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Functionality of openair package in air pollution assessment and modeling — a case study of Krakow

Funkcjonalność pakietu openair w ocenie i modelowaniu stanu zanieczyszczenia powietrza na przykładzie Krakowa

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Słowa kluczowe: jakość powietrza, projekt R, openair, trajektorie wsteczne, OSPM

Abstract
The paper presents the possibilities of selected functions from openair package for R programming environment in urban air pollution assessment. Examples of data analysis were based on the measurements from continuous air quality monitoring stations in Krakow (Poland). In order to present additional functionality of this software, modeling results of back trajectories and air pollution dispersion were used. Functions and visualization methods included in openair package make scrutiny of large data sets easier and less time consuming. They allow for analysis of measurement data with the determination of general relationships between parameters, additional complex spatial analyses for back trajectories, and validation of air pollution dispersion models. Openair package is, therefore, a valuable and functional tool that can be successfully used as a support in the air quality management system.

Streszczenie
W pracy przedstawiono możliwości wykorzystania wybranych funkcji pakietu openair, będącego częścią środowiska programistycznego R, w ocenie stanu zanieczyszczenia powietrza miejskiego. Przykładowe analizy wykonano na podstawie danych pomiarowych pochodzących ze stacji ciągłego monitoringu jakości powietrza w Krakowie (Polska). W celu przedstawienia dodatkowych funkcjonalności pakietu wykorzystano również wyniki modelowania trajektorii wstecznych i dyspersji zanieczyszczeń w powietrzu. Funkcje i metody wizualizacji danych zawarte w pakiecie openair przyspieszają i ułatwiają pracę z dużymi zbiorami danych. Umożliwiają one przeprowadzenie analizy danych pomiarowych i wyznaczanie zależności pomiędzy poszczególnymi parametrami, wykonanie złożonych analiz przestrzennych dla trajektorii wstecznych i walidację modeli dyspersji. Pakiet openair stanowi zatem wartościowe i funkcjonalne narzędzie, które z powodzeniem może być stosowane na potrzeby wsparcia systemu zarządzania jakością powietrza.

1. INTRODUCTION

In recent years, a significant amount of digital data including air quality monitoring data, dispersion modeling results, and other information concerning air pollution is stored and freely available online. For that reason, the necessity of tools capable of handling and analyzing large data sets became of substantial importance. One of the examples providing solutions and functions helpful in air quality assessment and other related research is openair package [Carslaw, Ropkins 2012] for R programming environment. It was developed as a NERC knowledge exchange project by the Environmental Research Group at King's College London [www.openair-project.org]. Functions in this package comprise tools for importing and analyzing air quality data, determining potential sources of pollutants using polar plots, defining correlations between parameters, and performing operational model performance evaluation and analysis of HYSPLIT back trajectories using additional statistic methods [Carslaw 2015].

For the past few years, openair package has been proved to be useful in air quality research and study worldwide. It has been successfully applied to tentative determination of potential emission sources based on the continuous urban ambient air measurements as reported by Munir et al. [2016], Oleniacz et al. [2016a], and Czernecki et al. [2016] as well as for single campaigns [Crilley et al. 2017], studies concerning pollution exposure [Pattinson et al. 2016], and natural events [Salvador et al. 2014; Schweizer, Cisneros 2014]. Frequently, functions provided in this package are combined to give comprehensive information about the analyzed data, especially when multiple variables and air pollutant drivers are taken into account as described by Leuchner et al. [2016], Crilley et al. [2015], and Jang et al. [2016], and to study physical and chemical properties of substances [Bigi et al. 2017; Sheridan et al. 2015; Stojić et al. 2016]. Model evaluation tools have been commonly applied in the evaluation of air pollutant dispersion modeling systems [Munir 2016; Barnes et al. 2014; Rzeszutek, Bogacki 2016]. Trajectory clustering, Concentration Weighted Trajectory (CWT), and other analyses have been used to study the origins of pollutants, for example, in India [Ghosh et al. 2015] and Southern Europe [Di Gilio et al. 2015].

The study was conducted in order to help identify trends and general relations between parameters as well as causation of poor air quality episodes in Krakow (Southern Poland) for the period of 2012–2015 using openair package. The paper was extended with CWT analysis using back trajectories calculated in HYSPLIT model for the urban background station and evaluation of modeling results in the OSPM system for the urban traffic station located in a street canyon. Krakow has been struggling with poor air quality for many years, which mainly results from its location in the Vistula valley and limited ventilation within the city center, and also from cumulative impacts of local, regional, and transboundary emissions. Only in 2015, PM_{10} concentrations in Krakow exceeded the 24-h permitted level of 50 μg m^{-3} during 109 days at the urban background station up to 200 days at the urban traffic station. Additionally, excessive levels of annual NO_2 concentrations are observed at the location of the traffic urban station, reaching 63 μg m^{-3} in 2015 (158% of annual permissible value) [monitoring.krakow.pios.gov.pl]. Therefore, the development of new methods enabling identification and assessment of the reasons behind this condition and their further application for air quality management is necessary.

2. MATERIALS AND METHODS

Performed analysis of correlations and trends was based on collected measurement data (concerning both pollutant concentrations and meteorology) from three of the air quality monitoring stations in Krakow (Figure 1): Kurdwanow (the urban background station), Krasinskiego (the urban traffic station), and Nowa Huta (the industrial station) [monitoring.krakow.pios.gov.pl]. These data comprise 1-h results of measurements for the years 2012–2015 in Central European Time (UTC+1).

Considered time range was chosen because of the availability of both air pollutants concentrations and meteorological measurements at concerned air quality continuous monitoring sites. The relationship and trends of concentrations, including PM_{10}, $PM_{2.5}$, SO_2, NO_2, NO_x, CO, and O_3 and meteorological parameters such as wind speed and direction, mixing-layer height, temperature, and relative humidity were examined using the following functions: timeVariation, timeProp, corPlot, scatterPlot, and polarPlot. Values of mixing-layer height in the area of the air quality monitoring stations were estimated using CALMET model according to Oleniacz et al. [2016b].

Calculations of 72-h back trajectories performed every 3 h for urban background station in Krakow in the year 2015 were carried out using openair package initializing the HYSPLIT model [Stein et al. 2015]. Simulations were driven with NCEP/NCAR meteorological reanalysis data set available at 17 pressure levels and for surface layer every 6 h in a global grid of 2.5 degree latitude–longitude resolution. In the paper, the CWT analysis was presented.

Model evaluation was conducted using the PM_{10} and NO_2 modeling results in OSPM system [Kakosimos et al. 2010] obtained for Krasinskiego urban street canyon in Krakow in 2012. The air pollutant emission rates were estimated using EEA CORINAIR methodology [EEA 2013]. Meteorological conditions were obtained from measurement station located approx. 1.5 km from considered street canyon and using CALMET diagnostic model [Scire et al. 2000]. Air pollutants background concentrations were set accordingly to the measurements at Krakow–Kurdwanow urban background station [Rzeszutek, Bogacki 2016].

3. RESULTS AND DISCUSSION

3.1. Trend analysis and relationships

Exemplary results of initial examination of trends and cyclic variability of pollutant concentrations observed at Krakow air quality monitoring stations were presented for NO_2 in Figure 2. The results explicitly reveal that regardless of the measurement station type, the variability of this pollutant concentration is conditioned by road transport emission, where daily and weekly variation corresponds to the cyclical nature of traffic volume. Consequently, during weekend days, the morning peak is not as clear as during weekdays for all stations. The highest concentrations of this pollutant are observed at Krasinskiego urban traffic station with overall mean of 65.83 μg m^{-3} during analyzed period. For Kurdwanow and Nowa Huta stations, mean values reach roughly 30.08 and 26.51 μg m^{-3},

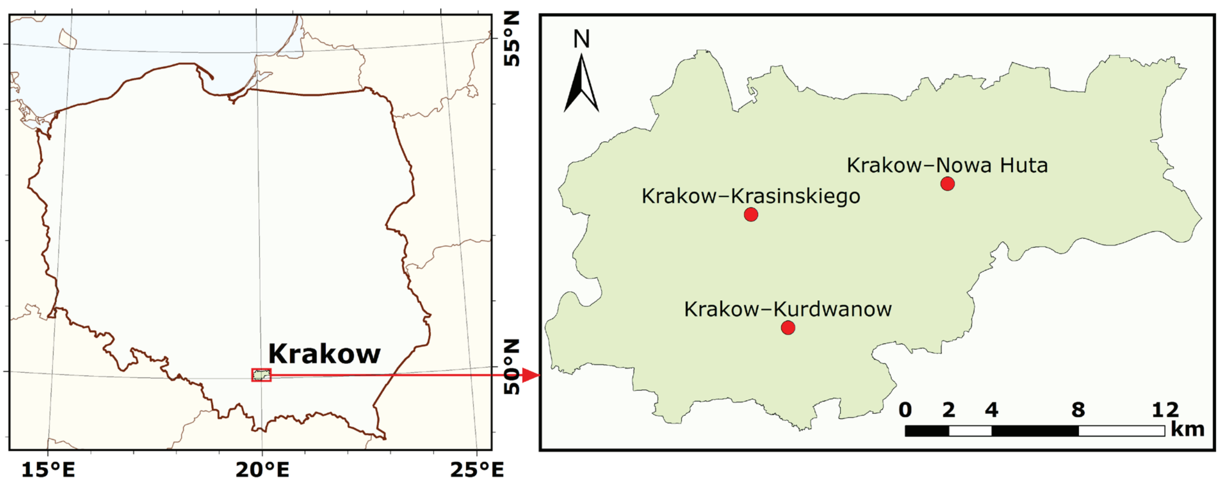

Figure 1. Location of considered air quality monitoring stations (red dots) in Krakow.

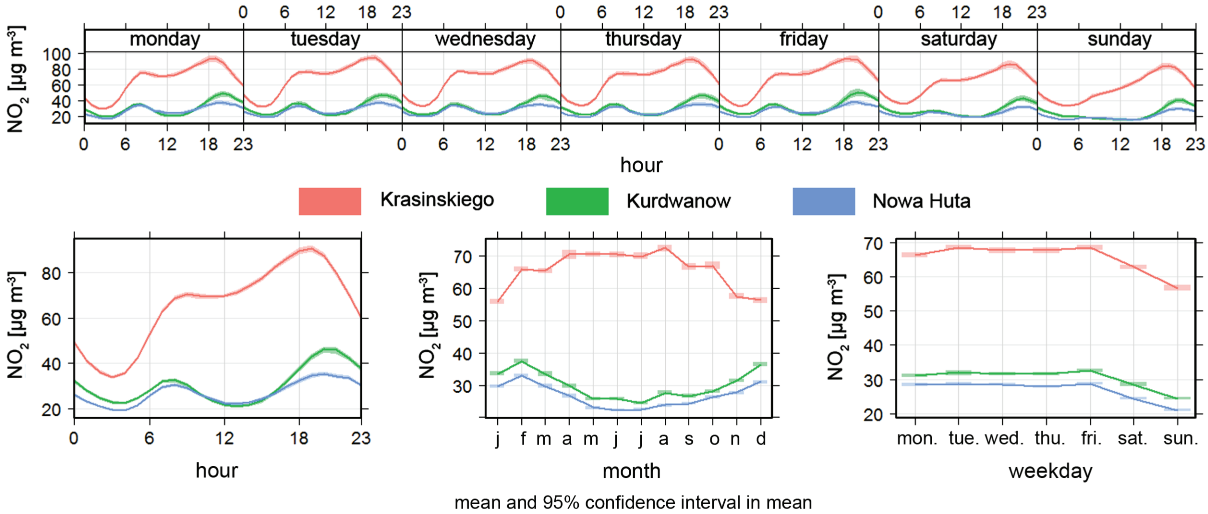

Figure 2. Mean NO_2 concentrations [µg m^{-3}] at air quality stations in Krakow calculated for hourly mean during weekdays and a single day, monthly, and daily mean (2012–2015).

respectively. It is noteworthy that the concentration of NO_2 during summer months observed at Krasinskiego station is considerably higher than that in winter, while for the other two stations, the character of this tendency is reversed. This is strongly related to the intensity of photochemical transformations of NO, which is substantially lower during days with limited sunlight. The effect of NO_2 formation is, therefore, noticeable at more remote sites, but at stations located in close vicinity of the road, higher concentrations of NO during winter are expected.

When meteorological data are available, the other functions showing trends over time can be applied and reveal possible relations between parameters. Relationship between wind direction and daily average concentrations of PM_{10} presented in Figure 3 clearly indicates that high episodes of PM_{10} levels are primarily related to winds from the south (S) and southwest (SW) directions and occur more often at low wind speeds during heating season. Higher wind speed is noticeably associated with northeast (NE) and north (N) directions and can be responsible for greater PM_{10} concentrations as well. However, there is a clear indication that temporary wind gusts contribute to the dilution of pollutants during colder part of the year.

Pearson linear relations can be defined in openair using corPlot and scatterPlot functions, which provide information about general behavior of the parameters with possible division into time periods (years, seasons, weekdays, etc.). Optionally, scatter plots can be presented using three variables, with color scale labeling the values of additional parameter. Correlation matrix between all parameters available for Krakow–Kurdwanow station (Figure 4a) indicates that, in general, most of the air pollutants are negatively correlated with meteorological variables. As mixing layer and temperature are usually higher in the summer, during that season, lower concentrations of air pollutant are expected. As it was emphasized earlier, higher wind speed is responsible for better ventilation within city center resulting in dilution of air pollutants.

Secondary pollutants such as ozone (O_3), formed as a result of photochemical reactions, are positively correlated with wind speed, because their concentration depends on the inflow of precursors. Formation of this pollutant during intensive insolation episodes explains strong positive relationship between O_3 air concentration and both mixing-layer height and temperature (Figure 4a), while the relationship between O_3 and NO_2 or NO_x ($NO + NO_2$) air concentrations (Figure 4b) is negative.

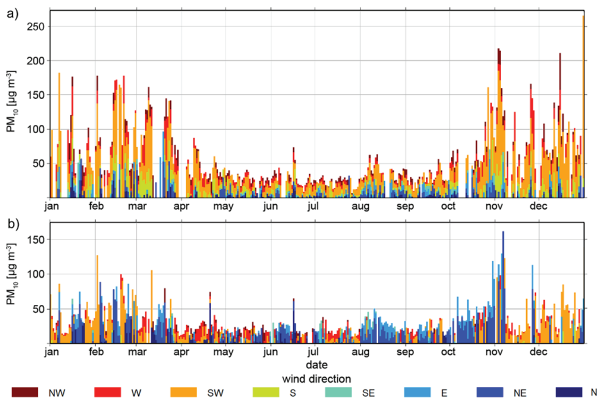

Figure 3. Wind direction contribution weighted by mean air concentrations of PM_{10} [µg m^{-3}] and daily averaged for Krakow–Kurdwanow station in 2015 for wind speed below median of 0.8 m s^{-1} (a) and above median value (b).

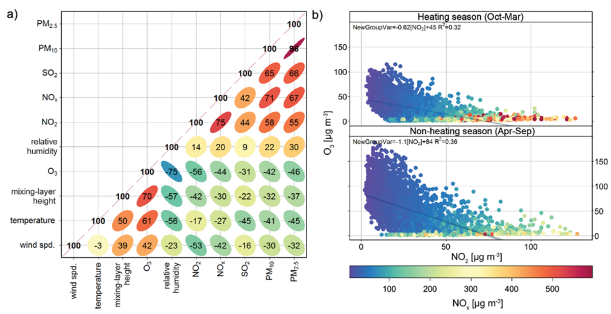

Figure 4. Strength of the Pearson linear relation between selected parameters (a) and a scatter plot with division to heating and non-heating season (b) for Krakow–Kurdwanow station (2015).

3.2. Emission source apportionment

Bivariate polar plots with wind direction presented on a radial scale provide information about the potential emission sources of analyzed air pollutants [Carslaw, Beevers 2013]. Apart from mean concentration, this function can be plotted against specified percentile or using CPF (Conditional Probability Function) analysis. Additional approach involves creating heat maps using temperature instead of wind direction on a radial scale. This can be helpful as well when examining basic relations between parameters.

NO_2 concentration distribution in the period of 2012–2015 presented for Krakow–Nowa Huta station as a function of wind speed and direction (Figure 5) explicitly demonstrates that high levels of NO_2 are associated mainly with low wind speed and the inflow from nearby road on weekdays. During analyzed years, this tendency is constant; however, additional inflow from northeast (NE) direction is noticeable in 2012. The presence of high concentrations at wind speed ranging from 3 to 4 m s^{-1} indicates potential impact of industrial sources located in the Nowa Huta district as well.

Heat maps for different air pollutants observed at Krakow–Nowa Huta station in 2012 (Figure 6) indicate that for PM_{10}, SO_2, and CO, the highest concentrations occur only during low temperatures, which results mostly from domestic heating systems and combustion. However, for NO_2, elevated concentrations are observed at higher temperatures as well, which points to the influence of road transport throughout the year. Similar dependences have also been observed in recent years for other air quality monitoring stations in Krakow.

3.3. Back trajectories analysis

As an extension to HYSPLIT functionalities, openair package provides additional analysis that can be performed using calculated back trajectories. These involve, inter alia, calculating gridded differences in occurrence for high concentrations of air pollutants compared with conditions over the whole year and the CWT analysis to identify flow directions of most polluted air masses using trajLevel function.

Presented gridded CWT analysis for PM_{10} concentrations at Krakow–Kurdwanow station (Figure 7) clearly indicates that air masses inflowing from the south, southwest, and southeast directions are responsible for the highest levels of this pollutant and they are associated with low wind speeds. Simultaneously, the inflow from northern directions may contribute to periodic dilution of air pollutant concentrations and better ventilation within the area of Krakow. Identified directions are consistent with the observations based on concentration distribution in Figure 3. Despite the fact that the pathways cross regions with increased emissions in Europe (e.g., Balkan countries, Ostrava-Mošnov Strategic Industrial Zone (SIZ)), the entrainment time of pollutants into the air masses is undetermined. Thus, the contribution of local sources in high PM_{10} concentrations may be significant, in particular during low wind speed episodes and heating season. It is noteworthy that tracking the concentration of PM_{10} along the pathways may narrow down its possible entrainment time and area of origin.

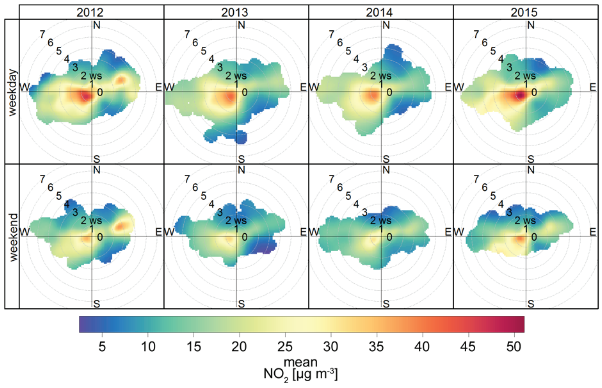

Figure 5. PolarPlot function used for the identification of potential source contribution with respect to wind speed (ws) [m s^{-1}] for NO_2 concentrations at Krakow–Nowa Huta station (2012–2015).

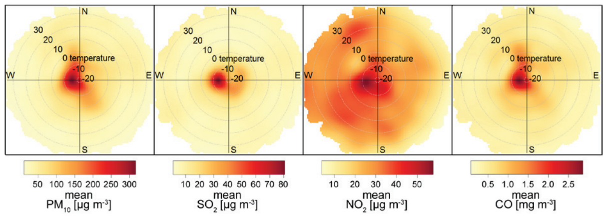

Figure 6. PolarPlot function plotted against temperature to create heat map for concentrations of different substances at Krakow–Nowa Huta station (2012).

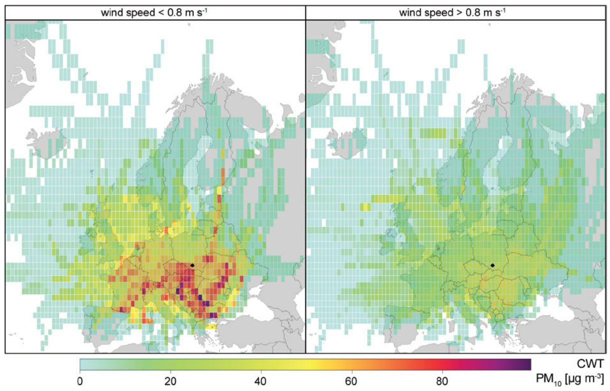

Figure 7. CWT analysis for Krakow–Kurdwanow station starting location (based on calculated 72-h back trajectories in 2015 for PM_{10} concentrations [μg m^{-3}]).

3.4. Operational model evaluation

Visualization methods of model performance evaluation include Taylor Diagram and conditional quantile plots, which combine a set of parameters to determine the quality of modeling results. Evaluation of OSPM model performance was carried out for PM_{10} and NO_2 street canyon (Krakow–Krasinskiego station).

Taylor diagram presented for PM_{10} modeling results (Figure 8a) reveals that the largest deviations from the observations are noticeable in autumn and winter with Mean Bias (MB) of −20.74 and −23.91 μg m^{-3}, respectively. This is most likely connected to the strong impact of local municipal emissions of air pollutants associated with the heat consumption during this period, which hinders the accurate determination of air pollution background. During warmer part of the year, the model performs better and mean biases reach roughly from −1.92 μg m^{-3} in summer to −8.42 μg m^{-3} in spring. Figure 8b illustrates that the model quite correctly represents the actual levels of PM_{10} with general underestimation confirmed by mean bias of −13.32 μg m^{-3} for the whole year. Presented histograms indicate that in particular, the underestimation occurs within the area of high concentrations, which can be also connected to the other random events such as periodic cleaning of the streets [Rzeszutek, Bogacki 2016].

Evaluation of OSPM model performance for NO_2 air concentrations revealed that the accuracy of modeling results is similar for all seasons of the year (Figure 9a). MB ranges from −4.67 μg m^{-3} in spring to 9.07 μg m^{-3} during summer. Noticeable overestimation during warm season and high concentrations of O_3 may result from oxidation scheme used in the model, which describes conversion of NO to NO_2. Overall MB error of −0.11 μg m^{-3} in 2012 proves good agreement with observations of modeling results of OSPM for NO_2 (Figure 9b).

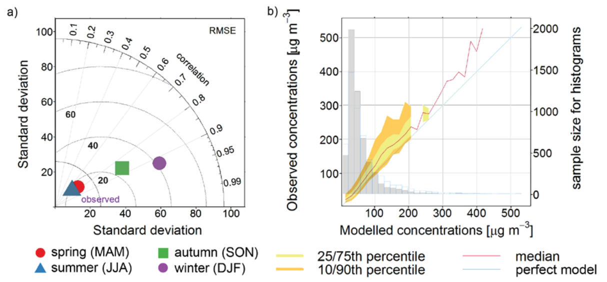

Figure 8. Taylor diagram (a) and conditional quantile plot (b) used for defining overall OSPM model performance with respect to PM_{10} air concentrations in the urban street canyon (Krakow–Krasinskiego station, 2012).

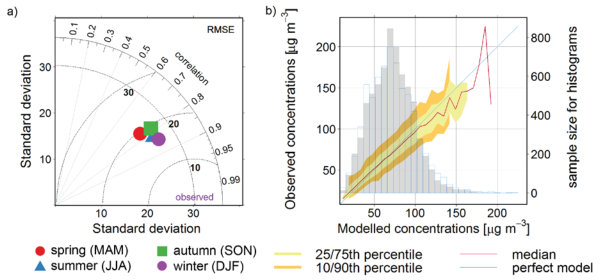

Figure 9. Taylor diagram (a) and conditional quantile plot (b) used for defining overall OSPM model performance with respect to NO_2 air concentrations in the urban street canyon (Krakow–Krasinskiego station, 2012).

4. CONCLUSIONS

Openair package allows for initial assessment of air pollution data as well as more advanced analysis using backward trajectories and evaluation of atmospheric dispersion model performance. Functions provided with the package are particularly suitable for the identification of general relationships between air pollutant concentrations and meteorological conditions, as well as for the characterization of temporal and directional variation of the concentrations, which may help determine the emission sources responsible for air quality at a given point.

In the case of Krakow, unfavorable meteorological and orographic conditions cause stagnation of the air in the cite center. These factors contribute greatly to poor air quality episodes (e.g., large PM_{10} air concentrations) throughout the year resulting from the activity of various emission sources (mainly from the residential sector in the heating season and from road transport). Compared to other substances, in the case of NO_2 levels, the seasonal variation is not as significant. However, a strong weekly and daily variability of NO_2 concentrations is noticeable, which points to the fact that it is associated with traffic volume. Furthermore, in the area of urban traffic station, located in street canyon and exposed to very heavy traffic, the levels of PM_{10} and NO_2 are significantly higher compared to the urban background station. It was demonstrated that OSPM system can be successfully used to assess temporal variability of concentrations within street canyons.

Concentration trends against wind speed and direction revealed that Krakow is struggling with poor air quality especially during episodes of calm winds and the inflows from south and southwest. Simultaneously, stronger winds from northern directions contribute to periodic dilution of air pollutants and improvement of ventilation conditions in the city. These findings were confirmed by the CWT analysis, indicating that air masses inflowing from the southern directions are the most polluted in terms of PM_{10}. To some extent, this may be explained by the influx of fine particles from areas at greater distances from Krakow, including those beyond Polish borders. This statement, however, requires more detailed research regarding modeling of backward trajectories for selected episodes, greater number of starting locations with more accurate meteorological data.

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