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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 can not 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.

Keywords: PM_{10}, WRF-Chem, air quality forecast, Poland

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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. temporarily 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 48h 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 have an important role in Earth's climate system (Kirtman et al., 2013). Particulate matter 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 particulate matter can be changed considerably within the atmosphere due to factors such as location, temperature, humidity and the presence of other pollutants (Sloss & Smith 2000). Therefore, the PM_{10} concentration in the air is affected by both human activities and meteorological factors (Saliba et al., 2010). Due to the fact that 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 to PM_{10} concentrations can be studied by Chemistry Transport Models (CTMs), e.g. by focusing on the physical and chemical processes of gases and particulate matter. 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 1h, 3h or 6h 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 on-line model WRF-Chem version 3.5 (Skamarock & 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 on-line 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 particulate matter. 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 24h and 48h lead time and for both the summer and winter period.

Methodology

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 & Dudhia 2001), YSU boundary layer physics (Hong et al. 2006), RRTMG long and short wave radiation scheme (Iacono et al. 2008), Grell 3D parameterisation with radiative feedback and shallow convection (Grell 2002), the Lin microphysics scheme (Lin et al. 1983). The simulations are driven by the GFS meteorological data, available every 3h, at a 0.5^o x 0.5^o spatial resolution. Emissions are the TNO MACC II data set at a 1/8° x 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 01 January and 01 July uses a 2-week spin-up, with the model simulations initialized 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 initialize the next day's forecasting simulation.

Table 1. Model configuration used in WRF-Chem simulations*

Model evaluation

The PM_{10} concentrations' 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 (Fig. 1, 2). Forecasting quality was evaluated by using forecasting lead time as defined by World Meteorological Observation, separately for 24h and 48h lead time (Tab. 2). This means that the first day will correspond to 0 day lead time (0h-23h forecasts) and the second day to 1 day lead time (24h-47h forecasts). Taking into account all available stations 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 (Fig. 3, Fig.4). Mean Bias for 48 lead time is also presented spatially for individual stations separately for winter and summer season (Fig. 2).

Figure 1. Height above sea level of the innermost model domain [m].

Figure 2. Mean PM_{10} concentrations for winter (Jan-Feb 2014, upper) and summer (Jul-Aug 2014, lower) period in SW Poland, for 48 hour lead time. Mean Bias statistic marked with dots (MB=model-observation, different scale for winter and summer).

Results

Spatial distribution of modelled mean PM_{10} concentration for winter and summer period is presented in Fig. 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 neighboring emission sources and also with the region of Kłodzko which favors 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 (Tab. 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 24h lead time compared to the 48h lead time during winter and lower during summer (Tab. 2).

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

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).

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

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

The model generally captures the observations at Działoszyn (winter and summer) and Nowa Ruda (summer, Fig. 3) and most of the model-observation pairs are between the lines 1/2 and 2/1 (dotted lines, Fig.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 (Fig. 5).

Figure 5. Vertical cross-section of temperature at Nowa Ruda station, 5 – 18 January 2014.

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, this issue) 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 can not 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 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 (1km x 1km) 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.

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Tables

Table 1. Model configuration used in WRF-Chem simulations*

Category	Model setup
Forecasts period	01st January – 28th February 2014, 01st 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 Denvenyi (2002) for d1 and d2
Shortwave & 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

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

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

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

Author

Figures

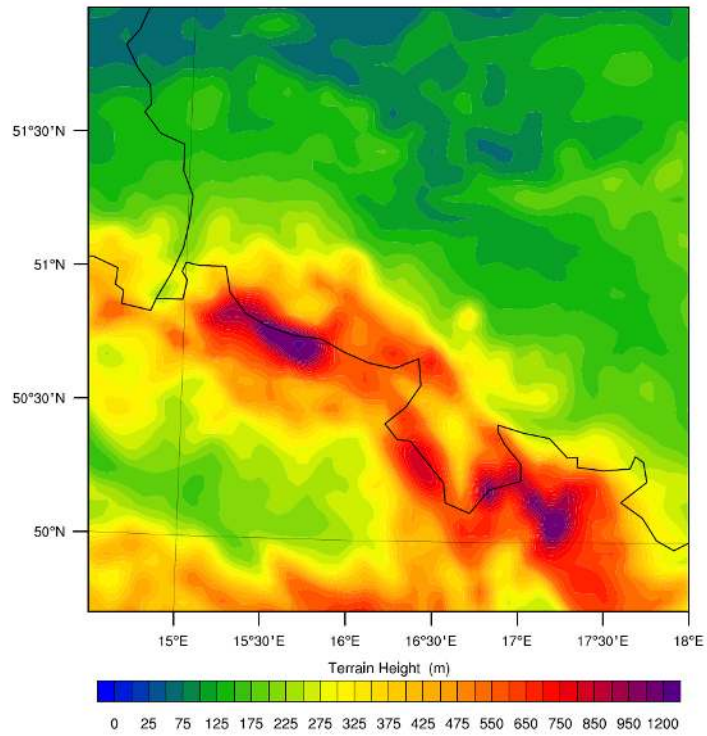

Figure 1. Height above sea level of the innermost model domain [m].

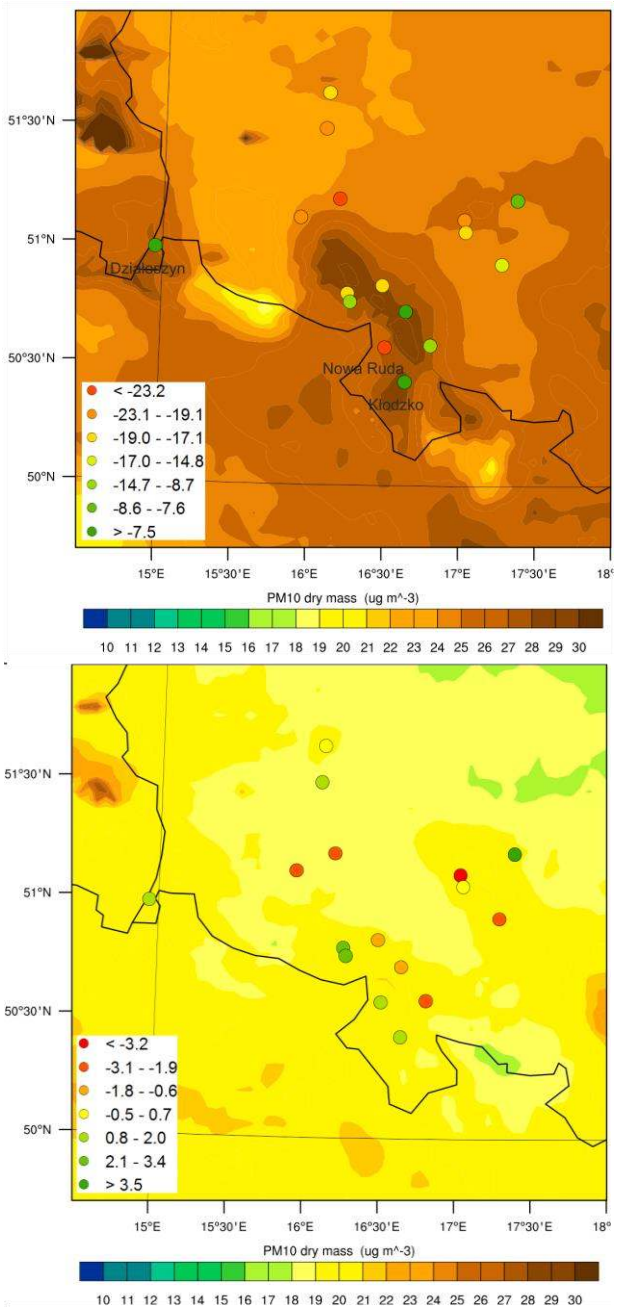

Figure 2. Mean PM_{10} concentrations for winter (Jan-Feb 2014, upper) and summer (Jul-Aug 2014, lower) period in SW Poland, for 48 hour lead time. Mean Bias statistic marked with dots (MB=model-observation, different scale for winter and summer).

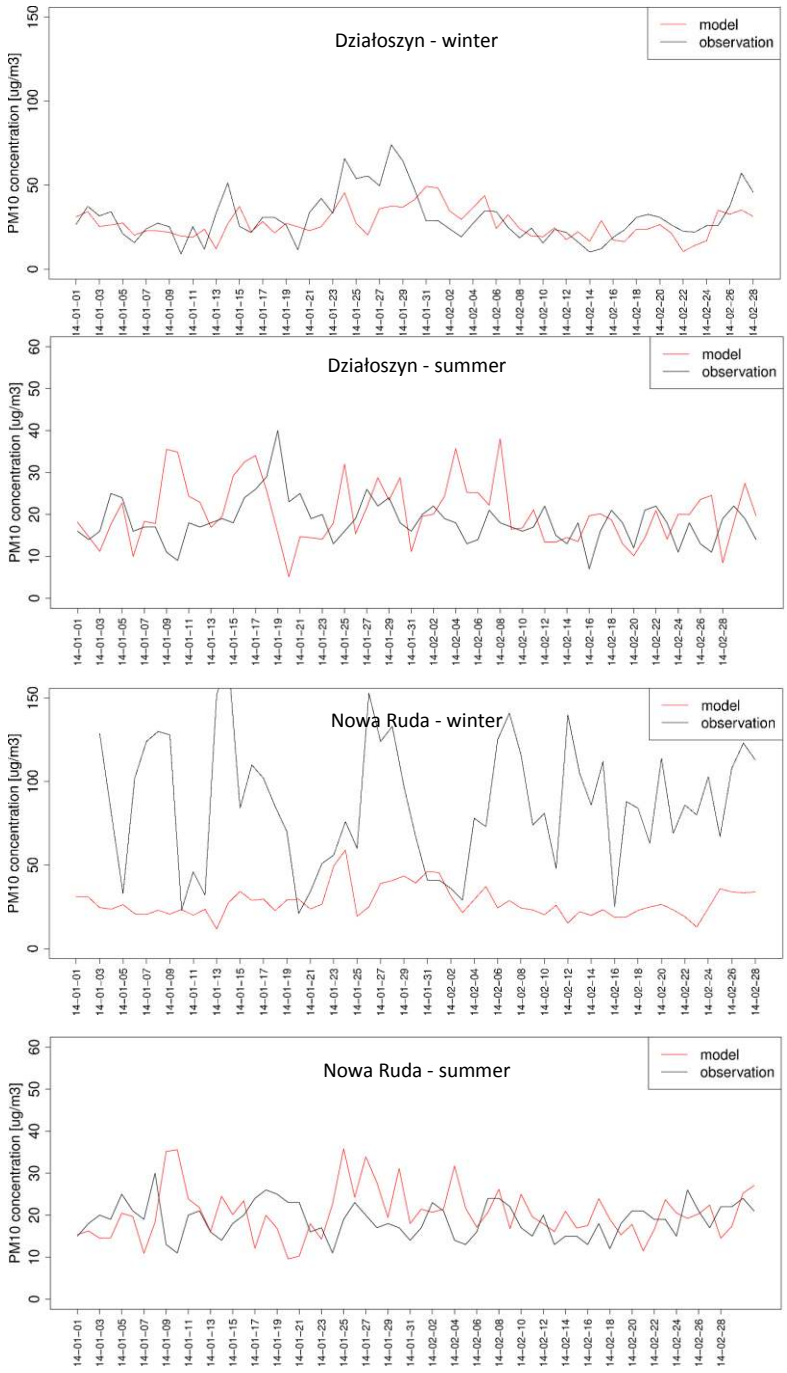

Figure 3. Time series of PM_{10} concentration for the 48h lead time of the forecasts for two selected stations (different y-axis scale is for winter and summer).

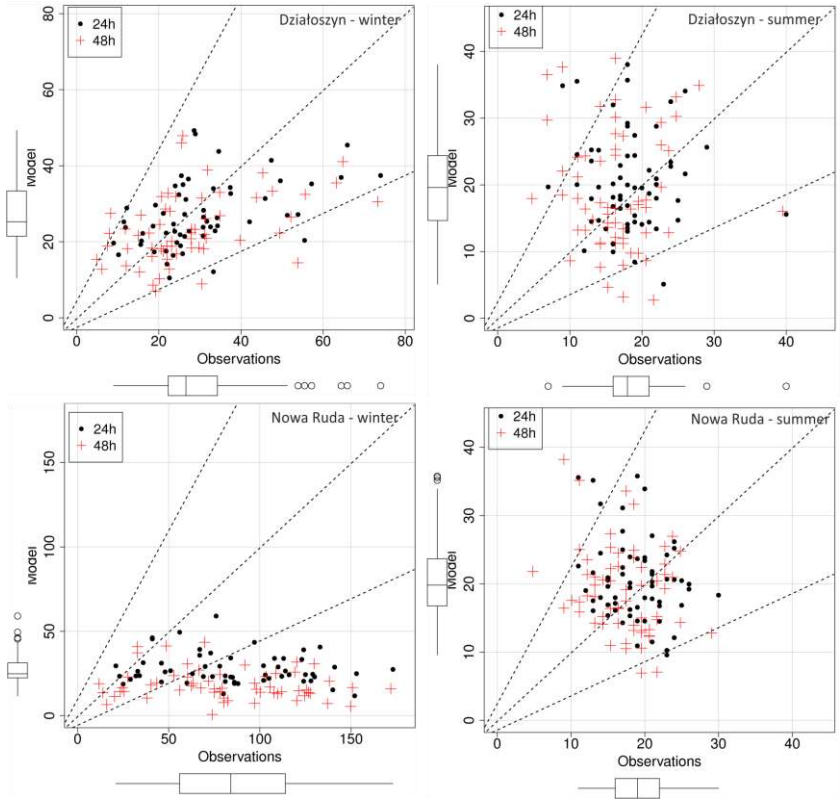

Figure 4. Scatter plots for two selected stations for winter and summer, presenting both 24h and 48h lead time (unit: µg m^{-3}).

Author

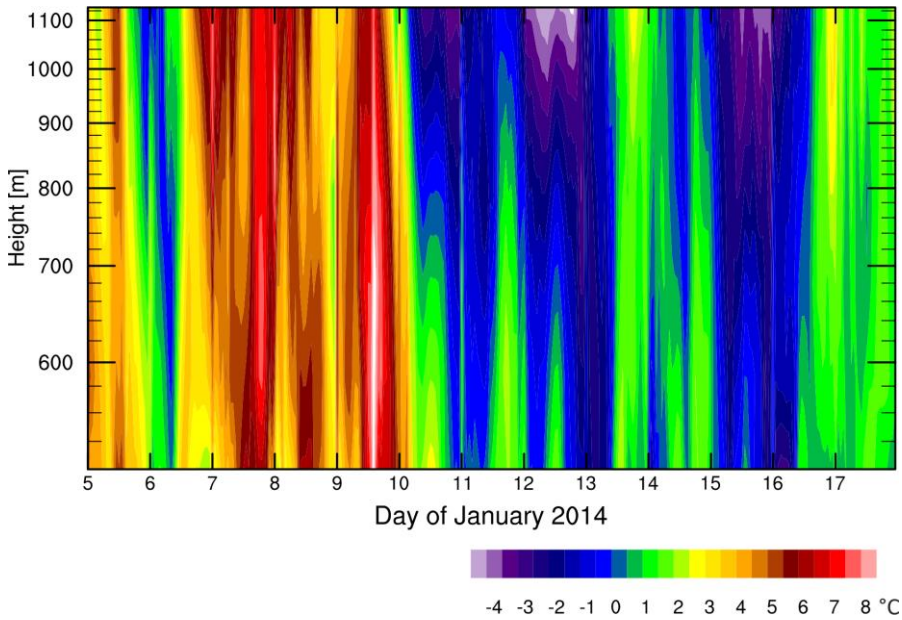

Figure 5.

Vertical cross-section of temperature at Nowa Ruda station, 5 – 18 January 2014