An urban scale validation of the CALPUFF model

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Abstract

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}, $PM_{2.5}$, NOx, 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.

Keywords: urban air pollution, emission inventory, computer modeling, model validation

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 abo

ut 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. CALLPUF/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 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 odour dispersion, and Oshan et al. (2006) in the urban case study – show good agreement between the two models, while Dresser and Huiser (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., 3013), 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

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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.

Figure 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);

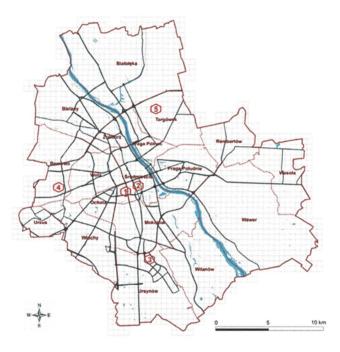- Linear sources (the urban transport system).

Fig. 1. The study area; location of the monitoring stations

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

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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 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 µg/m3 for PM_{10} and 30 µg/m3 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, PM2.5, also exceeds the limit value – 25 µg/m3 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 µg/m3 (SO2), 10000 µg/m3 (CO), 5 µg/m3 (C6H6).

Table 1. Characteristics of the monitoring stations

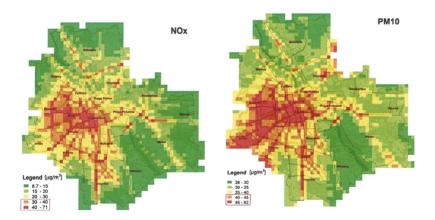| Station	Coordinates [°]	Pollutants measured	Site type
#1	(21,005;52,219)	NO_X, PM_{10}, $PM_{2.5}$, C_6H_6, CO	Roadside
#2	(21,019; 52,225)	SO_2, NO_X, CO	Urban background
#3	(21,034; 52,161)	SO_2, NO_X, PM_{10}, $PM_{2.5}$, C_6H_6	Urban background
#4	(20,909; 52,226)	SO_2, NO_X	Industrial impact
#5	(21,042; 52,291)	SO_2, NO_X, PM_{10}, $PM_{2.5}$, CO	Urban background

Fig. 2. The exemplary, annual mean concentration maps of NO_X (left) and PM_{10} (right)

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 before, there are five contributing emission categories considered: high and low point sources, area sources (residential sector), linear sources (transportation system) and trans-boundary inflow from the outside emission sources (incorporated as boundary conditions). Two exemplary receptor points are selected to illustrate how the share of emission categories depends on the location of the receptor point. Fig. 3 (left) shows a receptor located in the central district, near monitoring site #1 (roadside, street canyon site), and Fig. 3 (right) – a receptor located in the neighborhood of station #5 (housing, local street). Generally, higher concentration values occur in the center. The vicinity of a traffic artery means the dominating contribution of linear sources, especially for NO_X and PM_{10}, which both violate admissible concentration limits, 30 $\mu g/m^3$ and 40 $\mu g/m^3$, respectively (CAFE, 2008). The more significant share of area sources occurs in the residential district, especially with PM_{10} and $PM_{2.5}$ compounds. Also the trans-boundary inflow considerably contributes to both fractions of particular matter pollution. For SO_2 a balanced contribution of source categories is observed, with concentration below the limit value, 20 $\mu g/m^3$. CO concentration depends mainly on line sources, similarly to C_6H_6, where the share of the point emission is remarkable.
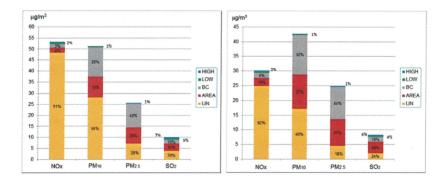
Fig. 3. The source apportionment depending on receptor location. The vicinities of the monitoring sites: station #1(left) and station #5 (right)

3. Assessment of the model performance

3.1 Annual mean concentrations

The annual mean concentrations based on the observation data were compared with the calculated values at the same receptor sites. Each station listed in Table 1 measures the selected set of compounds. For the pollutants considered in the study, the following numbers of measurement results are available: $NO_X - 5$, $SO_2 - 4$, $PM_{10} - 3$, $PM_{2.5} - 3$, $CO - 3$, $C_6H_6 - 2$. The commonly used simple metrics, employed to quantify the difference between modeled and observed concentrations, is the FAC2 index (Chang and Hanna, 2004; Dernwent et al., 2010; Juda-Rezler, 2010), based on a scatter plot of points, where the fraction of the measurement to observation is within the constraints:

$$0.5 \leq FAC2 = C_m/C_o \leq 2$$

where: C_o, C_m – observed and modeled concentrations, respectively. The perfect model, due to the above metrics, would have FAC2 = 1.

The diagrams shown in Fig. 4 depict assessments of FAC2 index for the above 6 basic compounds. Most of the scatter plots in Fig. 4 show that the modeling results satisfy the

performance standard, $0.5 \leq FAC2 \leq 2$. The only exception is related to the monitoring station #1, where the model (60 µg/m^3) underestimates the measured NO_X concentration (about 140 µg/m^3). This case, however, is caused by traffic observation, where the point-wise, street-canyon measurement is performed, while the model calculates spatially averaged concentration. A similar underestimation of NO_X pollution at this receptor site is also seen for short-term predictions (compare Fig. 6).
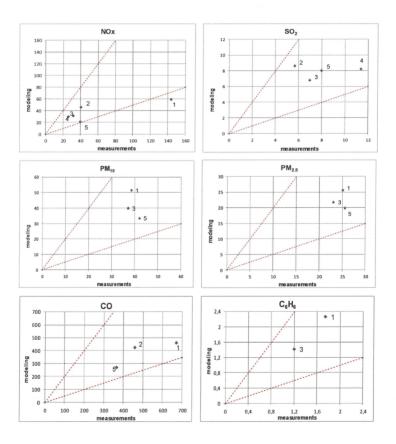

Fig. 4. Modeling vs. measurements – the annual mean concentrations [µg/m^3] at the monitoring stations (compare Table 1)

The calculated results show slight underestimation of CO and similar overestimation of C_6H_6 concentrations (compare Fig. 4), however FAC2 criteria are satisfied. CO pollution is mainly due to the mobile sources' emission with a significant share of the transboundary inflow. Moreover, linear emission is a dominating contributor to C_6H_6 in the central districts, while high point sources (major power plants) or low point sources (local industry) have a substantial share locally, e.g. in some peripheral districts.

A similar approach is proposed for the assessment of modeling performance in (CAFE, 2008) Directive. Annual average predicted concentrations should be in the range: SO_2 and NOx ($\pm 30\%$), PM_{10} and $PM_{2.5}$ ($\pm 50\%$), C_6H_6 ($\pm 50\%$). There is no limit for CO. Table S5 (Supporting material) shows the respective values for the above pollutants in five receptor points. The more significant underestimation due to the above limits occurs for NOx at #1 receptor point (roadside).

3.2 Daily average PM_{10} concentrations

Regarding PM_{10} pollution, an alternative index of air quality is that 24-h average PM_{10} concentration can exceed the limit value 50 $\mu g/m^3$ no more than 35 times in a year (CAFE, 2008; ME, 2012; ETC/ACM, 2011; ETC/ACM, 2013). The availability of short term measurements is very limited. However, there are some literature results which indicate a relationship between the number of days with 24-h average PM_{10} concentration exceeding 50 $\mu g/m^3$ limit and the annual mean value. Stedman et al. (2007) derived this relationship based on the United Kingdom monitoring data for the years 1992—1999, including supplementary measurements for 2004. The conclusion is that the annual mean concentration of 31.5 $\mu g/m^3$ is equivalent to the number of 35 days with 24-h mean concentration exceeding 50 $\mu g/m^3$.

On the other hand, in (Kiesewetter et al., 2014) the 36th highest daily mean PM_{10} concentration is suggested as an alternative index, which can stand for the daily mean limit. Also for this index a relationship is shown that the 36th highest daily average value

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corresponds to 29.6 µg/m^3 of annual mean PM$_{10}$ concentration. In this case the last result is based on the observation data from the Air Base, the European air quality database (2009). In both cases the relationship was directly applied to assess the 24-h concentration based on the annual mean concentration resulting from a model simulation. The general conclusion from the above results is that the daily mean concentration limit 50 µg/m^3 (CAFE, 2008) is a more restrictive air quality index in comparison with the annual mean 40 µg/m^3.
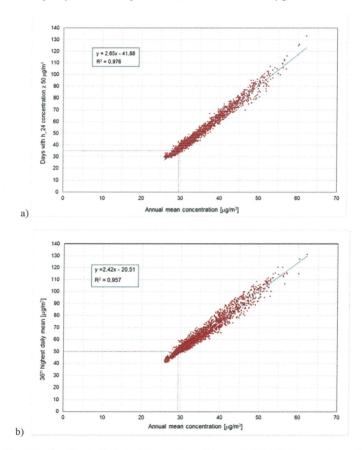
a)

b)

Fig. 5. Daily average limits: (a) the number of days with 24-h limit exceedance, (b) the 36th highest daily mean concentration vs. the annual mean concentrations

The above two approaches have been verified in the Warsaw case study and the CALPUFF modeling results. Figure 5 presents the respective scatter plots of the resulting concentrations – the daily mean index vs. the annual mean concentration – at 2248 receptor points. For both daily mean indices: (i) the number of the violations of 50 $\mu g/m^3$ standard (Fig. 5a) and (ii) the 36th highest daily mean PM_{10} concentration (Fig. 5b) – the corresponding annual mean threshold is approx. 29.5 $\mu g/m^3$. This confirms the previous findings of Kiesewetter et al. (2014) as well as the adequacy of the CALPUFF model in the analysis of the correspondence of annual/daily mean limit concentrations. On the other hand, as shown below, direct application of the CALPUFF model in short term forecasting of air pollution is not recommended.

3.3 Short term average concentrations

The basic time resolution of the input emission data applied in the CALPUFF simulation is 1-hour step. Also the recorded modeling results contain 1-h average concentrations at receptor points. The resulting concentrations can be compared with the 1-h mean observations recorded at the automatic monitoring stations (see Table 1). Figures 6–7 show comparison of 1-h average concentrations of NO_X, PM_{10}, $PM_{2.5}$, SO_2 computed and observed at 2 monitoring sites, stations #1 and #3. Exemplary graphs for January (the set of 744 values of 1-h concentrations) were selected for this presentation. This month is representative for the year 2012, when the temporal share of the over-predicted concentration is considered. There are approximately 2–4 computed peaks per month in 2012, and they occupy about 3% of the total modeling period (such an episode usually lasts 6–10 hours). As follows from the wind rose (Fig. S1) the frequency of the weak wind episodes (below ~2 m/s) is similar.

The most apparent effect which appears in the recorded set of the modeling results relates to very high concentration peaks which appear at some specified time moments. In all
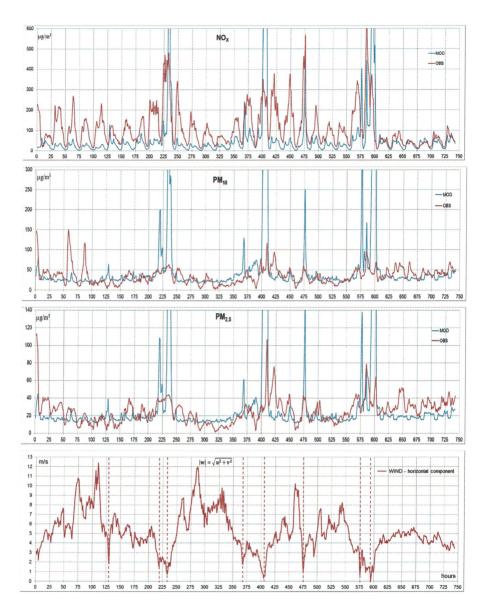
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Fig. 6. The 1-h average concentrations of NO_X, PM_{10} and $PM_{2.5}$ (#1 monitoring station Jan 2012). Bottom graph – the related horizontal wind velocity
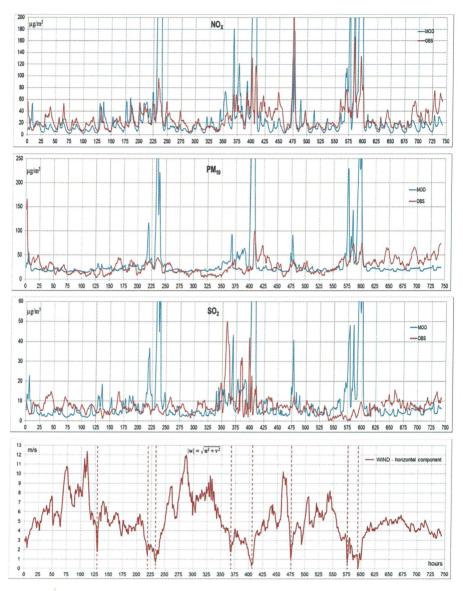
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Fig. 7. The 1-h average concentrations of NOX, PM10 and SO2 (#3 monitoring station, Jan. 2012). Bottom graph – the related horizontal wind velocity

figures and polluting compounds these peaks strictly coincide with the same meteorological episodes (compare the identical wind rose graphs for distant stations, Fig S1), representing the very weak velocity of the horizontal wind. For this reason, each plot of the resulting concentration values in Figs 6–7 is compared with the temporal characteristics of the wind velocity. The most evident, sharp maxima occur in the hours when the horizontal wind speed in the bottom layer is close to or below 1 m/s. This is an evident effect of poor representation of turbulent diffusion in such meteorological episodes and limits the applicability of CALPUFF to long term modeling.

Furthermore, it can be observed that the temporal correlation of the calculated and observed data is relatively good for NO_X concentrations, since the linear emission data reflects the daily variability of the traffic intensity. A similar correlation can be observed at all monitoring sites stations. Since station #1 represents a typical street canyon site, the model definitely underestimates 1-h average data. Certain correlation of the observed and calculated data can be also observed for PM concentrations, where the contribution of linear sources is also apparent (especially for PM_{10}). Much worse is the agreement of the short term data for SO_2 concentration.

4. Summary

The paper presents selected results of an urban scale analysis of air quality, based on the CALPUFF model simulations. Calculations are carried out in the Warsaw metropolitan area, basing on the emission and meteorological dataset for the year 2012. The total emission field consists of the following source categories: pointwise (energy sector, industry), area (housing), linear (urban transport). The transboundary inflow of the main pollutants is also included. The main results present the spatial distributions of the year average concentrations 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 exceedances of the air quality limits due to (CAFE,

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2008) are related to NO_X, PM_{10} and $PM_{2.5}$ pollution, mainly in the central and S-W districts of the city.

The principal subject of the paper is the CALPUFF model validation, referred to the temporal scale of the forecast and the time averaging step. To this end model predictions were compared with the observation data from 5 monitoring stations (Table 1). Satisfactory compatibility of the modeling results with measurements can be observed for annual mean concentrations. In this case, the validation is based on the FAC2 index (Chang and Hanna, 2004; Dernwent et al., 2010; Juda-Rezler, 2010). The required standards are satisfied for all polluting compounds and monitoring sites. The only exception is NO_X pollution at the street canyon site #1, where the calculated concentrations are definitely underestimated compared to the observed values. A similar relation was observed for short term episodes.

The European Directive (CAFE, 2008) defines two limit values of PM_{10} pollution: 40 $\mu g/m^3$ for annual mean concentration and (for the protection of human health) 50 $\mu g/m^3$ for daily mean concentration, not to be exceeded more than 35 times in a calendar year. Some literature results (Stedman et al., 2007; Kiesewetter et al., 2014) indicate a correlation of the above measures, basing on the UK and European monitoring results. Moreover, Kiesewetter et al. (2014) show that the standard 24-h average limit (CAFE, 2008) can be replaced by an equivalent index – the 36th highest daily mean concentration. A similar comparison was performed within this study based on the CALPUFF modeling results. The scatter plots presented in Fig. 5 confirm the equivalence of the above two indices, and also show that each 24-h limit value corresponds to approximately 29.5 $\mu g/m^3$ of annual mean concentration.

Figures 6–7 present sample performance assessments of the short-term, 1-h average concentrations (results for January 2012 are displayed as a representative example). The comparison of the calculated and observed concentrations shows significant discrepancies, especially in certain determined temporal moments during one month period which is

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displayed. Very high calculated concentration peaks coincide with episodes of very low wind speed in the bottom layer of the atmosphere. This effect is independent of the receptor's location and is exactly the same at all monitoring sites and it concerns all the polluting compounds. The effect follows from the intrinsic properties of the model and is probably related to the parameterization of the turbulent diffusion effect in week wind episodes. This signifies rather poor performance of the CALPUFF system in the short term analysis, especially for some meteorological scenarios.

Another question is the consistence of the modeled and observed time series, depending on the specific pollutant and on the characteristics of the emission source. It follows from Figs 6–7, that the consistence of the model-measurements time series is relatively good for NO_X, less apparent for PM_{10} and poor for SO_2. The dominating contribution of linear sources in the case of NO_X (compare Fig. 3) means the coincidence of the spatial location of the source and receptor site. Moreover, the emission strength of the mobile sources reflects the daily variability of the traffic intensity, which is seen both in the observed and calculated data (compare Figs 6–7). The contribution of linear sources is much lower for PM pollution, but the significant share of transboundary inflow flattens the concentration graphs. Worse model-measurement agreement occurs for SO_2 where the share of all emission categories is important, including significant contribution of distant sources. The above properties also confirm the low applicability of CALPUFF in short term pollution analysis.

References

Brode, W.R., 2012. CALPUFF Near-field validation. 10th Conference on Air Quality Modeling. Research Triangle Park, NC, March 13, 012 (//epa.gov/scram001/10thmodconfpres.htm).

Buchholz, S., Krein, A., Junk, J., Heinemann, G., Hoffmann, L., 2013. Simulation of Urban-Scale Air Pollution Patterns in Luxembourg: Contributing Sources and Emission Scenarios. *Environmental Modeling and Assessment* 18, 271–283.

Bussini, V., Capelli, L., Sironi, S., Nano, G., Rossi, A.N., Bonati, S., 2012. Comparison of CALPUFF and AERMOD Models for Odour Dispersion Simulation. *Chemical Engineering Transactions*, 30, 205–210.

CAFE, 2008. Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe.

Calori, G., Clemente, M., De Maria, R., Finardi, S., Lollobrigida, F., Tinarelli, G., 2006. Air quality integrated modelling in Turin urban area. *Environmental Modelling & Software* 21, 468–476.

Carnevale, C., Finzi, G., Pisoni, E., Volta, M., Guariso, G., Gianfreda, R., Maffeis, G., Thunis, P., White, L., Triacchini, G., 2012. An integrated assessment tool to define effective air quality policies at regional scale. *Environmental Modelling & Software* 38, 306–315.

Chang, J.C., Hanna, S.R., 2004. Air quality model performance evaluation. *Meteorology and Atmospheric Physics*, 87, 167–196.,

Dernwent, D., Fraser, A., Abott, J., Jenkin, M., Willis, P., Murrells, T., 2010. Evaluating the Performance of Air Quality Models, No 3, June 2010. (*http://naei.defra.gov.uk/reports? report_id=616*).

Dresser, A.L., Huizer, R.D., 2011. CALPUFF and AERMOD model validation study in the near field: Martins Creek revisited. *Journal of the Air & Waste Management Association*, 61, 641 -657.

Elbir, T., 2003. Comparison of model predictions with the data of an urban air quality monitoring network in Izmir, Turkey. *Atmospheric Environment* 37, 2149–2157.

Escoffier, Ch., 2013. CALPUFF model overview and some applications. DMUG meeting, St martin in the fields, London, 9 Dec. 2013. (iaqm.co.uk/download/CEscoffier_DMUG2013.pdf)

ETC/ACM, 2011. Technical Paper 2011/9 (L. Malherbe, A. Ung, A. Colette, E. Derby). Formulation and quantification of uncertainties in air quality mapping.

ETC/ACM, 2013. Technical Paper 2013/11 (R. Rouil, B. Bessagnet, eds). How to start with PM modelling for air quality assessment and planning relevant to AQD.

Fox, T.J., 2012. CALPUFF Status and Update. 2012 R/S/L Modelers Workshop. April 30, 2012. (http://www.cleanairinfo.com/regionalstatelocalmodelingworkshop/archive/2012/presentations/2-5_CALPUFFstatus_TFox.pdf).

Holmes, N.S., Morawska, L., 2006. A Review of Dispersion Modelling and its application to the dispersion of particles: An overview of different dispersion models available. *Atmospheric Environment* 40, 5902–5928.

Holnicki, P., Kałuszko, A., 2014. *Supporting management of air quality in an urban area.* Systems Research Institute, Research Report RB/5/2014, Warsaw.(http://www.ibspan.waw.pl/~kaluszko/Raport_RB_5_2014.pdf).

Holnicki, P., Nahorski Z., 2015. Emission Data Uncertainty in Urban Air Quality Modeling – Case Study. *Environmental Modeling and Assessment,* DOI 10.1007/s10666-015-9445-7.

Juda-Rezler, K., 2010. New Challenges in Air Quality and Climate Modeling. *Archives of Environmental Protection* 36, 3–28.

Kiesewetter, G., Borken-Kleefeld, J., Schöpp, W., Heyes, C., Thunis, P., Bessagnet, B., Terrenoire, E., Fagerli, H., Nyiri, A., Amann, M., 2014. Modelling street level PM_{10} concentrations across Europe: source apportionment and possible futures. *Atmospheric Chemistry and Physics. Discussions* 14, 18315–18354.

Lim, L.L., Hughes, S.J., Hellawell, E.E., 2005. Integrated decision support system for urban air quality assessment. *Environmental Modelling & Software* 20, 947–954.

ME, 2012. Ministry of the Environment. Decree 1031, 24 Aug. 2012, On the admissible levels of some substances in the air (Polish).

Mediavilla-Sahagún, A., ApSimon, H.M., 2006. Urban scale integrated assessment for London: Which emission reduction strategies are more effective in attaining prescribed PM10 air quality standards by 2005? *Environmental Modelling & Software,* 21, 501–513.

NCAR, 2008. A description of the advanced research WRF Version 3. NCAR Technical Note, TN–475+STR. Boulder, Colorado, USA June 2008.

Oshan, R., Kumar, A. & Anand,M., 2006. Application of the USEPA's CALPUFF model to an urban area. *Environmental Progress & Sustainable Energy*, 25, 12–17.

Pisoni, E., Carnevale, C., Volta, M., 2010. Sensitivity to spatial resolution of modeling systems designing air quality control policies. *Environmental Modelling & Software* 25, 66–73.

Rood, A.S., 2014. Performance evaluation of AERMOD, CALPUFF, and legacy air dispersion models using the WINTER Validation Tracer Study dataset. *Atmospheric Environment*, 89, 707–720.

Stedman, J.R., Kent, J.A., Griece, S., Bush, T.J., Dernwent, R.G. 2007. A consistent method for modelling PM_{10} and $PM_{2.5}$ concentrations across the United Kingdom in 2004 for air quality assessment. *Atmospheric Environment* 41, 161–172.

Scire, J.S., Strimaitis, D.G., Yamartino, R.J., 2000. A User's Guide for the CALPUFF Dispersion Model. Earth Technology Inc.

Tartakovsky, D., Broday, D. M., Stern, E., 2013. Evaluation of AERMOD and CALPUFF for predicting ambient concentrations of total suspended particulate matter (TSP) emissions from a quarry in complex terrain. *Environmental Pollution* 179, 138–145.

Trapp, W., 2010. The application of CALMET/CALPUFF models in air quality assessment system in Poland. *Archives of Environmental Protection* 36, 63–79.

WIOŚ, 2012. Environment Quality in Mazovian Voivodship in the year 2012. Voivodship Inspectorate of Environment Protection (WIOŚ). Report for the year 2012 (in Polish).

SUPPORTING MATERIAL

Content

Text S1. Emission inventory

The aggregated emissions from the basic sectors in Warsaw agglomeration in the year 2012 are presented in Table S1 (WIOŚ, 2012). The main activities influencing Warsaw air quality which were taken into account, are: energy production and industry (point sources), residential heating (area sources), road transport (line sources). The table shows the emission volumes of the main pollutants and the share of each sector in the total emission.

The nominal emission data of area and line sources are distributed over 0.5 km x 0.5 km grid elements. The emission of each energy or industrial installation is assigned to the respective point emission source, according to its location coordinates and technological parameters. The daily variability of traffic intensity is reflected by the emission intensity of line sources. Similarly, the seasonal variability of emissions from the energy sector and residential heating correspond to the seasonal changes in fuel combustion. The emission data are finally entered as a sequence of 1-h episodes (8785 time steps) which cover the simulation year.

Table S1. Emission volumes by sector in Warsaw agglomeration

Sector	SO_2		NOx		PM_{10}		$PM_{2.5}$		CO		C_6H_6	
	[Mg]	[%]	[Mg]	[%]	[Mg]	[%]	[Mg]	[%]	[Mg]	[%]	[Mg]	[%]
Energy/industry	12478	87,6	7781	40,0	803	10,5	264	8,8	2504	7,5	-	-
Residential	931	6,5	614	3,2	2105	27,4	1603	53,3	8830	26,5	0,075	0,0
Transport	837	5,9	11051	56,8	4772	62,1	1141	37,9	21955	66,0	317,4	100,0
Total	14246	100	19446	100	7680	100	3008	100	33289	100	317,5	100

Table S2. The share of the primary and re-suspended fractions in the transport emission

Emission	PM_{10}		$PM_{2.5}$	
	[Mg]	[%]	[Mg]	[%]
Primary	862	18,1	575	50,4
Re-suspended	3910	81,9	566	49,6
Total	4772	100	1141	100

Text S2. Meteorological data

The real data sequence for 2012 (wind rose shown in Fig. S1) are re-analyzed by the meso-scale numerical WRF model (NCAR 2008). The data utilized encompass main meteorological fields, such as wind, pressure, temperature, humidity, cloudiness, precipitation intensity. These fields are then transferred by the CALMET preprocessor to a meteorological dataset accepted by CALPUFF. The additional parameters required by the main model, such as inversion height and atmospheric stability class, are also generated. Terrain orography and land coverage are utilized to assess the aerodynamic roughness parameter and generate the final wind field which is interpolated to the 0.5 km x 0.5 km grid used by the forecasting model. The data (similarly as for the emissions) are finally prepared as a sequence of 1-h episodes (8785 time steps) which cover the year.

Average meteorological conditions, based on WRF model simulation (WIOŚ 2012), for the Warsaw area are shown in Tables S3, S4 and Figure S1.

Table S3. Temperature and precipitation in Warsaw in the year 2012 (WIOŚ 2012)

No	Month	Mean temperature [$^{\circ}$C]	Mean precipitation [mm]
1	January	-0,8	58,8
2	February	-6,3	36,6
3	March	5,6	21,2
4	April	10,4	66,2
5	May	16,0	33,3
6	June	18,3	73,8
7	July	22,9	45,2
8	August	20,1	35,8
9	September	16,1	20,1
10	October	9,7	51,6
11	November	6,3	33,6
12	December	-1,9	33,1

Table S4. Atmospheric stability conditions in the year 2012 (WIOŚ 2012)

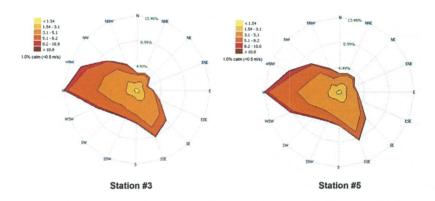| No	Stability class	Frequency [%]
1	A – very unstable	0,1
2	B – unstable	8,8
3	C – slightly unstable	15,5
4	D – neutral	42,0
5	E – slightly stable	21,3
6	F – stable	12,3

Fig. S1. Wind rose for two monitoring stations in the year 2012 (WIOŚ 2012)

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Table S5. Assessment of the modeling performance due to (CAFÉ 2008) regulations

Receptor	SO_2 Cm/Co [%]	NO_X Cm/Co [%]	PM_{10} Cm/Co [%]	$PM_{2.5}$ Cm/Co [%]	C_6H_6 Cm/Co [%]
#1		-56,7	30,8	4	35,3
#2	38,3	12,2			
#3	-2,9	6,3	32,4	-4,3	16,7
#4		20			
#5	0	-47,5	-19	-23,1	