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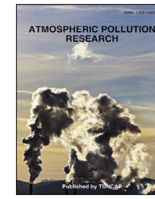

Original article

An urban scale application and validation of the CALPUFF model

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A B S T R A C T

The paper presents selected results of an urban scale analysis of air quality. Calculations are carried out for the Warsaw area, basing on the emission and meteorological dataset for the year 2012. The regional scale CALMET/CALPUFF modeling system has been used to link the emission data with the resulting concentration maps of the selected polluting substances that characterize the urban atmospheric environment: PM_{10}, $PM_{2.5}$, NO_x, SO_2, CO, C_6H_6. The emission field encompasses the basic activities in an urban area: the energy sector, industry, traffic and the municipal sector. The basic simulation results present the annual mean concentrations of pollutants at the receptor points and indicate the areas where air quality limits are exceeded. The presentation is focused on the assessment of the model performance. The calculated annual mean concentrations are verified against the measurement data at 5 monitoring stations. Moreover, for selected modeling periods (January 2012), performance estimates are also presented for 1-h concentration results. The good performance of the model is shown for the annual mean predictions, while the temporal agreement of the short-term, 1-h average concentrations is much less accurate, especially for the low-wind meteorological episodes.

1. Introduction

Air pollution dispersion models and the Integrated Assessment Models (IAM) (Lim et al., 2005; Calori et al., 2006; Mediavilla-Sahagún and ApSimon, 2006; Carnevale et al., 2012) are often applied for supporting decisions in air quality control and emission abatement. The key module of the system is an air pollution transport model which links the emission input data with the resulting environmental impact. The purpose of the mathematical model is to provide a quantitative assessment of the intensity of the dispersion processes and their results in the form of pollution concentration maps. These data are in turn the basis for the evaluation of resulting environmental risk and for supporting the necessary planning actions (Mediavilla-Sahagún and ApSimon, 2006; Pisoni et al., 2010; Carnevale et al., 2012). The quality of the final environmental decisions directly depends on the model performance and also reflects the uncertainty related to the input data and the model's intrinsic simplifications and parameterization (ETC/ACM, 2011; Holnicki and Nahorski, 2015). The full information about the model's strengths and weaknesses is a key factor for investigating effective strategies of emission abatement and improving air quality.

The applied implementations of air quality models usually depend on the temporal and spatial scale of the forecast (global, regional, urban, local), characteristics of the domain, the structure of the emission field, composition of the key polluting compounds and on the application where the modeling results are to be used. CALPUFF/CALMET modeling system (Scire et al., 2000) is often applied in analysis of the atmospheric environment in regional and urban areas (Elbir, 2003; Calori et al., 2006; Trapp, 2010; Buchholz et al., 2013; Holnicki and Nahorski, 2015). CALPUF is a non steady state, Gaussian puff dispersion model, which operates in the Lagrangian system of coordinates and considers the geophysical data, the temporal and spatial variability of meteorological conditions in three dimensions. It is a multi-layer model designed to investigate the dispersion of gases and particles, using space and time varying meteorology based on similarity equations. Emission strengths, turbulence, transformation and removal are the main processes included. It is able to analyze different source types: point, line, volume and area using an integrated puff formulation incorporating the effects of plume rise (Holmes and Morawska, 2006; Tartakovsky

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et al., 2013). The model calculates dry deposition, using the resistance method with inputs for deposition velocities and the wet removal using a scavenging coefficient approach as a function of precipitation intensity and type. CALPUFF uses three-dimensional meteorological fields computed by the CALMET preprocessor.

Many studies address the application and validation of the CALPUFF predictions. A wide overview of near-field to far-field CALPUFF applications is presented by Escoffier (2013). Model validations are often based on the comparison of CALPUFF and AERMOD models in near-field applications. Rood (2014), using the Winter Validation Tracer Study dataset, Bussini et al. (2012), for odor dispersion, and Oshan et al. (2006) in the urban case study – show good agreement between the two models, while Dresser and Huizer (2011), assess the performance of CALPUFF better than that of AERMOD (the short-term and the annual average model predictions of SO_2 compared with the measurements). In the results presented in (Tartakovsky et al., 2013), for prediction of TSP dispersion in a complex terrain, the results of the AERMOD model show better agreement with the measurements. On the other hand, strong over-predictions in short-term CALPUFF forecasts are pointed out in (Brode, 2012) as well as in the presentation by Fox (2012). Similar conclusions can be found in (Holmes and Morawska, 2006).

This study presents a case study application of CALPUFF model on an urban scale. Selected modeling results are utilized to assess the performance of model predictions depending on the time horizon of analysis and the temporal resolution step. In particular, good performance of the model is shown for long-term forecasts (computation of the annual mean concentrations), while the weaknesses of the system appear for 1-h averaged pollution data. In particular, it is shown that over-predictions of short-term forecasts coincide with weak wind meteorological episodes. The base of the analysis within this study is the contents of the paper (Holnicki and Kałuszko, 2014), where air quality analysis for Warsaw, Poland is presented.

In Section 2 selected results of air quality modeling are presented, and model validation is discussed in Section 3.

2. The Warsaw case study – air quality assessment

In the paper (Holnicki and Kałuszko, 2014) the CALMET/CALPUFF modeling system was used to analyze dispersion of the main polluting compounds in the Warsaw Metropolitan Area, Poland. The emission field comprises industrial and domestic heating sources, the urban transportation system and the transboundary inflow of primary and secondary pollutants from distant sources. The modeling domain covers the area of about 520 km^2 with the grid spacing of 500 m. The aim of the simulation was to obtain spatial maps of the annual average concentrations of the main urban pollutants, to determine the regions where pollution limits are exceeded, and to identify emission sources which are mainly responsible for these violations. Such results are the key factors in the formulation of the respective regulatory actions and emission reduction strategy. Within this study the above modeling results are utilized to evaluate the performance of the CALPUFF model predictions.

Fig. 1 shows the computational domain and the spatial discretization grid. The numerical simulation is based on the emission and meteorological dataset for the year 2012. The annual mean concentrations of the main pollutants, which characterize an urban environment, were recorded at 2248 fictitious receptor points which are located in the centers of the elementary grid elements, at 1.5 m level (compare Fig. 1). The inventory of emission sources encompasses the following categories of emission sources:

- High point sources (energy sector and major industrial emitters;
- Low point sources (other industrial and local sources);
- Area sources (residential sector and distributed industrial sources);
- Linear sources (the urban transport system).

The total emission field also includes the close emission outskirt of Warsaw, the belt of about 10–20 km wide. General characteristic of the emission field in Warsaw is shown in Text S1 and Tables S1–S2 (WIOŚ, 2012). The point sources, including technological and emission parameters, are located according to geographic coordinates. Area and linear sources are represented by 0.5×0.5 km^2 grid elements. The temporal variability of emission intensity takes into account the seasonal changes of energy sector emission (point sources) or residential sector emission (area sources). Daily emission variability of the linear sources reflects changes of traffic intensity. The emission data, similarly as meteorology, are finally entered as a sequence of 1-h episodes (8785 time steps) which cover the year considered. Some details concerning emission can also be found in the report (Holnicki and Kałuszko, 2014).

The supporting material (Tables S3–S4, Fig. S1), based on (WIOŚ, 2012), presents general characteristics of the meteorological conditions in Warsaw in the year 2012 (temperature, precipitation, atmospheric stability, wind rose). The final set of the data used by the main model is re-analyzed and preprocessed by WRF (NCAR, 2008) and CALMET models (Text S2).

The performance of a dispersion model is a crucial factor in supporting decisions concerning urban air quality. This factor is discussed in Section 3, referring to the Warsaw implementation. The model predictions considered in this study comprise the following selected pollutants: NO_X, SO_2, PM_{10}, $PM_{2.5}$, CO, C_6H_6. Concentration of particulate matter is calculated as a result of: the primary emission (all sources), the re-suspended emission (linear sources – Table S2), the sulfate and nitrate aerosols computed by CALPUFF. The calculated concentrations are compared with the measurement data recorded at 5 automatic monitoring stations, the locations of which are indicated in Fig. 1, while Table 1 shows the main technical parameters.

The paper (Holnicki and Kałuszko, 2014) presents concentration maps for the main polluting factors and indicates the most polluted regions, where air quality limits are exceeded. In particular, significant exceedances of air quality standards occur for NO_X and PM_{10}. The respective concentration maps are shown in Fig. 2. In both cases the quality limits for the annual mean concentrations: 40 $\mu g/m^3$ for PM_{10} and 30 $\mu g/m^3$ for NO_X (CAFE, 2008; ME, 2012) are violated, mainly in the center and S–W districts of the city. The concentration of the fine fraction of particulate matter, $PM_{2.5}$, also exceeds the limit value – 25 $\mu g/m^3$ by about 25% in the S–W peripheral district (compare the research report by Holnicki and Kałuszko, 2014), mainly due to individual housing emission. The other pollutants discussed in this study attain annual average concentrations below the official admissible values: 20 $\mu g/m^3$ (SO_2), 10,000 $\mu g/m^3$ (CO), 5 $\mu g/m^3$ (C_6H_6).

Fig. 2 shows that concentrations of both pollutants are strongly correlated with the topography of the main arterial streets. It mainly relates to NO_X which is a typical, traffic related pollution. The area sources of the local heating as well as the trans-boundary inflow from distant emission sources also contribute to the overall PM_{10} pollution.

Due to the linear structure of the CALPUFF model, it is possible to individually compute the contribution of each source to the overall concentration at any receptor site. This approach has been applied to assess the source apportionment at the selected receptors. The diagrams in Fig. 3 present the source apportionment for the main pollutants, i.e. PM_{10}, $PM_{2.5}$, NO_X and SO_2. (As said