scheme, 4 soil layers, unified Noah land-surface model.

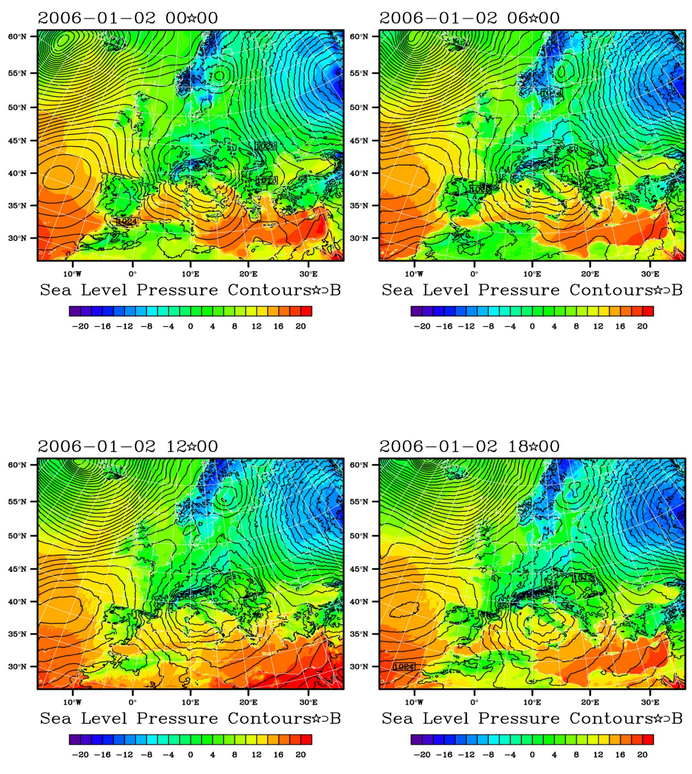
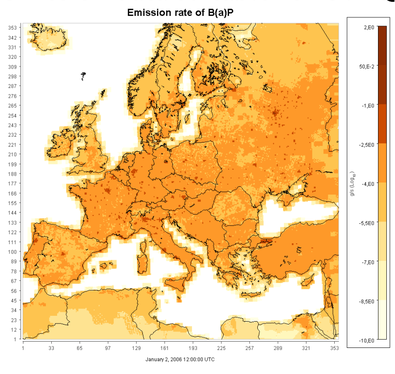


Figure 3: Example of WRF output for 2 January 2006 - Temperature at 2 m and sea level pressure.

Emissions input data

The emission model SMOKE is the official emission model of the United States Environmental Protection Agency (US EPA) and is one of the most used emission models worldwide (Houyoux et al. 2000). SMOKE was originally created by the MCNC Environmental Modeling Center (EMC) and developed further by the US EPA. It is the official emission model of the Models-3 Community Modeling and Analysis System (CMAS) and creates emission data suitable for CMAQ (Byun & Ching 1999 and 2006).



Although SMOKE is highly specialized for usage with officially reported data in the US, there have been several successful attempts to apply it to other regions. A modified version of SMOKE, SMOKE for Europe (SMOKE-EU), was developed by the Institute for Coastal Research of the Helmholtz Centre Geesthacht (Bieser et al. 2011). The emission data set was prepared for CMAQ 4.7.1.

Figure 2: B(a)P emission rates (January 2, noon)

Computational domain for CMAQ and model set up

Spatial resolution 12 x 12 km (357 x 357 cells), 17 (non-hydrostatic sigma-p) vertical layers, chemical mechanism CB V, aerosol module aero5. Concentrations of B(a)P were scaled from primary carbonaceous particle (fixed ratio of B(a)P and PM_{10} emission factors, f_{BaP}/f_{PM10}).

Modified CMAQ 5.0.1 – Preliminary Simulation Results (CMAQ-POPS)

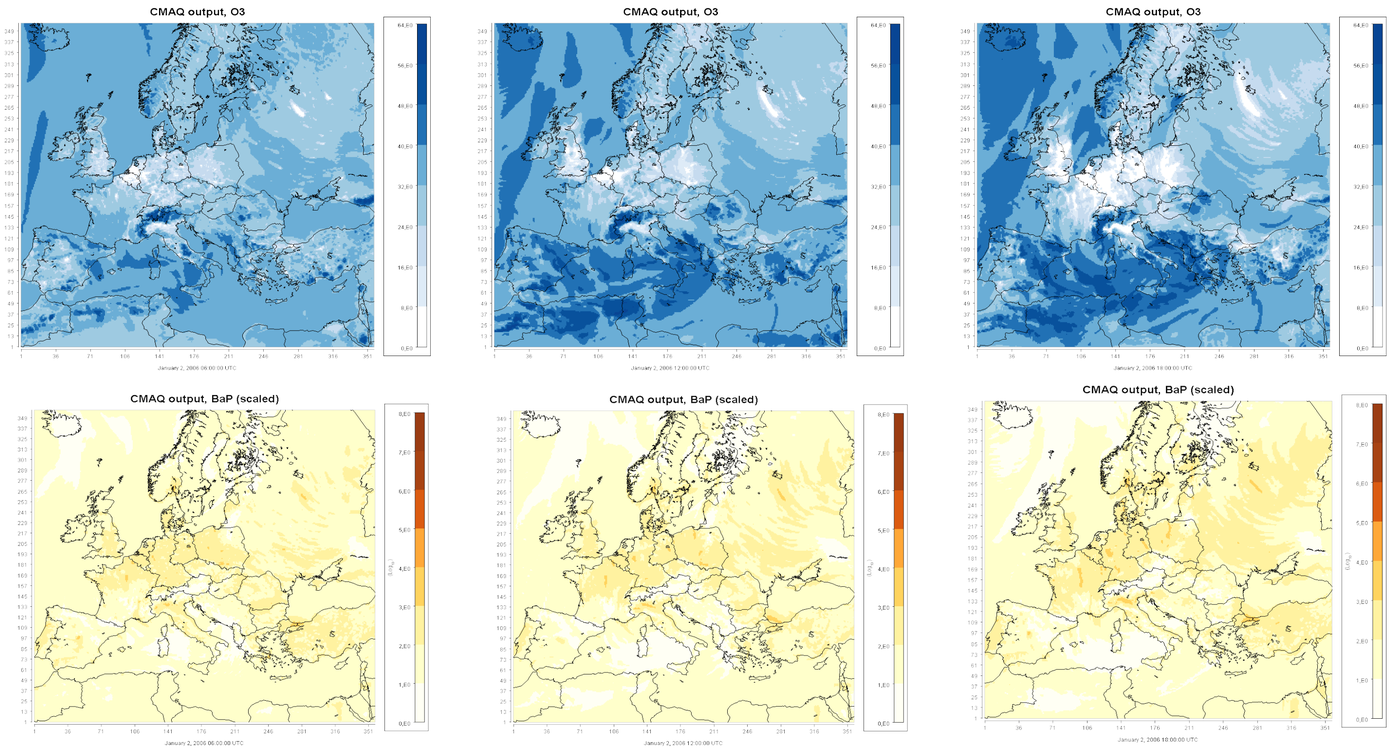
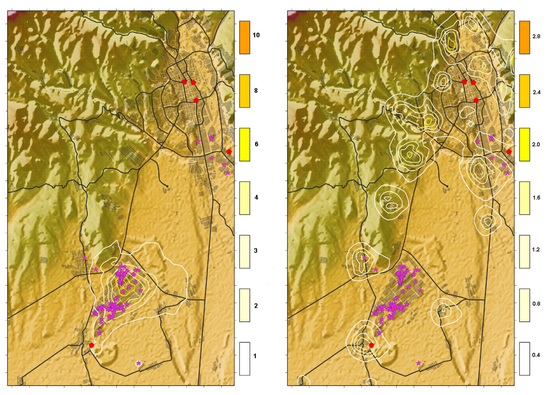


Figure 4: CMAQ output for ozone (upper row, ppbV) and BaP (lower row, ng m^{-3}) for 2 January 2006 without spin-up.

LOCAL STUDY
- comparison of point and area sources of B(a)P

Model used, computational domain

The Lagrangian puff model CALPUFF (Scire et al. 2000) was used for the local study, focused on the comparison of emission sources in Slovakia. The primary aim was the source apportionment of PM_{10}. The domain of the size 13.5 x 22 km, with metallurgy and coke production (large industrial point source) and several areas of domestic heating was selected for modelling of B(a)P. The spatial resolution of the domain was 500 m x 500 m. The simulation of PM_{10} for the year 2008 was run for each source type separately. No sink of B(a)P was included (dry and wet deposition switched off, no chemical degradation). An estimate of the annual mean concentration of B(a)P for each source type was obtained from the annual mean concentration of PM_{10}, scaled by the ratio of the emission factors, i.e. $f_{B(a)P}/f_{PM10}$. Emission factors used for the reporting to the Convention on Long-Range Transboundary Air Pollution (CLRTAP) were used (SRIIR 2010). In domestic heating, only wood combustion was taken into account, as the amount of coal used for residential heating is negligible.



Detailed information on the simulation setup, input data acquisition and processing is presented in a companion paper (→ *HARMO 2013 poster No. H15-50*; Krajčovičová et al. 2013)

Figure 5. Annual mean concentration of B(a)P (ng m^{-3}) from large point source (metallurgy, on the left) and domestic heating (on the right).

Legend:
pink = point sources, red = air quality stations.
B(a)P is measured at the southernmost air quality station only.

Results and discussion

A regional-scale simulation was run for selected days of January 2006. B(a)P concentration was obtained in coherence to the method used for the local study - from the primary carbonaceous pollutants scaled by the ratio of B(a)P and PM_{10} emission factors, $f_{B(a)P}/f_{PM10}$. The dominance of strong area sources (urban areas including strong point sources) for the B(a)P distribution can be recognized (Figure 4). In the next step chemical degradation by O_3 will be included.

Atmospheric concentrations of B(a)P provided by the local-scale study were comparable to the concentrations measured at the air quality station close to the industrial source addressed. Concentrations of B(a)P in the range of 1.2 – 5.3 ng m^{-3} were measured in January 2008. The local study (Figure 5) confirmed the expectations that a large industrial point source contributes more significantly to B(a)P levels in the vicinity of this source than domestic heating does. However, according to the measurements of B(a)P on other air quality stations in Europe (EEA 2011), it is possible that urban background sites , where domestic heating can be the only significant source of air pollution, are exposed to high annual mean concentrations of B(a)P. This will be addressed by simulations of the year 2010, which will combine local and regional modelling approaches under various emission scenarios.

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