Application of WRF-Chem to forecasting PM$_{10}$ concentration over Poland

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Abstract: The meteorological and chemical transport model WRF-Chem was implemented to forecast PM$_{10}$ concentrations over Poland. WRF-Chem version 3.5 was configured with three one-way nested domains using the GFS meteorological data and the TNO MACC II emissions. The 48 hour forecasts were run for each day of the winter and summer period of 2014 and there is only a small decrease in model performance for winter with respect to forecast lead time. The model in general captures the variability in observed PM$_{10}$ concentrations for most of the stations. However, for some locations and specific episodes, the model performance is poor and the results cannot yet be used by official authorities. We argue that a higher resolution sector-based emission data will be helpful for this analysis in connection with a focus on planetary boundary layer processes in WRF-Chem and their impact on the initial distribution of emissions on both time and space.

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1   Introduction

Forecasting air quality provides important information to the public. Air quality forecasts are especially important to sensitive individuals, e.g., children, elderly or asthmatic patients. Forecasts assist local authorities in preventive steps (e.g., temporary shutting of major emission sources; Ying et al., 2004). Saide et al. (2011) suggest that preventive steps to limit high concentrations require that air quality forecast is available with at least 48 h lead time. A key parameter in air quality forecasts is PM_{10} concentration (Saide et al., 2011). According to current knowledge, particulate matter (PM) consists of a complex mixture of solid and liquid particles of organic matter, mineral dust, secondary inorganic aerosols, trace metals and sea salt aerosols, as well as water and unspecified compounds. PM affects air quality and, in turn, human and ecosystem well-being, and also has an important role in Earth's climate system (Kirtman et al., 2013). PM pollution is probably the most pressing issue in air quality regulation worldwide (Fuzzi et al., 2015) and our study is focused on forecasting of PM_{10} concentrations over one of the most problematic regions in Europe in the context of air pollution.

PM_{10} pollution results from both primary emissions and secondary formation through complex photochemical and heterogeneous chemical pathways. Both natural processes and human activities release PM_{10} into the atmosphere. Potential sources from human activities include among others coal-fired power plants, industry, residential heating and road transport. The chemical and physical nature of emitted PM can be changed considerably within the atmosphere due to factors such as location, temperature, humidity and the presence of other pollutants (Sloss and Smith 2000). Therefore, the PM_{10} concentration in the air is affected by both human activities and meteorological factors (Saliba et al., 2010). Because PM_{10} is a sum of various different elements, a total uncertainty of PM_{10} concentrations is a sum of uncertainties of emissions and concentrations modelling of individual gaseous and particle pollution. This makes the prediction of temporal and spatial distribution of PM_{10} concentrations more difficult than modelling of individual species (Vautard et al., 2007; Werner et al., 2014).

Causes of PM_{10} concentrations can be studied by chemistry transport models (CTMs), e.g., by focusing on the physical and chemical processes of gases and PM. The majority of CTMs are offline models meaning that the meteorology is calculated prior to the chemistry such as CHIMEREv4.5 (Bessagnet et al., 2008; Pay et al., 2010), CMAQ (Matthias, 2008) or EMEP (Simpson et al., 2012; van Loon et al., 2007). Usually, the meteorology for these models is available at a 1 h, 3 h or 6 h resolution. The online integration of numerical weather prediction with atmospheric chemistry, transformation and transport allows all meteorological three-dimensional fields to be used at each time step (Kukkonen et al., 2012), varying from seconds to a few minutes. This reduces inconsistencies in processes that relate to aerosols, chemistry and meteorology (Baklanov et al., 2014). It also enables feedback effects from air pollution (e.g., those due to aerosol) on meteorological processes (Kukkonen et al., 2012; Forkel et al., 2012). A recent review has highlighted a number of important areas to focus on in relation to online modelling (Baklanov et al., 2014). These areas include focus on mixing processes in the planetary boundary layer (PBL) and improved time-dependence on atmospheric conditions.

In this study, we apply the online model WRF-Chem version 3.5 (Skamarock and Klemp, 2008; Grell et al., 2005) to forecast PM$_{10}$ concentration over Poland, with a focus on the south-west part of the country called the Lower Silesia region. The forecasting system described in the paper is developed within the LIFE European project (http://ec.europa.eu/environment/life/). The first operational version of the system is presented, where the focus is to study the influence of the meteorological conditions, independent of the – well-known but uncertain – large temporal variations in the emissions. The final version of the system will be based on information from this study in relation to the relevant meteorological processes and also will include up-to-date temporal variation in emission. The approach used here, therefore, enabled us to study the influence of meteorological conditions on air quality and the potential feedback mechanisms, which are important components in air quality forecasting systems using complex online models like WRF-Chem.

The PM$_{10}$ forecasts were tested during the winter (1st January–28th February) and summer (1st July–31st August) period of 2014. Winters in Poland often contain episodes with high concentrations of PM. These episodes are due to both high coal consumption used for residential heating and meteorological conditions preventing mixing and dilution of air pollutants. The forecasts are evaluated by comparison with observations separately for 24 h and 48 h lead time and for both the summer and winter period.

2   Methodology

2.1   The WRF-Chem model setup

WRF-Chem is used in nested mode with a summary of the model configuration in Table 1. These include the Noah Land Surface Model (Chen and Dudhia, 2001), YSU boundary layer physics (Hong et al., 2006), RRTMG long and short wave radiation scheme (Iacono et al., 2008), Grell and Devenyi (2002) 3D parameterisation with radiative feedback and shallow convection, the Lin microphysics scheme (Lin et al., 1983). The simulations are driven by the GFS meteorological data, available every 3 h, at a 0.5° × 0.5° spatial resolution. Emissions are the TNO MACC II dataset at a 1/8° × 1/16° spatial resolution (Pouliot et al., 2012). Temporal variations in emissions are restricted to emissions from nature, while the TNO MACC II emissions are assumed constant during the entire simulation. The chemical boundary conditions of trace gases consist of idealised, northern hemispheric, mid-latitude, clean environmental profiles based upon the results from the NOAA Aeronomy Lab Regional Oxidant Model (Liu et al., 1996). The first 48 h forecasting cycle on the 1 January and 1 July uses a two-week spin-up, with the model simulations initialised with the GFS meteorology for initial and boundary conditions. From the 2nd of January and July, the model uses chemistry cycling, and the WRF-Chem run for the last hour on the previous day is used to initialise the next day's forecasting simulation.

Table 1   Model configuration used in WRF-Chem simulations*

Category	Model setup
Forecasts period	1st January–28th February 2014, 1st July–31st August
Domains	Europe (36 km) – Poland (12 km) – SW Poland (4 km)
Vertical resolution	35 layers
PBL process	YSU (Hong et al., 2006)
Land-surface process	NOAH LSM
Cumulus	Grell and Devenyi (2002) for d1 and d2
Shortwave and longwave radiation	RRTMG
Microphysics	Lin et al. (1983)
Gas-phase mechanism	RADM2
Aerosol model	MADE/SORGAM
Photolysis scheme	Fast-J
Wet deposition	Simplified parameterisation for wet scavenging

Note: *Please refer to the WRF and the WRF-Chem user's guides for a complete
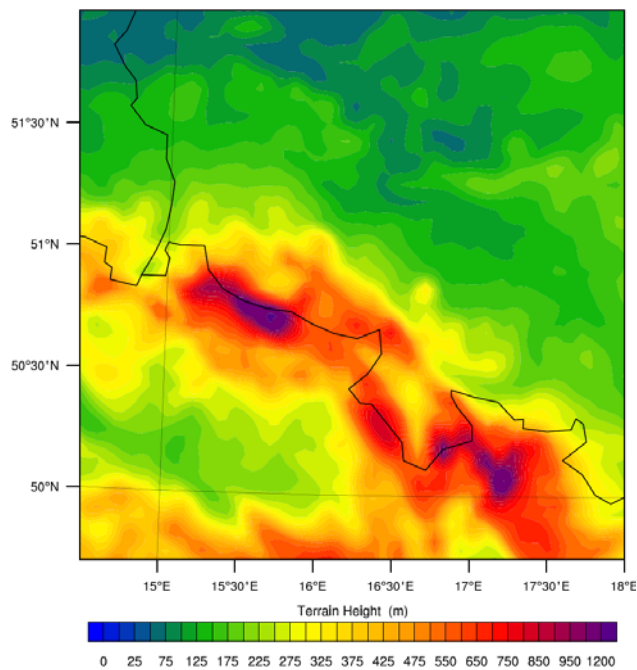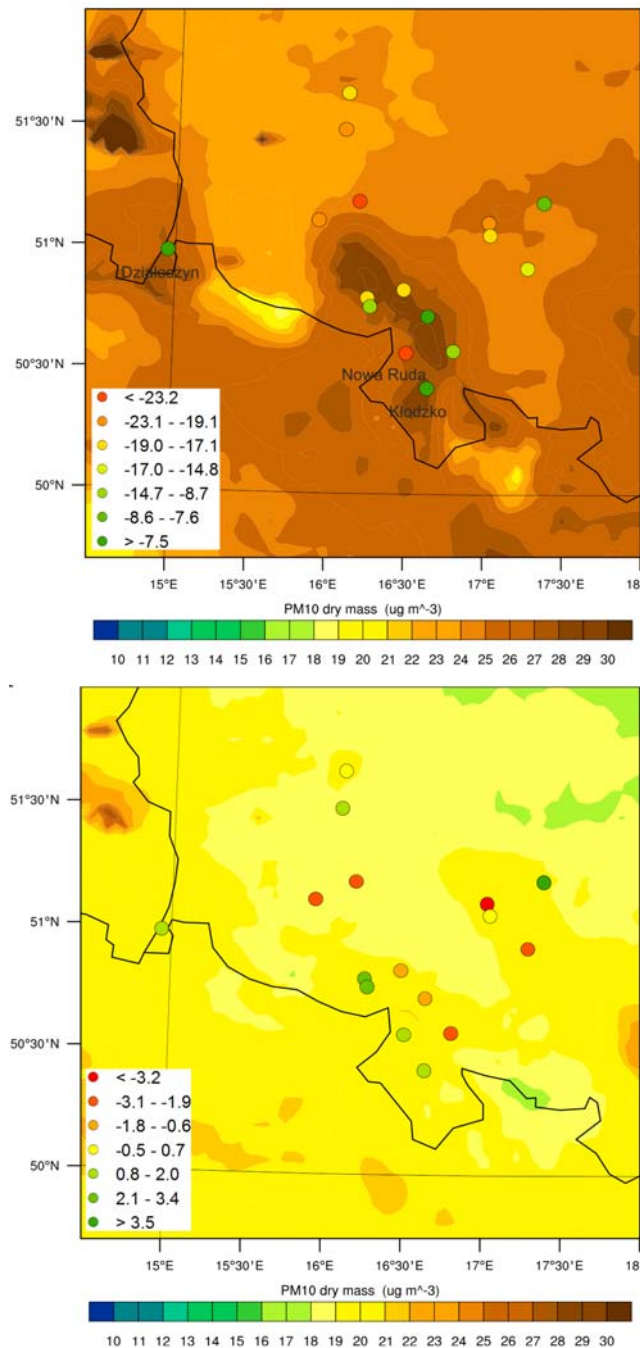description of the options.

Figure 1   Height above sea level of the innermost model domain [m] (see online version
for colours)

Figure 2 Mean PM$_{10}$ concentrations for winter (January–February 2014, upper) and summer (July–August 2014, lower) period in SW Poland, for 48 hour lead time (see online version for colours)

Note: Mean bias statistic marked with dots (MB = model-observation, different scale for winter and summer).

Figure 3   Time series of PM$_{10}$ concentration for the 48h lead time of the forecasts for
two selected stations (different y-axis scale is for winter and summer)
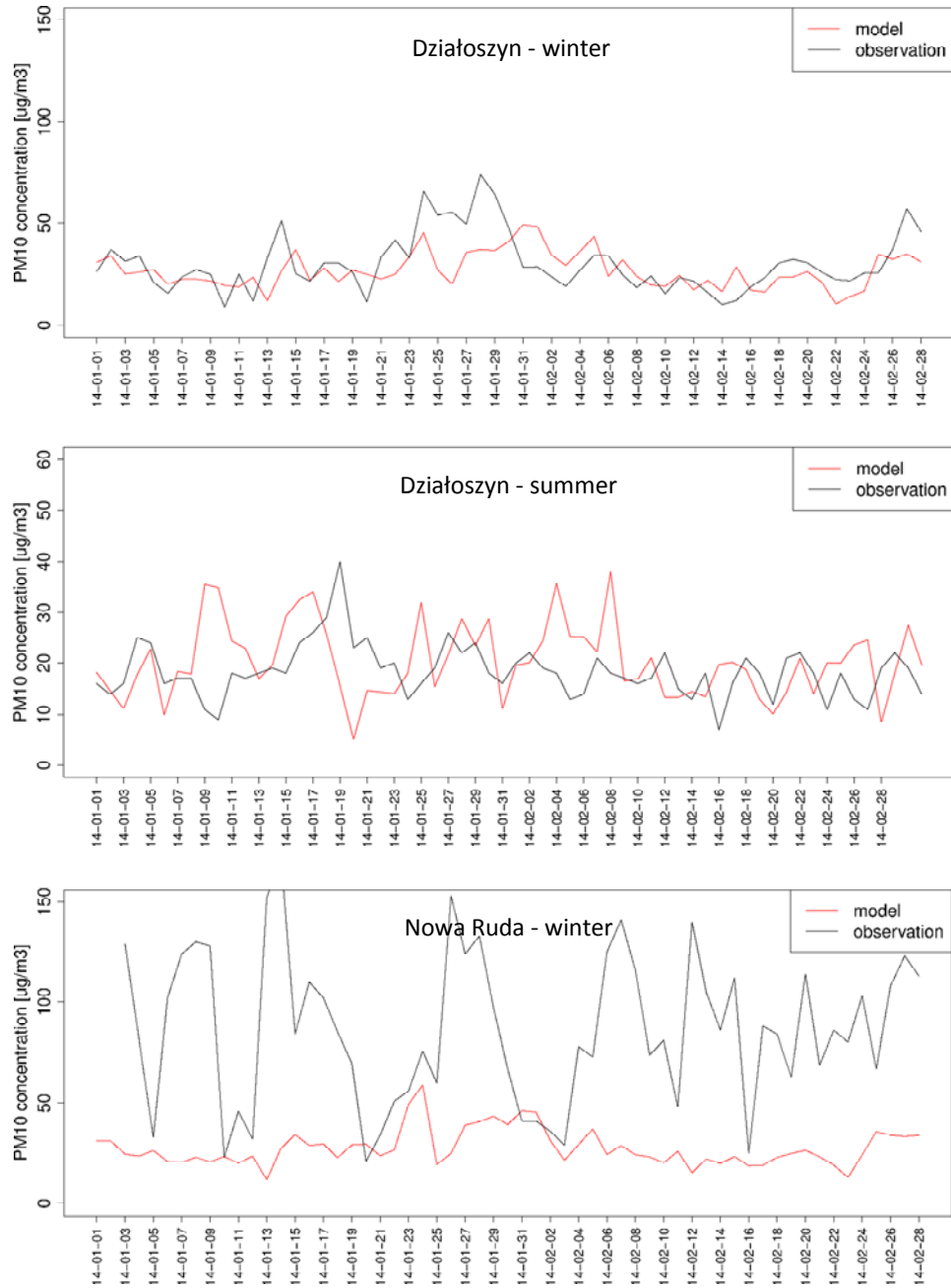(see online version for colours)

Figure 3   Time series of PM$_{10}$ concentration for the 48h lead time of the forecasts for
two selected stations (different y-axis scale is for winter and summer) (continued)
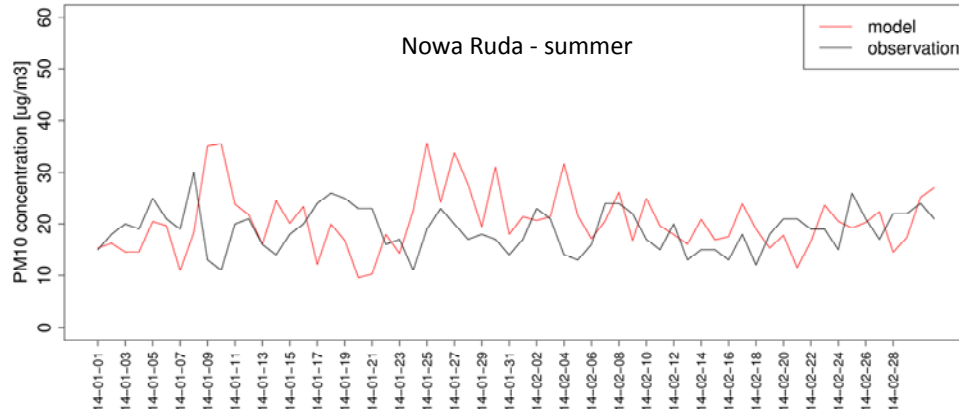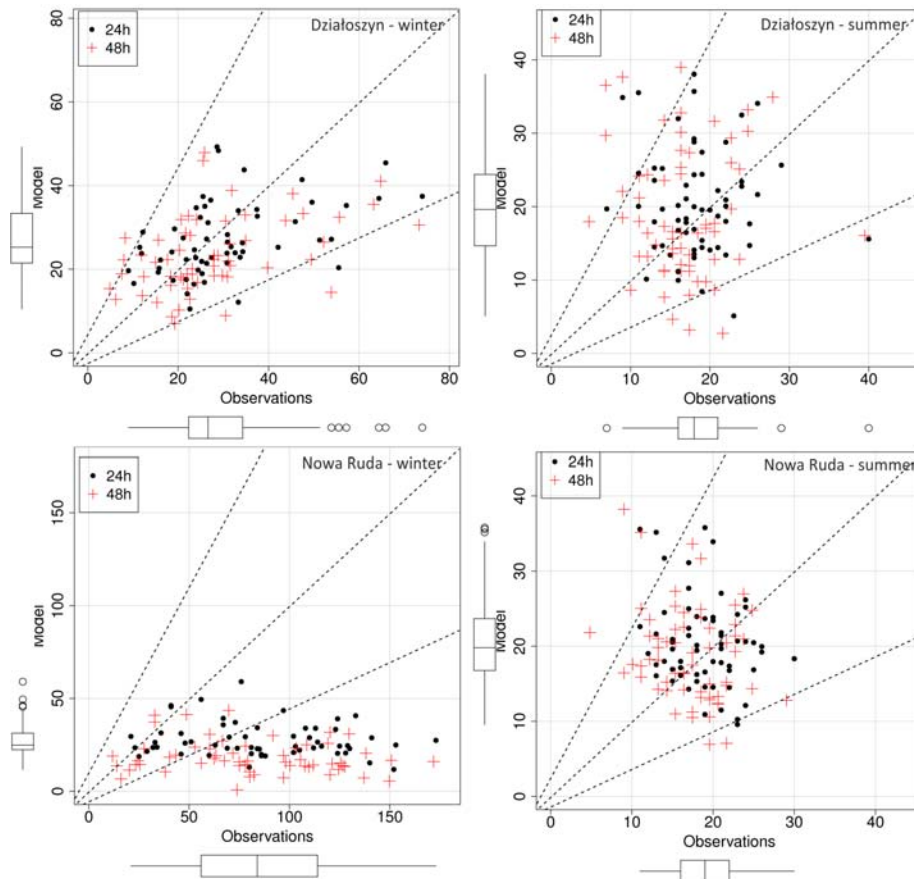(see online version for colours)

Figure 4   Scatter plots for two selected stations for winter and summer, presenting both 24h and
48h lead time (unit: µg m^{-3}) (see online version for colours)

2.2 Model evaluation

The PM_{10} concentration forecasts were compared with daily mean observations gathered by the Voivodeship Inspectorate of Environmental Protection for 16 stations in the Lower Silesia region in SW Poland (Figures 1 and 2). Forecasting quality was evaluated by using forecasting lead time as defined by World Meteorological Observation, separately for 24 h and 48 h lead time (Table 2). This means that the first day will correspond to 0 day lead time (0 h–23 h forecasts) and the second day to 1 day lead time (24 h–47 h forecasts). Taking into account all available stations the following statistics have been calculated: mean bias (MB), factor of two (FAC2), normalised mean bias (NMB) and root mean square error (RMSE). Time series and scatter plots for one station with the lowest and one with the highest MB (calculated for the winter period) are given as examples (Figure 3 and Figure 4). Mean bias for 48 lead time is also presented spatially for individual stations separately for winter and summer season (Figure 2).

3   Results

Spatial distribution of modelled mean PM_{10} concentration for winter and summer period is presented in Figure 2. Mean PM_{10} concentration in the winter period is slightly higher than in summer (24.0 and 18.0 μg m^{-3}, respectively), however, maximum value is about 70% higher in winter than in summer (47.8 and 29.0 μg m^{-3}, respectively).

For winter, the lowest values are in the Sudety Mountains and the highest are related to neighbouring emission sources and also with the region of Kłodzko which favours appearance of temperature inversion as well as gathering and stagnation of air pollution.

The mean observed PM_{10} concentration from 16 stations is 42 μg m^{-3} during winter and 19 μg m^{-3} during summer period. Very high concentrations were observed between 25th and 28th of January and between 25th and 28th of February. Model performance is noticeably better for summer in comparison to winter, with FAC2 respectively equal to 0.84 and 0.65 (Table 2). Measured concentrations are underestimated by the model during cold and slightly overestimated during warm season. NMB for summer is close to 0. Generally, the simulated forecast performance is slightly better for the 24 h lead time compared to the 48 h lead time during winter and lower during summer (Table 2).

Table 2   Model performance for the 24h and 48h lead time, separately for the winter and summer period (n – number of observations)

Forecast range	Winter						
	n	*FAC2*	*MB*	*MGE*	*NMB*	*NMGE*	*RMSE*
00–23 h	977	0.65	−16.49	21.10	−0.39	0.50	29.46
24–48 h	977	0.65	−16.65	21.23	−0.39	0.50	29.73
	Summer						
00–23 h	994	0.84	0.12	7.55	0.01	0.39	10.03
24–48 h	994	0.82	0.55	7.59	0.03	0.40	10.01

The lowest absolute MB, from all stations during winter, is for Kłodzko and Działoszyn, whereas the highest is for Nowa Ruda (Figure 2). It does not correspond to the model performance during summer where the lowest NMGE is calculated for Nowa Ruda.

Figure 5 Vertical cross-section of temperature at Nowa Ruda station, 5–18 January 2014
(see online version for colours)
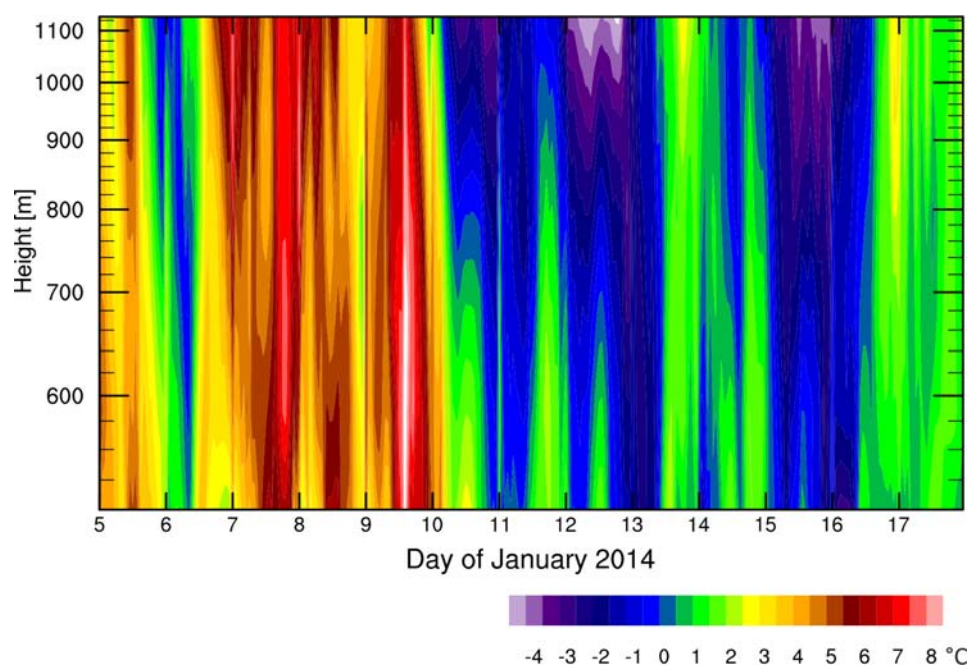
The model generally captures the observations at Działoszyn (winter and summer) and Nowa Ruda (summer, Figure 3) and most of the model-observation pairs are between the lines 1/2 and 2/1 (dotted lines, Figure 4) in the scatter plot. In the case of Nowa Ruda in winter, the model is not able to reproduce the observations during a series of episodes with very high PM$_{10}$ concentrations. In fact, the observations show much higher variability than the model calculations for that site only (e.g., compare the variability in all four scatter plots). There are two main factors responsible for this situation in winter season. The station is located in a river valley surrounded by hills and in the station vicinity dominate family houses heated by coal and wood burning. The first is responsible for the air stagnation and the second for high emission from residential heating, for which emission inventory is highly uncertain. An investigation of the meteorology in WRF-Chem showed that several of these episodes (e.g., within 5–17 of January) coincided with days that are either characterised by temperature inversion or relatively low T2 temperature (below 0ºC), which forces people to heat their houses (Figure 5).

4   Summary and conclusions

We have presented the results of WRF-Chem PM$_{10}$ forecasts for south-west Poland. The 48 hour forecasts were run for each day of the winter and summer period of 2014 and there is only a small decrease in model performance for winter with respect to forecast lead time. We have found that WRF-Chem tends to underestimate measurements in winter and slightly overestimate in summer, with much better error statistics for summer.

The model in general captures the variability in observed PM$_{10}$ concentrations for most of the stations. However, the highest observed peaks in winter are in general underestimated by the model. The lowest performance for this period was obtained for the Nowa Ruda station, which is located in a deep valley. This area has a high contribution of the emissions from coal fired residential heating, which is highly uncertain. Such circumstances could cause high PM$_{10}$ observed concentrations peak during certain weather types such as winter time inversions. Recent paper by Kryza et al. (2016) shows that the WRF model overestimates the PBL height for this area and for the winter season. This overestimation of PBL height may lead to underestimation of the observed concentrations of air pollutants.

For some locations and specific episodes, the model performance is poor and the results cannot yet be used by official authorities. We argue that a higher resolution of sector-based emission data will be helpful for this analysis in connection with a focus on PBL processes in WRF-Chem and their impact on the initial distribution of emissions on both time and space. In the next step, we are planning to adopt a high resolution (1 km × 1 km) up to date regional emission database and temporal emission profiles. This will also give an opportunity to study the impact of the more detailed emission inventory and application of temporal emission profile on the quality of the air chemistry forecasts.

Acknowledgements

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