21st International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
27-30 September 2022, Aveiro, Portugal

ASSESSMENT OF THE IMPACT OF THE RESIDENTIAL HEATING EMISSIONS ON CONCENTRATIONS BY LOCAL AND REGIONAL AIR-QUALITY MODELS

Dušan Štefánik[1], Jana Krajčovičová[1], Juraj Beňo[1] and Katarína Belohorcová[2]

[1] Slovak Hydrometeorological Institute, Jeséniova 17, 833 15, Bratislava, Slovakia
[2] Ministry of Environment of the Slovak Republic, Námestie Ľ. Štúra 1, 812 35 Bratislava, Slovakia

Abstract: Comparison of three models differing in resolution and mathematical formulation - CALPUFF Lagrangian puff model, CMAQ Eulerian chemical transport model and IFDM Gaussian dispersion model - is presented. Modelling results for $PM_{2.5}$ concentrations coming from residential heating emissions over a selected local domain in Slovakia are compared and the differences as well as the usability of the models for local source apportionment is discussed.

Key words: *residential heating, $PM_{2.5}$, chemical-transport model, Lagrangian puff model, Gaussian dispersion model*

INTRODUCTION

Residential heating is the main contributor to the adverse air quality during winter periods in many regions in Central and Eastern Europe. In Slovakia, there are many villages and small towns without connections to central heating systems or natural gas distribution. Therefore, the local heating using solid fuel (mainly wood) is mostly used there. Moreover, the increasing energy prices also contribute to households leaning towards cheaper solid fuel. The consequence of this development is that the annual concentration limits for benzo(a)pyrene and $PM_{2.5}$, and the number of daily PM_{10} exceedances continue to occur at many air quality monitoring stations situated near residential areas. Since the number of air quality monitoring sites is rather limited, there is a need for reliable modelling outputs not only to assess the concentrations at locations without monitoring stations, but also to carry on the source apportionment at monitoring sites. In this paper, we attempt to compare the modelling results for $PM_{2.5}$ concentrations of several models differing in resolution and mathematical formulation: CALPUFF Lagrangian puff model, CMAQ Eulerian chemical transport model and IFDM Gaussian dispersion model. The local modelling domain includes the town of Jelšava, which according to the measurements is one of the locations with the worst air-quality due to PM in Slovakia, as well as the whole mountain valley NW of Jelšava with the town of Revúca and several smaller villages with solid fuel heating. The simulations are only performed for the residential heating emissions. The results are demonstrated using $PM_{2.5}$ as it represents almost all of PM_{10} emissions from residential heating.

SIMULATION DOMAIN AND EMISSIONS

Simulations were performed for the whole month of January 2021 for the domain of Jelšava, which is a mountain valley with adverse dispersion conditions especially in winter time. The size of the domain is roughly 13 km x 10 km.

The emissions from residential heating were computed using emission model REM_v2 (Krajcovicova et. al, 2020). PM emission totals in January 2021 for the whole domain are as follows: PM_{10} = 13.1 t and $PM_{2.5}$=12.8 t. 47 % of $PM_{2.5}$ emissions represents organic carbon and 10% black carbon. Figure 1 shows the simulation domain with residential heating emissions resolution of 50 m for CALPUFF and IFDM and 2 km for CMAQ. The diurnal and monthly emission profiles used in CMAQ and CALPUFF simulations are displayed in Fig. 2. The diurnal profile is adopted from CAMS methodology (Guevara et al., 2021) and the monthly profile is based on mean daily temperatures measured at meteorological station in Revúca. The emission rate at each hour is calculated as annual emission total multiplied by diurnal and monthly profile values from Fig. 2 divided by 8760. Constant emission profile was used for IFDM simulation.

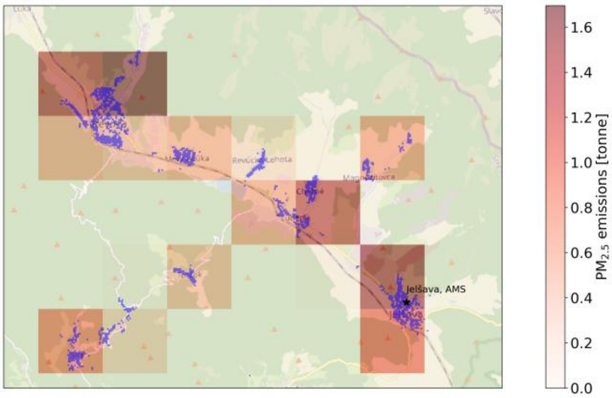

Figure 1. Red squares: $PM_{2.5}$ emissions for January in CMAQ model. Blue raster: distribution of $PM_{2.5}$ emissions to the IFDM and CALPUFF models (the emission flux is not shown).

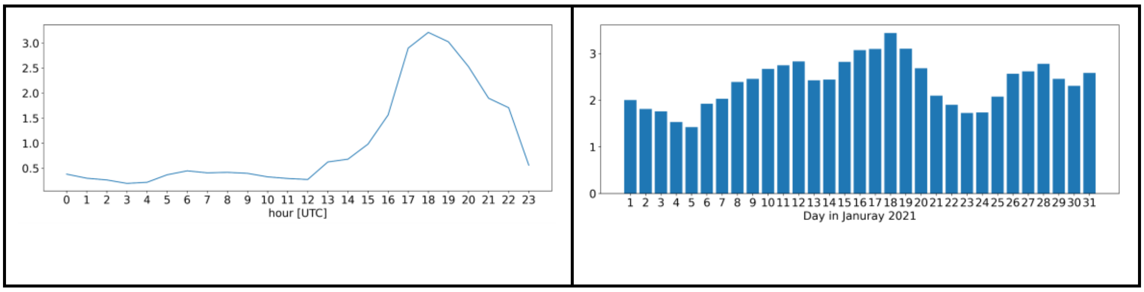

Figure 2. Emissions profiles for residential heating: diurnal (left) and monthly (right) used in CALPUFF and CMAQ calculations.

MODELS

ALADIN forecasting model (Termonia et. al., 2018, Derkova et. al., 2017) meteorological data output with the resolution of 4.5 km was used as input to IFDM and CALPUFF. For the CMAQ model a complex set of meteorological 2D and 3D parameters from model Aladin with 2 km resolution were used.

CALPUFF

CALPUFF (Scire et al, 2000a) version 7.2.1 was used to model concentrations of $PM_{2.5}$. CALPUFF is a Lagrangian puff model which is capable of treating complex terrain, low wind and calm situations which frequently occur in the mountain valleys. CALMET (Scire et al, 2000b) version 6.5.0 meteorological fields was used to process ALADIN meteorological inputs to high resolution grid. CALMET is a diagnostic meteorological model for computation of high resolution terrain-following winds and micrometeorological parameters necessary as inputs for CALPUFF model. The emissions were represented as volume sources corresponding to the emission squares of 50m.

CMAQ

The Community Multiscale Air Quality (CMAQ) model is a third-generation Eulerian mathematical air quality model (Byun and Schere, 2006). It can be used on various spatial scales from local to hemispheric and for corresponding time scales. It simulates ozone, particulate matter (PM), toxic airborne pollutants, visibility, and acidic and nutrient pollutant species throughout the troposphere. In the simulation, the

CMAQ meteorological inputs are taken from the model Aladin, corresponding to the model resolution of 2 km. Boundary conditions are zero except for the ozone. The CMAQ model version 5.3.3 was used (US EPA, 2021). The residential heating emissions are represented as area sources with 2 km resolution.

IFDM

IFDM (Immission Frequency Distribution Model) is a bi-Gaussian dispersion model developed by VITO to calculate the local dispersion of pollutants in the atmosphere based on meteorological data such as wind speed, wind direction and temperature (Lefebvre et al., 2011a, 2011b). It does not explicitly include the influence of the terrain and is unable to capture calm wind periods. However, as the meteorology for a particular source is always taken from the nearest Aladin gridpoint, a terrain influence is indirectly included through the wind speed and direction from the meteorological model. Emissions gridded in the 50 m squares were represented as point sources at the centres of grid cells. Results were interpolated into the regular grid with 10 m resolution.

Model	**CALPUFF**	**IFDM**	**CMAQ**
Type	Lagrangian puff	Gaussian	Eulerian CTM
Horizontal (terrain) resolution	250 m	no terrain included	2 km
Model output resolution	250 m	10 m	2 km
Number of vertical layers	11	NA	19
Top layer height	3 000 m	NA	17 000 m

Table 1. Selected parameters of the models.

RESULTS

Mean monthly concentrations in January

Mean $PM_{2.5}$ concentrations for the whole simulation period resulting from CALPUFF and IFDM models are shown in Fig. 3. These local models provide outputs at high resolution. On the other hand, CMAQ, being a CTM model, requires a lot of computer resources and therefore its typical resolutions are several km. Fig. 4 shows mean $PM_{2.5}$ concentrations computed by CMAQ, together with the downgraded results from CALPUFF and IFDM models. We can see that the CMAQ concentrations are rather low in comparison with other models even if those are downgraded to the 2 km resolution corresponding to CMAQ, while CALPUFF model gives the highest concentrations of all. Domain-wide statistics are as follows: CALPUFF vs. CMAQ: BIAS = 8.2 , RMSE = 9.0, r =0.77; IFDM vs. CMAQ: BIAS = 0.27, RMSE = 1.0, r =0.90; IFDM vs. CALPUFF: BIAS = -7.7 , RMSE = 8.3, r =0.80. The statistics show the closest similarity between the IFDM and CMAQ model results. Comparing these two models, CMAQ gives lower concentrations for all grid cells but those with small emissions and bad dispersion conditions caused by the terrain.

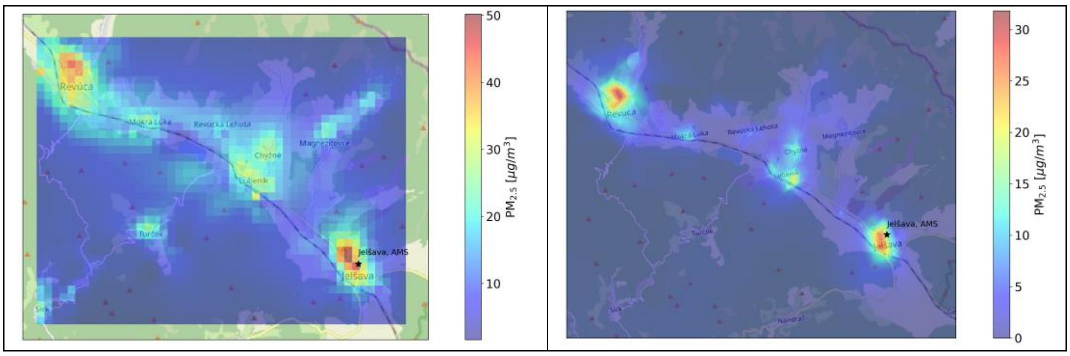

Figure 3. Mean $PM_{2.5}$ concentrations from residential heating in January 2021 calculated by a) CALPUFF model (left panel); b) IFDM model (right panel)

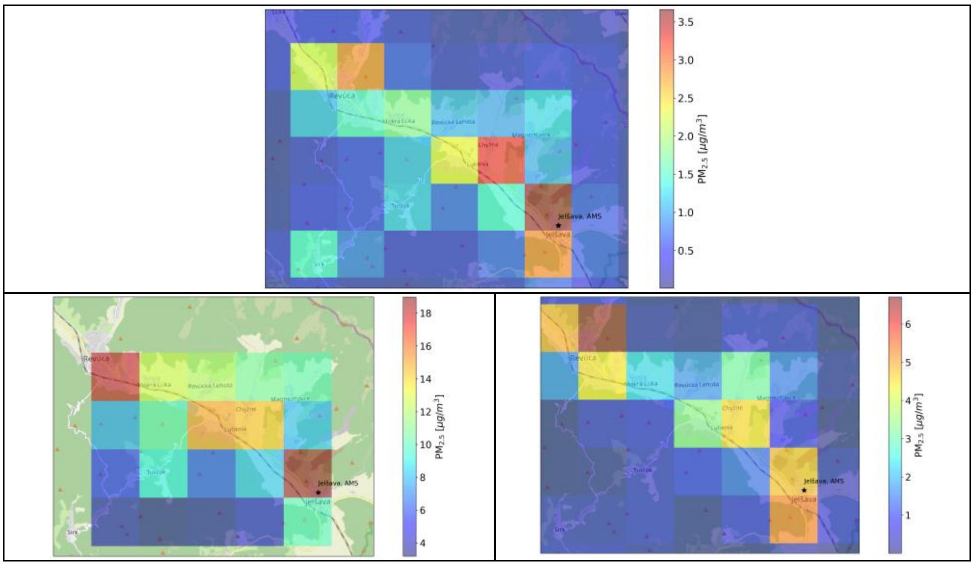

Figure 4. Mean $PM_{2.5}$ concentrations from residential heating in January calculated by CMAQ model (top).$PM_{2.5}$ concentrations resampled to the CMAQ resolution: a) CALPUFF model (bottom left); b) IFDM model (bottom right)

Concentrations at the monitoring station

The predicted hourly $PM_{2.5}$ concentrations at the monitoring station location in Jelšava, together with the measured values are presented in Fig. 5. CMAQ model underestimates the concentrations since the 2 km resolution is not capable of seeing this hot-spot. On the other hand, CALPUFF and to a certain degree IFDM give values for some hours which highly exceed measured concentrations. Therefore, in case of CALPUFF simulations we experimented with different diurnal profiles. It turned out that the unrealistic high peaks decreased when constant diurnal profile was used (Fig. 6) and monthly mean domain maximum also decreased by ~15%. .

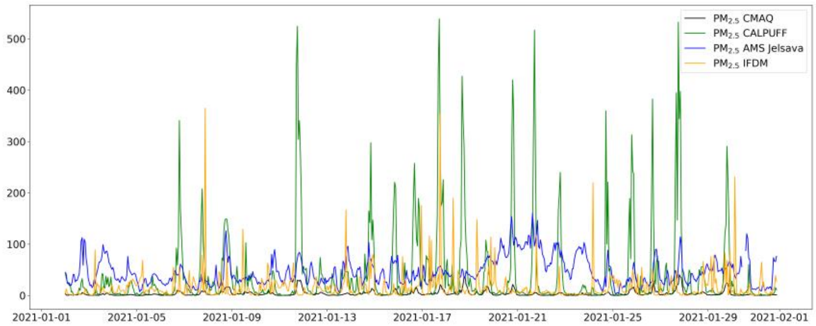

Figure 5. Hourly $PM_{2.5}$ concentrations at Jelšava monitoring station – models and measurements.

CONCLUSIONS

The simulations demonstrated the expected result that the resolution of the model is crucial to obtain realistic concentration values in hot-spots, especially in complex mountainous locations. Besides this, we learned that the diurnal emission profile is also very important, especially in case of CALPUFF model using high resolution terrain-adjusted meterology. After downgrading two local models to the 2 km resolution, seemingly comparable concentrations were obtained using CMAQ and IFDM models, while CALPUFF seemed to overestimate especially when CAMS emission profile was used. This can not be interpreted in the way that IFDM and CMAQ results are better than CALPUFF, as their higher correlation may be accidental (they use completely different diurnal emission profiles - completely constant versus CAMS profile with high amplitude). Further simulations and more insight into the differences in the meteorological fields in relation to the modeling results is necessary, as well as to the impact of the diurnal emission profiles, especially in case of IFDM and CALPUFF models As it seems that local models are sensitive to diurnal emission profiles, it is also necessary to develop emission profiles for residential heating which would be as close to reality as possible.

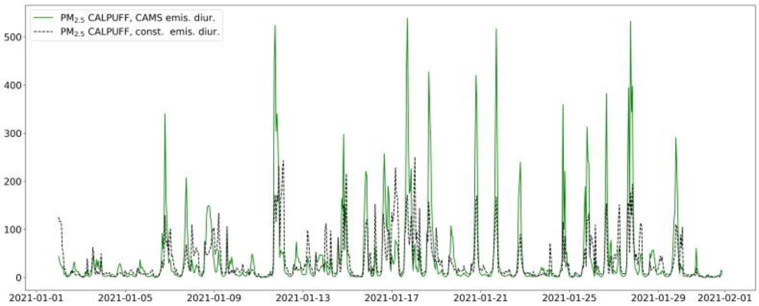

Figure 6. Calpuff hourly $PM_{2.5}$ concentrations with constant and CAMS diurnal emission profiles at Jelšava monitoring station.

REFERENCES

Derková et. al., 2017: Recent improvements in the ALADIN/SHMU operational system. *Meteorological Journal*, Vol.**20**, No. 2, pp 45-52.

Byun, D., Schere, K., 2006. Review of the governing equations, computational algorithms, and other components of the Model-3 Community Multiscale Air Quality (CMAQ) *Modeling System. Appl. Mech. Rev.* **59** (2), 51–77. https://doi.org/10.1115/1.2128636.

Guevara, Marc Jorba, Oriol Tena Medina, Carles Denier van der Gon, Hugo Kuenen, Jeroen Elguindi, Nellie Darras, Sabine Granier, Claire Pérez García-Pando, Carlos. (2021). Copernicus Atmosphere Monitoring Service TEMPOral profiles (CAMS-TEMPO): global and European emission temporal profile maps for atmospheric chemistry modelling. *Earth System Science Data*. **13**. 367-404. 10.5194/essd-13-367-2021

Lefebvre, W., Fierens, F., Trimpeneers, E., Janssen, S., Van de Vel, K., Deutsch, F., Viaene, P., Vankerkom, J., Dumont, G., Vanpoucke, C., Mensink, C., Peelaerts, W., Vliegen, J., 2011a. Modeling the effects of a speed limit reduction on traffic-related elemental carbon (EC) concentrations and population exposure to EC. Atmospheric Environment 45, 197e207. http://dx.doi.org/10.1016/j.atmosenv.2010.09.026.

Lefebvre, W., Vercauteren, J., Schrooten, L., Janssen, S., Degraeuwe, B., Maenhaut, W., de Vlieger, I., Vankerkom, J., Cosemans, G., Mensink, C., Veldeman, N., Deutsch, F., Van Looy, S., Peelaerts, W., Lefebre, F., 2011b. Validation of the MIMOSA-AURORA-IFDM model chain for policy support: modeling concentrations of elemental carbon in Flanders. Atmospheric Environment 45/37, 6705e6713. http://dx.doi.org/10.1016/j.atmosenv.2011.08.033.

Scire J.S., Robe F.R., Fernau M.E., Yamartino R.J., 2000b: A User's Guide for the CALMET Meteorological Model, Earth Tech, Inc., Concord, MA

Scire, J.S., Strimaitis, D.G. and Yamartino, R.J., 2000a: A User's Guide for the CALPUFF Dispersion Model, Earth Tech, Inc., Concord, MA.

United States Environmental Protection Agency. (2020). CMAQ (Version 5.3.2) [Software]. Available from https://doi.org/10.5281/zenodo.4081737

Termonia et.al., 2018: The ALADIN System and its Canonical Model Configurations AROME CY41T1 and ALARO CY40T1. *Geosci. Model Dev*., Vol. **11**, pp 257-281.