Validation of CMAQ chemical-transport model and its meteorological inputs

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Abstrakt

Modelovanie znečistenia ovzdušia v sebe spája atmosferické a chemické modelovanie, za účelom predpovedí koncentrácií znečisťujúcich látok v ovzduší. Aktívne sa využíva ako podpora monitoringu súčasného stavu ovzdušia a taktiež predstavuje jediný nástroj, vďaka ktorému vieme ohodnotiť dopady navrhovaných opatrení pre znižovanie emisií na kvalitu ovzdušia v budúcnosti.

Projekt LIFE IP Malopolska in a Healthy Artmosphere sa zaoberá opatreniami pre znižovanie emisií domácností kúriacich pevným palivom v juhopoľskom regióne. Predpokladá sa, že tieto patrenia budú mať dopad aj na kvalitu ovzdušia v severných regiónoch Slovenska. SHMÚ sa podieľa na tomto projekte implementáciou chemicko-transportného modelu CMAQ za účelom ohodnotenia vplyvu týchto opatrení na kvalitu ovzdušia.

Dôverihodnosť predpovedí modelu vieme určiť na základe procesu validácie, ktorý je založený na porovnávaní modelových predpovedí s nameranými dátami na základe rôznych štatistických metód. Keďže meteorologické javy výrazne ovplyvňujú rozptyl a prenos znečisťujúcich látok v atmosfére, pre spoľahlivé výsledky predpovedí znečistenia ovzdušia sú potrebné aj kvalitné meteorologické predpovede.

V tejto práci bol validovaný meteorologický model WRF pre potreby modelovania znečistenia ovzdušia modelom CMAQ, ktorý používa výstupné dáta z WRF ako meteorologické vstupy. Modelové predpovede boli porovnávané s nameranými dátami z meteorologických staníc Slovenska.

Model CMAQ bol validovaný pre predpovede koncentrácií NO_2, SO_2, O_3 a prachových častíc (PM_{10} a $PM_{2.5}$) v ovzduší. Emisné vstupy do modelu CMAQ boli sprostredkované emisným modelom FUME. Modelové dáta boli porovnávané so sieťou monitorovacích staníc znečistenia ovzdušia v strednej Európe. Na záver sme sa pokúsili určiť veľkosť vplyvu meteorologických predpovedí modelu WRF na predpovede modelom CMAQ.

Anotácia

Meteorologický model WRF bol validovaný pre potreby modelovania znečistenia ovzdušia v modeli CMAQ, ktorý používa výstupné dáta z WRF ako meteorologické vstupy. Chemicko-transportný model CMAQ bol validovaný pre predpovede koncentrácií NO_2, SO_2, O_3 a prachových častíc (PM_{10} a $PM_{2.5}$) v ovzduší. Naším cieľom bolo tiež určíť veľkosť vplyvu WRF na predpovede v modeli CMAQ.

Kľúčové slová: model WRF, model CMAQ, modelovanie znečistenia ovzdušia, validácia.

Anotation

WRF meteorological model was validated for the purpose of air quality modelling in CMAQ model, which uses the WRF outputs as meteorological drivers. Chemical-transport model CMAQ was validated for predictions of NO_2, SO_2, O_3 and particulate matter (PM_{10} and $PM_{2.5}$) concentrations in the air. Our intention was also to

determine magnitude of an impact WRF has on CMAQ predictions.

Keywords: WRF model, CMAQ model, air quality modelling, validation.

Introduction

Air quality modelling is used for the assessment of current status of the air quality and the evaluation of impacts of proposed emission reduction measures on the future air quality. The air pollutants of major concern in Europe are particulate matter (namely, PM_{10} and $PM_{2.5}$), benzo(a)pyrene (BaP) and NO_2. As for PM and BaP, the border regions of Czech republic, Slovakia and southern Poland are considered as one of the hotspots in Europe.

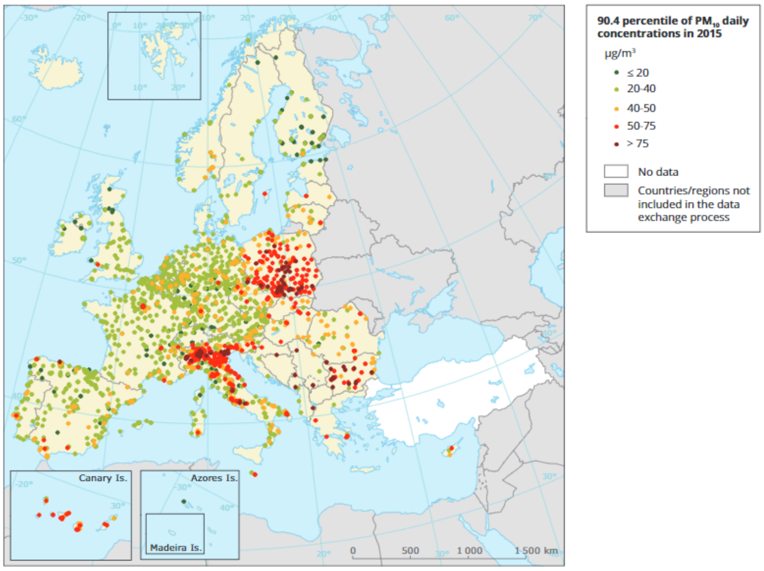


Figure 1: Concentrations of PM_{10} 2015 - daily limit value [1]

LIFE IP Project Malopolska in a Healthy Atmosphere [2] which is currently being implemented, is focused on the measures for decreasing the emissions from residential combustion of solid fuels. SHMI[1] participates in this project by implementing CMAQ regional air quality model, driven by WRF meteorological forecasting model, in order to estimate the impact of these measures on the air pollution.

The transport and diffusion of pollutants in the atmosphere is significantly influenced by the meteorological phenomena, thus it is necessary to provide the air quality models with good quality meteorological inputs. For that reason, the meteorological model that provides the meteorological inputs for the air quality model should be well evaluated. Evaluation is a sum of processes that assess individual aspects of the model performance. Validation is a component of evaluation which analyses whether the model predictions correspond sufficiently with the observations [3].

We validated WRF for surface level temperature, pressure, wind speed and wind direction and we tried to determine the factors that may have caused the differences between the model results and observations. We then use these findings in attempt to explain the variations in CMAQ validation results.

• **The Weather Research and Forecasting (WRF) Model** is a next-generation mesoscale (local to continental) numerical weather prediction system designed for both atmospheric research and operational forecasting

[1] Slovak Hydrometeorological Institute

applications. It is is a fully compressible and nonhydrostatic eulerian model [4].

• **The Community Multiscale Air Quality (CMAQ)** is a third-generation Eulerian mathematical air quality model, which is capable of handling multiple pollutants simultaneously [5]. 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 [5].

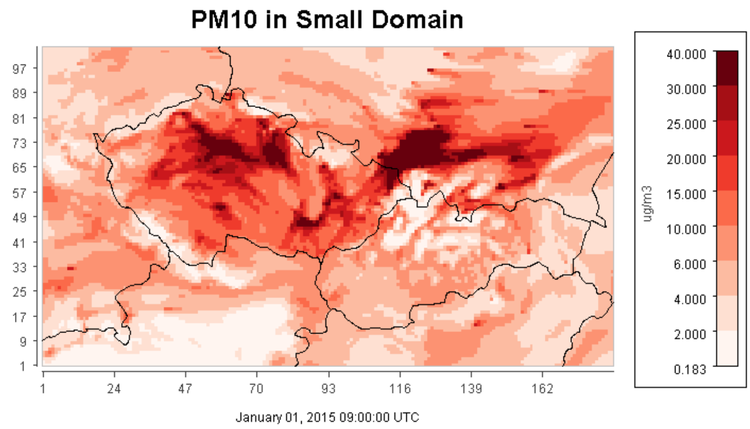


Figure 2: An example of CMAQ model PM_{10} prediction visualized in Verdi software

Validation

Model validation is a structured comparison of model predictions with experimental data and it is based on statistical analyses of selected variables [3]. There is a wide range of validation statistics that can be used to assess air quality model performance. However, no single statistic encapsulates all aspects of interest. For this reason, it is useful to consider several performance statistics [6].

For validation of WRF model we used some of the quality indicators for model evaluation as proposed in [7]: Mean Bias (MB), Mean Gross Error (MGE), Coefficient of Correlation (r), Index of Agreement (IOA) and Root Mean Square Error (RMSE). For validation of CMAQ we added two more indicators: Coefficient of efficiency COE and Fraction of predictions within a factor or two (FAC2) A description of these statistics with the corresponding formulae can be found in [6]. Ideal values for BIAS, MGE and RMSE are zero, for r, IOA, COE and FAC2 it is one.

For the model to be considered sufficient, it needs to fulfill certain benchmarks - its quality indicators should satisfy given limits. In our validation we utilized 9 benchmarks as stated in [7].

Simulations

Grid specification

WRF and CMAQ simulations were computed for the year 2015 in two domains. The small domain with 103x184 grid boxs of 4.7 km resolution was nested inside of the large domain with 133x169 grid boxs of 14.1 km resolution. Simulations were computed on SHMI's supercomputer using 64 cores.

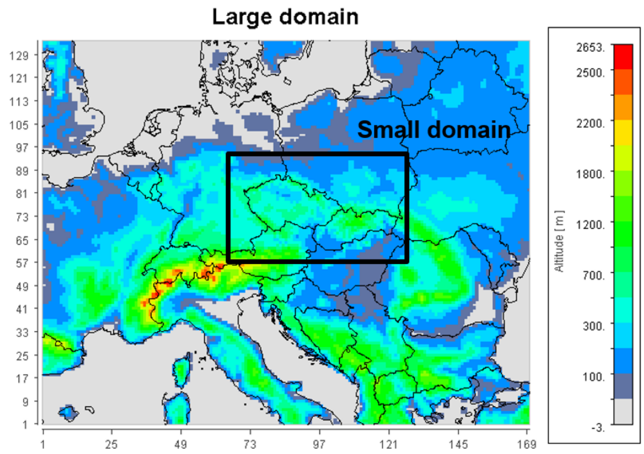


Figure 3: Large domain with nested small domain.

WRF simulations

The first WRF simulation was computed on the large domain using the ECMWF[2] reanalysis data as the boundary and initial conditions. The results of the large domain simulation became the boundary conditions for the small domain simulation. Simulations resulted in hourly data of 3D meteorological fields.

We validated WRF model predictions of pressure and temperature at standard 2 m height and wind speed and wind direction at standard 10 m height. With the validation, we intend to determine whether the current WRF model setup is suitable for use in air quality assessment. We compared model predictions with monitored data from 25 meteorological stations in Slovakia. Each station with its latitude (Lat) and longitude (Lon) is assigned to one grid box of a domain. Each grid box has its latitude and longitude given by center of the box. Thus, the final coordinates of each station in the grid are differing from the real ones, since the spatial resolution of the grid is limited. Every grid box has a given mean altitude of the whole covered area assigned to it so it may also differ from the real station altitude.

Since the model predicts the quantities at different altitudes than the real stations altitudes, we corrected the pressure and temperature predicted values to the real stations altitudes using the barometric formula and dry adiabatic temperature gradient.

CMAQ simulations

WRF model is used as a meteorological driver for CMAQ. Apart from meteorology inputs, air quality models also require information about emission sources. Those are acquired by emission models. For out simulations we used emission model FUME, which is currently being used for the air quality modelling in the Czech Hydrometeorological Institute and in several other projects [9].

The model results were compared to the observed concentrations from the air quality monitoring stations that lie within the domain area. We analyzed 5 pollutants: ozone (O_3), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), particulate matter with diameter smaller than 10 μm (PM_{10}) and particulate matter smaller than 2.5 μm ($PM_{2.5}$). For each pollutant there was a different number of available monitoring stations.

For validation we only used rural and suburban background stations - the model computes the mean concentrations for the whole grid box area, so background stations are more representative for the area then the stations in vicinity of emission sources.

[2]European Centre for Medium-Range Weather Forecast

Validation results

WRF validation results

We will only discus the results of the small domain, since the large one only served as the nesting domain an its results were overall worse. We present the statistics for the stations in Slovakia as simulated in the small domain in Table 1.

Table 1: Statistics for small domain

	Coverage	**BIAS**	**MGE**	**RMSE**	**r**	**IOA**
Pressure	99.35%	6.54	14.91	30.05	0.93	0.85
Pressure correction	99.35%	-0.23	1.24	1.91	0.99	0.99
Temperature	98.73%	0.56	2.33	3.06	0.95	0.85
Temperature correction	98.73%	-0.11	2.32	3.08	0.95	0.85
Wind speed	98.45%	0.70	1.98	2.70	0.54	0.53
Wind direction	71.84 %	9.57	50.68	69.19	0.35	

The pressure and temperature correction in Table 1 stands for the pressure and temperature model values in the real station altitude computed with barometric formula and dry adiabatic temperature gradient. The reason why we also present the pressure as computed by the model is that CMAQ uses the meteorological data in the original grid box altitude.

BIAS, MGE and RMSE values are in units corresponding to respective quantities - pressure in hPa, temperature in K or °C, wind speed in $m{\cdot}s^{-1}$ and wind direction in degrees. r and IOA are dimensionless. Coverage stands for the percentage of successful observations.

As we can see from Table 1, pressure correction significantly improved all model statistics. Temperature corrections did not change the overall statistics much. From these results, only the pressure correction meets the corresponding benchmark as stated in [7] (MGE$(pressure) < 1.7$ hPa).

Looking at the single stations results, the ones with the model altitude close to the real station altitude show better results than the averaged statistics from Table 1.

We achieved one of the best results for Košice airport station, where the real altitude and model altitude differ by only 0.636 m. This station satisfied temperature, wind speed and pressure benchmarks even without the corrections - since the altitude difference is so small, the correction did not change the results much. This station did not satisfy only one of the wind direction benchmarks (MGE$(wind\ dir.) < 30°$).

One of the worst results was obtained for Chopok station, which is situated on a top of a mountain in a very mountainous area, with an altitude of 2005 m. The model altitude is 654.07 m lower that the real station altitude. Only two benchmarks were satisfied for this station: the pressure benchmark for corrected values and one of the wind direction benchmarks (BIAS$(wind\ dir.) < \pm 10°$). The pressure correction immensely improved the results, as can be seen in Figure 4. However, the temperature correction was not sufficient in this case (Figure 5).

Wind direction MGE for this station was better than in most other stations and we expect this to be the consequence of the stations position - since it sits higher than its surroundings, the effect of surrounding orography on the wind direction is reduced. Therefore, the local air flow is more similar to the wind at higher altitudes, which is not as influenced by the surface and is more stable in wind speed and wind direction than the near surface wind.

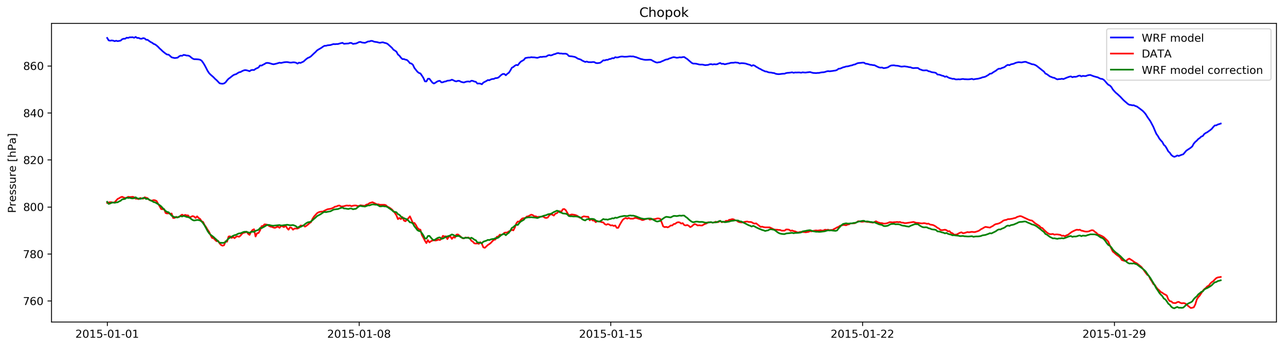


Figure 4: Pressure correction 2 at Chopok station, January 2015. The red line represents the observed data, blue line is the WRF model prediction and green line is the WRF model pressure correction 2. We can see that the correction matches the observations almost perfectly.

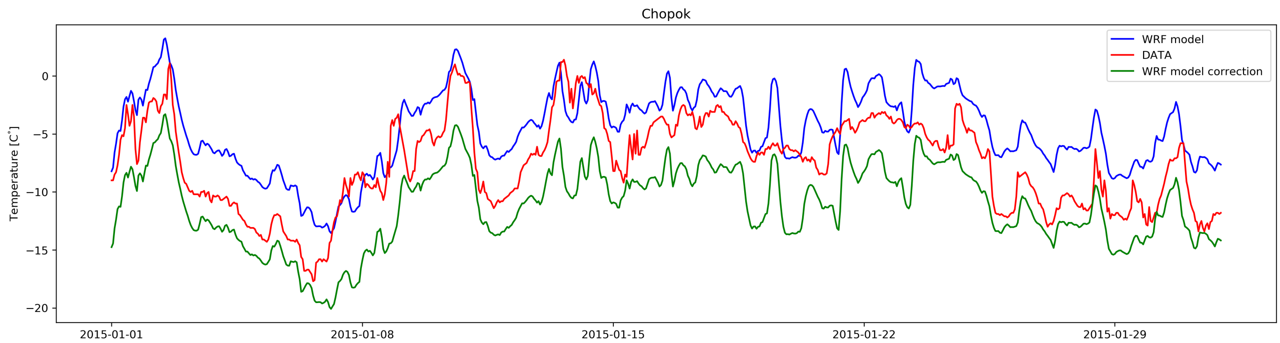


Figure 5: Temperature correction at Chopok station, January 2015. The red line represents the observed data, blue line is the WRF model prediction and green line is the WRF model temperature correction. We can see that the correction (the dry adiabatic gradient) was too large in this case.

Pressure correction significantly improved the results in all stations, we can therefore conclude, that the largest insufficiency of the model is due to limited spatial resolution of the domain, that causes large altitude differences between the model altitude and real station altitude. However, for the air quality modelling in CMAQ, only the uncorrected values can be used.

Out of 9 quality indicators that we used for validation, the wind direction MGE of 30° was not satisfied in any of the stations. The other indicators were achived with various rates, the most successful one was the temperature IOA benchmark (IOA$(temp.) \geq 0.8$) achieved at 22 out of 25 stations.

CMAQ validation results

The results of surface predictions for the small domain, using the FUME emission model are presented in Table 2. We analyzed the results of the simulation of the first 6 months of 2015. The model results were compared with the data from the stations of all countries within the small domain (Slovakia, Czech republic, Poland, Austria, Hungary and Germany) except of Ukraine, which does not provide the air quality data from the monitoring stations. Details about the stations with their observed values for each pollutant were acquired from [10].

Table 2: Statistics for the small domain using the FUME emission model

	Coverage	BIAS	MGE	RMSE	r	IOA	COE	FAC2
NO_2	93.49%	-5.83	8.66	13.42	0.44	0.52	0.04	0.47
SO_2	92.24%	-0.27	3.29	7.47	0.31	0.43	-0.13	0.39
O_3	94.94%	12.96	20.40	26.57	0.59	0.56	0.11	0.83
PM_{10}	94.22%	-9.43	11.38	16.92	0.49	0.48	-0.04	0.43
$PM_{2.5}$	82.72%	-5.47	7.96	13.11	0.54	0.57	0.13	0.52

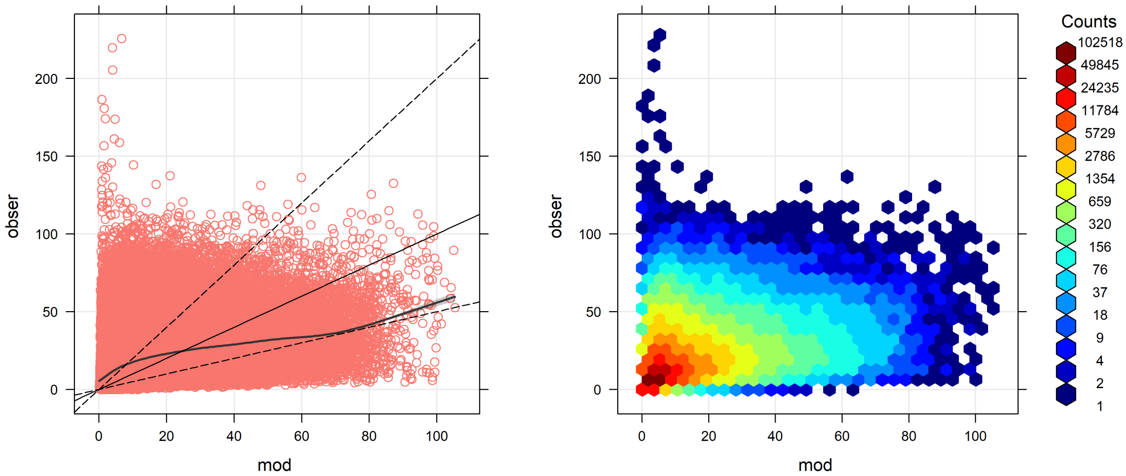
BIAS, MGE and RMSE in Table 2 are now in μg$\cdot$m^{-3}. COE and FAC2 are dimensionless. COE implies the models ability to predict - when COE$= 0$, the model is no more capable to predict the values then the observed mean value - the model has no predictive advantage [6]. Negative COE implies that the model is less effective than the observed mean in predicting variation in the observations.

In Table 2 we can see that O_3 reached the best values of r and FAC2 out of these pollutants, but it has the largest values of BIAS, MGE and RMSE. However, concentrations of ozone in the atmosphere usually reach higher values than the other pollutants, so the larger BIAS, MGE and RMSE are corresponding. Ozone also reached the second best result in IOA and COE values.

Predictions for $PM_{2.5}$ reached the best IOA and COE and its other statistics are also one of the best.

Negative COE for SO_2 and PM_{10} indicate no predictive advantage of the model for these two pollutants, for NO_2 the advantage is almost negligible. However, even for the O_3 and $PM_{2.5}$ the COE values are still rather low.

For a simple graphic illustration of correlation between the modeled and observed values, we also made 2 different scatter plots. For NO_2 they are presented in Figure 6 and for O_3 in Figure 7. We chose these two pollutants as a one with the worse and a one with the better results.

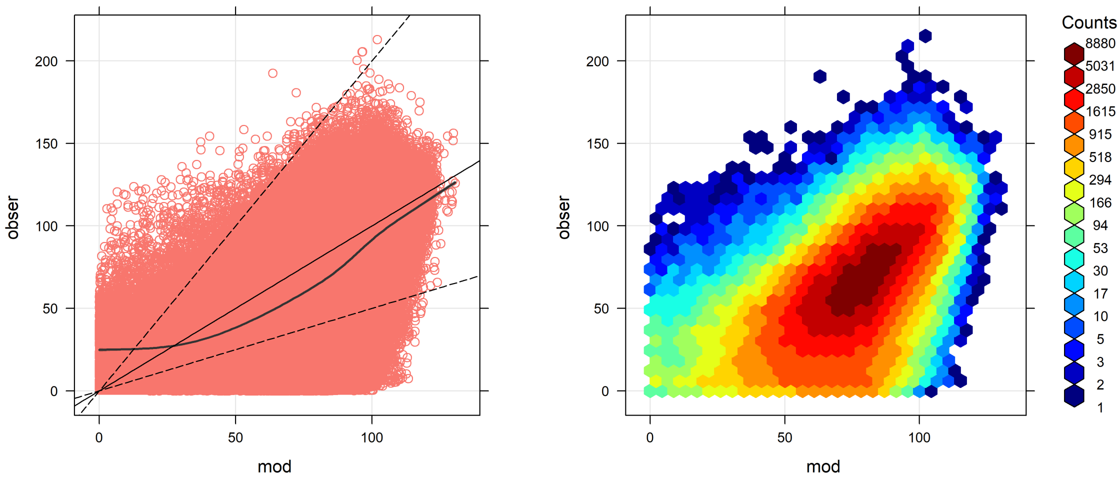


(a) Scatter plot 1 for NO2

(b) Scatter plot 2 for NO2

Figure 6: Scatter plots for NO_2

For both scatter plots, model values are on the x axis and the observed values are on the y axis. The scatter plot 1 makes one point for each pair of the observed value and the corresponding model value. The solid curved line is a fitted line. There are also 3 straight lines in scatter plot 1 - the solid middle one is a 1:1 relation, the top dashed one is a 1:0.5 relation and the bottom dashed one is a 1:2 relation. The solid middle line shows the relation for a perfect model and the dashed lines delimit the portion of points that lie within the factor of 2 (FAC2) [6].



(a) Scatter plot 1 for O_3

(b) Scatter plot 2 for O_3

Figure 7: Scatter plots for O_3

The scatter plot 2 divides the plot area into 'bins' that differ in color depending on the number of counts of occurrences in each bin [6]. This scatter plot reveals where most of the points lie, which is not apparent from the scatter plot 1.

In case of NO_2 from looking at a fitted line we can see that model underestimates the values slightly for small values and overestimates them for larger values. From scatter plot 2 we can see that number of occurrences does not descend much towards the axes, it is quite wide. A perfect model would have a narrow occurrence area close to the 1:1 relation line.

From the scatter plot 1 for O_3 (Figure 7 (a)) we can see that model underestimates the ozone values, but for larger values the correlation becomes quite favourable although a little overestimated. Large portion of the points lies within the FAC2. Scatter plot 2 (Figure 7 (b)) reveals that number of occurrences decreases around the 1:1 relation.

An impact of WRF and emission inputs on CMAQ predictions

In this section we try to determine causes of differences between the CMAQ predicted and observed values, based on the statistics for WRF meteorology predictions. We are limited by analyzing solely background air quality stations in Slovakia which also provide meteorology observations, which leaves us with only 4 stations - Bratislava Koliba, Chopok, Gánovce and Kojšovská hol'a out of which the later three measure only O_3 from the pollutants.

Bratislava Koliba station which is located at SHMI's main building is monitoring NO_2, PM_{10} and O_3. It is located in a suburban area on a hill. Its real altitude is 287 m and its model altitude is 148 m lower. It is marked as a background suburban station and it has no large emission sources around it, only households. To determine how might the WRF output influence the CMAQ predictions, we are presenting the statistics of WRF simulation results for the first 6 months of 2015 in the small domain in Table 3 . The results are presented only without the corrections, since CMAQ uses the uncorrected WRF predictions.

From these results, we can conclude that the altitude difference caused a rather large overestimation of the

Table 3: Statistics for WRF predictions in Bratislava Koliba station

	Coverage	BIAS	MGE	RMSE	r	IOA
Pressure	100%	17.56	17.56	17.63	0.98	-0.30
Temperature	100%	0.14	2.06	2.61	0.96	0.85
Wind speed	100%	1.34	1.72	2.15	0.62	0.33
Wind direction	48.16%	23.07	37.35	48.05	0.70	

pressure, however the temperature results are pleasant. The wind statistics are mostly above the average, especially the wind direction correlation. However, wind direction Coverage in this period is very poor and thus the statistics may not be reliable.

We present the results of CMAQ simulation for Bratislava Koliba station in the small domain for all monitored pollutants in Table 4.

Table 4: Statistics for CMAQ predictions in Bratislava Koliba station

	Coverage	BIAS	MGE	RMSE	r	IOA	COE	FAC2
NO_2	93.9%	-4.24	7.85	10.59	0.56	0.48	-0.04	0.67
O_3	97.44%	-1.71	15.56	20.15	0.68	0.64	0.28	0.94
PM_{10}	95.76%	-13.84	15.09	20.30	0.34	0.36	-0.29	0.36

Comparing these results with the average values from Table 2, we can see an improvement in NO_2's BIAS, MGE and RMSE and a large improvement in its r and FAC2. However, IOA and COE for NO_2 are worse than the average and negative COE also implies no predictive advantage of the model predictions in this station. Results for O_3 show a large improvement in all of the statistics. For PM_{10} all of the results are much worse than the average.

Chopok and Kojšovská hol'a stations (together with Lomnický štít station) reached the worst statistics for pressure and temperature in the WRF simulation due to the altitude difference of 654 m for Chopok and 490 m for Kojšovská hol'a station. Kojšovská hol'a also reached insufficient wind statistics. Chopok station wind statistics had a decent correlation in comparison with the other stations, although the wind speed was heavily underestimated. However, its wind direction statistics were even better than in some stations with otherwise much better results. Gánovce station has the altitude difference of only 7 m and its statistics for pressure and temperature were pleasant. However, its wind statistics were rather poor.

We present the results of O_3 CMAQ predictions for these stations in Table 5. We can see, that Chopok station has the best results - a decent correlation, COE above the average and FAC2 equal to one. It also has the smallest

Table 5: O_3 in small domain stations

	Coverage	BIAS	MGE	RMSE	r	IOA	COE	FAC2
Chopok	96.04%	5.65	10.49	12.80	0.68	0.59	0.18	1.00
Ganovce	82.16%	17.16	20.04	26.57	0.54	0.49	-0.03	0.86
Kojsovska hola	84.71%	22.99	24.21	26.98	0.68	0.13	-0.74	0.91

BIAS, MGE and RMSE. Kojšovská hol'a on the other hand has negative COE and very overestimated results. Ganovce station has the smallest correlation out of 4 stations monitoring ozone (including the Bratislava Koliba station). We present the scatter plot 1 for all four stations in Figure 8.

Looking at scatter plot in Figure 8, we can see that Chopok and Bratislava Koliba station have the best correlation and the least overestimated predictions out of these stations. Almost all of the points in their plots lie

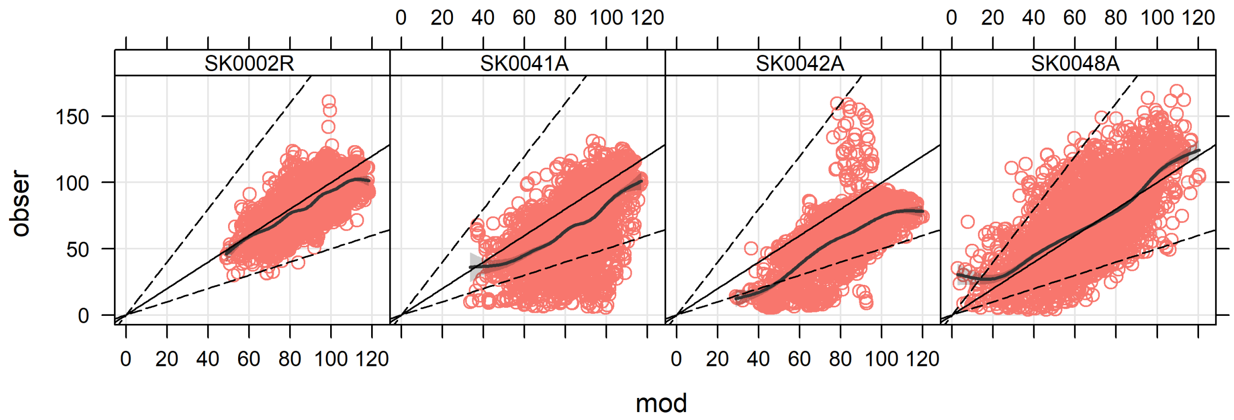


Figure 8: Scatter plot 1 for O3 measured at Chopok, Gánovce, Kojšovská hol’a and Bratislava Koliba stations, respectively

within the FAC2. The other two stations are much more overestimated but their correlation is still decent.

From these statistics, we can confirm that wind is the meteorological quantity which influences air quality the most, since we acquired better results for CMAQ predictions at stations with better wind statistics. We can suspect, that temperature and pressure solely do not influence the air quality as much, since we achieved the best results for Chopok station, where the WRF predictions of pressure and temperature were the worst out of these stations. Bratislava Koliba station also confirms this assumption, since it also has poor pressure statistics but its wind statistics are decent and so are its O_3 predictions. The Gánovce station had pleasant statistics for pressure and temperature, however its wind statistics were poor and its CMAQ predictions are also worse. Lastly, Kojšovská hol’a station had very bad statistics in all meteorological variables and also worse CMAQ predictions.

However, we should be careful with interpreting these results, since the model predicts at very different altitudes than the station altitudes for 3 out of these stations, including the Chopok and Koliba stations which achieved the best results for O_3 predictions from our 4 stations. Our results are also based upon a small portion of stations and for a definitive conclusion a much larger sample should be validated. Also we only compared these stations for ozone which had the best results in CMAQ simulations out of the analyzed pollutants.

Conclusion

Our intention was to validate WRF and CMAQ models with the aim to determine the amount of uncertainty that WRF model carries into the CMAQ predictions. The results for WRF overall did not satisfy the validation benchmarks from [7], but some stations with their altitude close to the corresponding grid box mean altitude achieved much better results. We were able to correct the pressure and temperature model values to the real station altitudes and improve the statistics this way in most of the stations for the validation. Thanks to the corrections we were able to determine that the difference between the station and model altitude which is caused by the spatial resolution of the domain being too large has the largest impact on the pressure and temperature results. However, the air quality modelling uses the uncorrected values and so the mistakes in the meteorological quantities are transferred into the CMAQ model via 3D meteorological input fields.

We validated CMAQ model (for the small domain) using the FUME emission set. The best results for CMAQ predictions were achieved for O_3 and this is probably caused by the fact that O_3 is not directly emitted into the atmosphere and thus it is not as dependent on the emission inputs as the other pollutants. The second best result was achieved for NO_2, then $PM_{2.5}$, PM_{10} and lastly SO_2.

We then wanted to analyze the influence of WRF meteorology predictions on CMAQ performance. Unfortunately, we were limited to only 4 background stations in Slovakia which monitor both meteorology and air quality. They were all monitoring O_3, only one station was monitoring also NO_2 and PM_{10}. We compared the meteorological and air quality results to determine that wind statistics are the most significant indicator of the air quality prediction success. We acquired the best results of the O_3 predictions for the Chopok station, which had one of the worst temperature and pressure statistics but it had a fairly successful wind correlations. A station with a pleasant temperature and pressure statistics but poor wind statistics had worse results in the O_3 predictions. However, we only analyzed a small sample of stations and we only compared ozone so our results should not be considered definite and more stations should be validated for more reliable conclusions.

Although it may seem like the CMAQ results were overall rather poor, this does not necessarily mean that the model is not convenient for use. There was a large diversity in the model predictions for individual stations. We can often determine the cause of unsatisfactory results and justify why some of the stations should not be used for validation. Bad validation results do not necessarily mean that the mean grid box concentrations computed by CMAQ are wrong - the differences in model and station values may be caused by an insufficient representativeness of the station. This may be improved by making the spatial resolution denser, however we would then have to face other problems such as inadequate spatial resolution of emission and meteorology inputs and also the computing time which would rise significantly.

We only analyzed the surface level predictions for both WRF and CMAQ. However, pollutants are often emitted by the high level sources, which can reach up to 300 m. For the purposes of the air quality assessment it is often needed to be able to predict the transport and diffusion of the pollutants in the close vicinity of the sources and in the corresponding heights. Therefore, a validation of the temperature and wind profiles of the WRF model is a necessary next step in our future validation work. Our intention to the future is also to improve the emission inputs since they can carry large inaccuracies into the model.

In the end, we need to realize that model results are not the predictions of the real world but rather they are predictions of a very limited representation of the real word, and they should be regarded accordingly. Model results will always contain simplifications of the real conditions as well as the mistakes that emerge from the simulations themselves, the limitations of spatial and temporal resolution and description of the atmospheric phenomena. Many factors influence the results and it is important to understand the underlying relations, otherwise we can not determine the reliability of the predictions.

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