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The impact of data assimilation into the meteorological WRF model on birch pollen modelling

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HIGHLIGHTS

GRAPHICAL ABSTRACT

- Data assimilation to WRF model reduces bias for air temperature.
- Small bias in air temperature leads to too early start of emissions.
- Data assimilation modifies the temporal distribution of emissions and pollen sums.
- Application of the emission scaling factor does not improve the season start/ end.

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ABSTRACT

We analyse the impact of ground-based data assimilation to the Weather Research and Forecasting (WRF) meteorological model on parameters relevant for birch pollen emission calculations. Then, we use two different emission databases (BASE – no data assimilation, OBSNUD – data assimilation for the meteorological model) in the chemical transport model and evaluate birch pollen concentrations. Finally, we apply a scaling factor for the emissions (BASE and OBSNUD), based on the ratio between simulated and observed seasonal pollen integral (SPIn) to analyse its impact on birch concentrations over Central Europe. Assimilation of observational data significantly reduces model overestimation of air temperature, which is the main parameter responsible for the start of pollen emission and amount of released pollen. The results also show that a relatively small bias in air temperature from the model can lead to significant differences in heating degree days (HDD) value. This may cause the

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HDD threshold to be attained several days earlier/later than indicated from observational data which has further impact on the start of pollen emission. Even though the bias for air temperature was reduced for OBSNUD, the model indicates a start for the birch pollen season that is too early compared to observations. The start date of the season was improved at two of the 11 stations in Poland. Data assimilation does not have a significant impact on the season's end or SPIn value. The application of the SPIn factor for the emissions results in a much closer birch pollen concentration level to observations even though the factor does not improve the start or end of the pollen season. The post-processing of modelled meteorological fields, such as the application of bias correction, can be considered as a way to further improve the pollen emission modelling.

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1. Introduction

Birch is a strong allergy-provoking tree with a European populationwide sensitisation that ranges from 8 to 16% (Biedermann et al., 2019). In a Polish epidemiological study, positive skin prick tests with birch pollen allergens were recorded in 14.9% of the representative population (Samoliński et al., 2014). Birch tree produces a huge amount of light pollen which can widely spread in the air (Puc et al., 2015). The mean daily concentration of birch pollen in Poland can often exceed 2000 (incidentally even 4000) pollen grains per cubic meter of air (grains m⁻³) (Myszkowska et al., 2021), whereas the first allergic symptoms for sensitive people in Poland can already occur at 20 grains m⁻³ (Rapiejko et al., 2004). Moreover, cross reactivity between birch and alder (Negrini, 1992) and also for certain fruits like apples, pears, and peaches has been proven (Berrens et al., 1990).

An increasing trend in pollen allergy in Europe, which was noted by Warm et al. (2013), Linneberg et al. (2000), and Kurganskiy et al. (2021), can be related to climate change and increasing temperature. Frei and Gassner (2008) noted that earlier flowering connected with increase in temperature is visible for birch. Bruffaerts et al. (2018) confirmed an increasing trend in birch pollen concentration in the air which can be connected to change in meteorological parameters, such as temperature, precipitation, and relative humidity. Sum of average daily temperatures is one of the most important weather variables influencing the start of pollen as the tree has to accumulate thermal energy to initiate flowering (Myszkowska, 2013; Severova and Volkova, 2017). Before flowering start, a chilling period is necessary to break the dormancy of the bud (Newnham et al., 2013; Severova and Volkova, 2017). Once the flowering has started, daily average temperature, wind speed and precipitation are the most important parameters influencing the count of birch pollen in the air (Khwarahm et al., 2014; Linkosalo et al., 2010). A study for south-west Poland has shown that warm, sunny and dry weather is connected with the highest pollen emissions and concentrations of birch and alder (Ojrzyńska et al., 2020).

Birch (Betula) is a tree which is most frequently represented in Poland by two species: *Betula pendula* and *Betula pubescens* (Puc et al., 2015), with a prevalence of the latter (Kubik-Komar et al., 2019). In a routine pollen observations Betula is treated without separation of species. Recent study of Depciuch et al. (2018) based on microscopy images has shown that the pollen grains of *Betula pendula* and *Betula pubescens* are similar in diameter as well as their results obtained from Fourier transform infrared spectroscopy indicated a similar chemical composition. This confirms that Betula can be treated as one group in the emissions and dispersion modelling.

There are two main methods that allow for estimating concentrations of pollen grains in the air: measurements and numerical modelling. An increasing trend in application of complex Eulerian chemical transport models to airborne pollen modelling has been observed in recent years. These models include a detailed description of physical and chemical processes in the atmosphere as well as the ability to estimate the co-exposure of air pollution and bioaerosols with the same modelling framework. The use of complex models for pollen modelling has been made possible by an enhanced computer processing power as well as development of methods for the preparation of input data to modelling such as coverage of plant species based on satellite (Hościło and Lewandowska, 2019) or lidar data (Bogawski et al., 2019a). Monitoring of Atmospheric Composition and Climate (MACC, http://www. gmesatmosphere.eu) has been the biggest European project which is focused on application of chemical transport models for pollen modelling over Europe (Sofiev et al., 2015b). Recently, the Weather Research and Forecasting model with Chemistry (WRF-Chem) has also been extended towards birch pollen modelling (Werner et al., 2020). The results showed that the model is able to correctly reproduce the main characteristics of the birch pollen season over Central Europe, although simultaneously several places for improvement still exist. For example, the start of the season was calculated too early compared to measurements, while peak pollen concentrations were shifted at some stations, which might suggest problems with meteorological or emissions data.

Previous studies have shown that data assimilation methods can improve meteorological and air pollution modelling (Bocquet et al., 2015; Zhang et al., 2012). Data assimilation is a combination of modelling with observational data. It could be applied with different objectives, i.e. to compute a field as close as possible to the "true" state, to enhance the initial conditions in order to improve forecasts, or to identify uncertain parameters such as the emissions flux (Tombette et al., 2009). In this paper, we focus on assimilation of meteorological data to improve results of the numerical meteorological model and verify the role of meteorological data in birch pollen modelling. We also check the impact of ground-based data assimilation to the Weather Research and Forecasting (WRF) meteorological model on: 1) modelled meteorological parameters relevant for pollen emissions, 2) calculations of heating degree days (HDD), and 3) birch pollen emission calculations. HDD is an important parameter as its threshold value determines the start date of pollen emissions. Second, we use two emission databases (one based on meteorological data without data assimilation (BASE), and another based on meteorological data with assimilation of observations (OBSNUD)) in a chemical transport model to analyse any further impact on birch pollen concentrations. Although the assimilation of meteorological data is a widely used method for improving meteorological and air pollution model performance (Bocquet et al., 2015), its impact on pollen modelling has not been previously considered. This is the first study which analyse the impact of observational data assimilation to meteorological model on pollen emissions modelling and in consequence also on calculations of the start/end of the season and pollen concentrations. Taking into account a significant increasing trend in the application of numerical models for pollen modelling, this task is important for further development and improvement of pollen modelling results. Finally, we applied a scaling factor for the emissions, based on the ratio between simulated and observed seasonal pollen integral, as previously used by Kurganskiy et al. (2020) for northern Europe and run additional simulations with the chemical transport model. We verify the impact of application of the scaling factor for the emission data on birch pollen dispersion modelling. Through this we also check which characteristics of the pollen season i.e. the start and end date of the season or pollen concentrations can be improved by the incorporation of pollen data in pollen source maps.

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2. Data and methods

2.1. Calculations of meteorology and birch pollen emissions and concentrations

2.1.1. Meteorology

Meteorological data was calculated using the Weather Research and Forecasting model version 4.2.1 (Skamarock et al., 2019). WRF is an open-source community mesoscale numerical weather prediction system design to apply to both meteorological research and weather prediction needs. The effort to support and maintain WRF is led by the National Center for Atmospheric Research (NCAR). The model source code is available at the WRF users' page (https://www2.mmm.ucar. edu/wrf/users/download/get_source.html).

In our study, the WRF model was run over Europe, with a spatial resolution of $12 \text{ km} \times 12 \text{ km} (285 \times 332 \text{ grids})$ and 35 vertical levels. Physics options included the Morrison double-moment scheme for microphysics, RRTMG (Rapid Radiative Transfer Model for General Circulation Models) scheme for longwave and shortwave radiation, ETA similarity scheme for the surface layer, Noah Land Surface Model, and the Mellor-Yamada-Janjic scheme for the planetary boundary layer. For cumulus parameterization, Grell 3D scheme was applied, with subsidence spreading turned on. The model was driven by the National Center for Environmental Prediction (NCEP) Final Analysis (FNL) Operational Global Analysis data with a horizontal resolution of 10×10 , 32 vertical levels, and a temporal resolution of 6 h. A similar configuration, but for WRF model version 3.8.1, was used earlier by Werner et al. (2018).

Earlier studies with the WRF model for this area have shown that the air temperature at 2 m is biased, e.g. it was underestimated for winter and overestimated for the spring and summer months of 2015 (Werner et al., 2018). Similar findings have been reported for the 1981–2010 period by Kryza et al. (2017). Pilguj et al. (2019) have shown that the assimilation of additional meteorological data may improve initial conditions and reduce bias in the modelled air temperature.

This bias in the WRF-modelled air temperature might be important for the accumulated values of air temperature, which are used to trigger the pollen emission in this study. This is why we have run two simulations with the WRF model. First, we run the model using only gridded NCEP FNL data for initial and boundary conditions (BASE run). Second, we run the model with the observational nudging option turned on (OBSNUD), with the aim of reducing the bias, especially for air temperature that triggers pollen emission.

Observation nudging is a technique in which artificial tendency terms are introduced into the model to "nudge" the model towards observations (Deng and Stauffer, 2006; Reen, 2016). Nudging belongs to the group of the four-dimensional data assimilation (FDDA) techniques, in which observations are used continuously throughout a model run, and not only at the initial phase (Deng and Stauffer, 2006). Recent findings presented by Yi et al. (2020) have shown that this technique may improve the simulation of surface meteorological variables, including air temperature, wind speed and humidity.

For the OBSNUD model run, observation nudging was turned on for air temperature (T2), moisture (RH), and wind components (WS). Observation data were taken from the NCEP Automated Data Processing (ADP) global surface observational weather data which include land and marine surface reports received via the Global Telecommunications System.

2.1.2. Birch pollen emission

Birch pollen emission was calculated based on the heating degree days (HDD) threshold parameterization method, which was originally described by Sofiev et al. (2013). First, we calculated the sum of daily temperature above a cut-off level (3.5 °C) from the 1st of March. If the calculated sum exceeded the temperature sum thresholds at any grid in the domain, the emission model would then start the emissions' calculation. The temperature sum threshold has been indicated based on the European phenological data (the date of the leaf unfolding) as

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described in Sofiev et al. (2013). We emphasize here that the start of emissions is distinct from the start of the pollen season which is indicated based on pollen concentrations. A release flux of pollen grains was dependent on hourly temperature. Additionally, wind speed, relative humidity and precipitation rate threshold values are used to correct the amount of released pollen (Sofiev et al., 2013). The calculated emission was multiplied by the fraction of the birch forest for each grid cell provided by the European Forest Inventory (EFI, https://www.efi.int/ knowledge/maps/treespecies). The end of the season is described via the open-pocket principle: the flowering continues until the initially available amount of pollen is completely released (Sofiev et al., 2013). A detailed description of the emission calculation procedure is given in Werner et al. (2020). The calculations were carried out using R 4.0.2 (R Core Team, 2021), the raster and ncdf4 packages. We used hourly meteorological data from the WRF model to feed the calculation of emissions. Following two meteorological model runs, the emission files were prepared in two versions - BASE (meteorological data from the WRF model with no observational data assimilation) and OBSNUD (meteorological data from the WRF model with assimilation).

2.1.3. Birch pollen concentrations

The Weather Research and Forecasting model with Chemistry (WRF-Chem, version 4.2.1) was used to estimate the impact of two emission data (BASE and OBSNUD) on modelled birch concentrations. WRF-Chem is an open-source tool that is widely used to study atmospheric chemistry, air quality, and aerosols. The development of WRF-Chem is a collaborative effort among the community. NOAA/ESRL (National Oceanic and Atmospheric Administration/Earth System Research Laboratories) scientists are the leaders and caretakers of the code which is available at https://ruc.noaa.gov/wrf/wrf-chem/. A long list of recent applications of WRF-Chem to study aerosols and their impact on air quality, climate at the regional scales and to analyse dust outbreaks is given in Ukhov et al. (2020). The model has been widely used for calculating air pollution concentrations in a re-analysis and forecasting mode in many countries around the world (Baklanov et al., 2014). The first application of WRF-Chem for bioaerosols modelling has been described in Werner et al. (2020), and that study includes a full description of the model parameterisation used. The birch pollen was included in the Goddard Chemistry Aerosol Radiation and Transport (GOCART) bulk aerosol scheme. The GOCART module includes algorithms for dry deposition and gravitational settling (Legrand et al., 2018; Ukhov et al., 2020). The gravitational settling parameterization is based on the calculation of settling velocity, which depends on the particle density and size. The wet deposition parameterization is based on the Jung scheme (Tsarpalis et al., 2018) and includes both in-cloud (rainout) and below-cloud (washout) scavenging. The computational domain covered the same area as the meteorological simulations with WRF (Fig. 1). We run two simulations with the WRF-Chem model, BASE and OBSNUD, which used emission based on WRF data without and with data assimilation, respectively.

Additionally, we calculated the relation between SPIn value from the WRF-Chem run and observations as previously suggested by Kurganskiy et al. (2020). We used this relation to scale the birch pollen emission. The scaled emission was then used for the last two runs with the WRF-Chem model – BASE_SPI and OBSNUD_SPI.

The simulations were started on 20 March 2019, which was two weeks before the season's start as indicated by aerobiological observations in Poland, and ended on 30 May 2019 (more than 3 weeks after the end of the seasons as calculated from observations).

A workflow showing the main steps of our study is shown in Fig. 1S.

2.2. Evaluation of the model results

2.2.1. WRF model results and emission model

The WRF model meteorological simulations (BASE and OBSNUD) were compared with observational data of T2, RH, and WS from 1

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Fig. 1. Simulation domain and the location of pollen stations in Poland used for the model evaluation.

March 2019 to 31 May 2019, which covered a period from the start of the temperature's accumulation for emissions' calculations till the end of the birch pollen modelling. The observational data at a 6-hour temporal resolution were made available from climatological stations of the Institute of Meteorology and Water Management National Research Institute (IMWM NRI). It should be emphasized that the location of these stations is different from that of stations used for the data assimilation. It comprised 64 stations for T2, 49 stations for WS, and 25 stations for RH. We calculated the standard statistical measures of model performance based on all stations for both simulations. The statistics were summarised in a table, while MB and IOA were plotted in maps to assess their spatial variability. Definitions of the statistics are given in Table 1.

Additionally, for each of the climatological stations, heating degree days were calculated from two WRF model runs (BASE and OBSNUD) and from observational data. Modelled and measured cumulated HDD time series were compared by calculating the statistic measures. The statistics were calculated for two periods: 1) from the start of T2 accumulation till the start of the season as indicated from observations (1 March–10 April), 2) for the start of the season as indicated from observations (4–10 April, season started at 90% of stations in this period).

For the locations of pollen stations, we compared the time series of birch pollen emissions based on meteorological data with and without data assimilation.

2.2.2. Birch pollen concentrations

The measured daily birch pollen concentrations from 11 stations for 2019 (Fig. 1) were provided by the Allergen Research Centre and cooperating university centres in Poland. Comparing SPIn for different

Table 1

Definitions of error statistics used in the study. O refers to observed values and P refers to predicted values.

Name	Formula	Range of values	Expected value
Mean bias (MB)	$MB = \frac{1}{N} \Sigma_1^N (P_i - O_i)$	[−Ō, +∞]	0
Normalized mean bias (NMB)	$NMB = \frac{\sum_{i=1}^{N} (P_i - O_i)}{\sum_{i=1}^{N} O_i}$	[−1, +∞]	0
Mean gross error (MGE)	$MGE = \frac{1}{N} \sum_{i=1}^{N} P_i - O_i $	[0, +∞]	0
Normalized mean gross error (NMGE)	$NMGE = \frac{\sum_{i=1}^{N} P_i - O_i }{\sum_{i=1}^{N} O_i}$	[0, +∞]	0
Pearson correlation coefficient (R)	$R = \frac{\sum_{i=1}^{N} (P_i - \overline{P}) (O_i - \overline{O})}{\left\{\sum_{i=1}^{N} (P_i - \overline{P})^2 \sum_{i=1}^{N} (O_i - \overline{O})^2\right\}^{\frac{1}{2}}}$	[-1, 1]	1
Index of agreement (IOA)	$IOA = 1 - \frac{\sum_{i=1}^{N} (P_i - O_i)^2}{\sum_{i=1}^{N} (P_i - \overline{O} + O_i - \overline{O})^2}$	[0, 1]	1

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Table 2

Mean statistics based on WRF modelled (BASE and OBSNUD) and observed meteorological parameters from Polish climatological stations available at 6 h temporal resolution over Poland for the period March 1–May 31, 2019.

	MB	NMB	MGE	NMGE	IOA
T2 BASE	0.80	0.13	1.85	0.24	0.95
T2 OBSNUD	0.48	0.09	1.38	0.19	0.98
RH BASE	0.99	0.03	11.39	0.18	0.84
RH OBSNUD	1.40	0.03	10.28	0.16	0.87
WS BASE	1.83	0.95	2.12	1.04	0.66
WS OBSNUD	1.91	0.99	2.18	1.07	0.67

For MB and MGE, the units are $^\circ C$ for T2, % for RH2, m s-1 for WSPD. NMB, NMGE and IOA are unitless.

Polish stations for the year 2019 with long-term values provided by Myszkowska et al. (2021) (years 1991–2018 for Kraków) or Grewling et al. (2012) (years 1996–2010 for Poznań) indicates that the year 2019 is characterised high birch pollen concentrations in Poland. At all stations, pollen data were collected with the use of Burkard 7-day volumetric pollen trap (Hirst 1952) and counted according to the guidelines of the International Association of Aerobiology (Galan et al., 2014). Pollen were counted for four longitudinal transects under a light microscope with 400 magnification and expressed as a daily mean value (Galán et al., 2017).

The modelled hourly birch pollen concentrations were aggregated into daily mean values for comparison with observations over Poland. To validate the modelling results, we compared modelled and measured values of the primary parameters describing the season, i.e. its start and Science of the Total Environment xxx (xxxx) xxx

end as well as the seasonal pollen integral (SPIn). The start and end of the season were calculated as the dates when 5% and 95% of the cumulative seasonal pollen sums of the observed pollen concentrations were respectively reached. The SPIn was calculated as the sum of daily pollen concentrations over the whole birch pollen season (Galán et al., 2017).

We also plotted the Taylor diagram to verify the model performance for birch pollen concentrations for four model runs (BASE, OBSNUD, BASE_SPI and OBSNUD_SPI). The Taylor diagram provides a concise statistical summary of how well patterns (in this case birch pollen concentrations) match each other in terms of their correlation, their root mean square difference, and the ratio of their variance (Taylor, 2001).

3. Results

3.1. The WRF model performance

Comparison of meteorological WRF model simulations (BASE – simulation without data assimilation, OBSNUD – simulation with data assimilation) with observations from Polish climatological stations for the period March 1, 2019 to May 31, 2019 is shown in Table 2. Statistics presented in the table aim to show if surface data assimilation to the meteorological model (OBSUND run) improves meteorological variables, which are relevant for pollen modelling. The results show that the assimilation of meteorological parameters to the WRF model mostly improves model performance. For temperature, the model tends to overestimate observed values for both simulations but the mean bias decreased from 0.80 °C for BASE to 0.48 °C for OBSNUD, while simultaneously MGE decreased from 1.85 °C to 1.38 °C. IOA is high (\geq 0.95) for both model runs. Spatial distribution of MB indicates that only in the



Temperature

Fig. 2. Spatial distribution of MB and IOA for the BASE (upper) and OBSNUD (lower) simulation for T2 for 1 March-31 May 2019. In the background - seasonal mean T2 for the BASE (upper) and OBSNUD (lower) simulation.

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mountainous region of southern Poland and at three stations in northern Poland does BASE run predict lower temperatures than observations (Fig. 2). For other stations, MB is close to or above 0. MB was improved for stations in northern Poland and partially for those in central Poland for the OBSNUD run compared to BASE. As a whole, MB for temperature was improved at 80% of stations for the OBSNUD simulation. IOA for the BASE run is slightly lower for stations in southern Poland (IOA < 0.97) compared to other areas; however, it was improved for the OBSNUD run for which at 95% of stations, IOA is above or equal to 0.97.

The MB for relative humidity is positive – it worsened from 0.99% for BASE to 1.40% for OBSNUD, while simultaneously MGE and IOA improved for OBSNUD compared to BASE (MGE changed from 11.95% to 10.09%). The MGE for both simulations is significantly higher than MB which, in relation to the positive MB, indicates that there are several stations for which the model underestimates the observed relative humidity. The spatial distribution of MB for BASE and OBSNUD shows that underestimation occurs mainly in central Poland in the belt from west to east of the country (Fig. 3). At most of the stations, IOA is above 0.82 for both simulations but with lower values in the mountainous area (0.82–0.88) compared to other regions (IOA mainly above 0.89).

Wind speed is overestimated by the model with slightly worse MB for OBSNUD (1.91 m s⁻¹) compared to BASE (1.83 m s⁻¹). In general, the highest overestimation and lowest IOA concern the mountainous region (Fig. 4). In this area, MB is above 1.91 m s⁻¹ while IOA is usually below 0.56 for both simulations.

3.2. Impact of data assimilation on HDD and emissions' calculations

The sums of daily temperature above the cut-off level (3.5 °C, called HDD) for each day of the period March 1–April 10 were calculated based

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on data from observations and from two model runs. The mean statistics for all stations based on cumulated HDD time series are shown in Table 3. For the BASE run, MB is below zero (MB = -1.55), which indicates that on average (for the location of meteorological stations) the model obtains the threshold value for the birch pollen emission start later than observations. For the OBSNUD run, MB is above zero while the absolute value is lower (MB = 0.71) than for BASE. The index of agreement is similar for both simulations at 0.89 and 0.90 for BASE and OBSNUD, respectively. The mean statistics of HDD for the starting period of birch pollen in Poland are shown in Table 4. Both simulations indicate overestimation of the measured HDD by the model with MB at 4.65 °C and 6.67 °C, respectively. The HDD value in the starting period of birch pollen has a direct impact on the start of pollen emission and in consequence on the start of the pollen season as well.

The time series of HDD for different locations in Poland are presented in Fig. 5. The plots indicate a significant variability between the stations. For some stations, HDD for BASE is below HDD for observations, e.g. Borucino and Olecko. For other stations, HDD for BASE, or both BASE and OBSNUD, is above observations (e.g. Jarocin, Jastrzębia), which might cause too early a start for birch pollen emissions.

Birch pollen emission, based on meteorology without BASE and with OBSNUD data assimilation, was calculated for the location of pollen stations (11 locations in Poland). The mean and maximum value (for all stations) for both BASE and OBSNUD emission is similar. The mean value is 22.3 and 22.2 μ g m⁻² h⁻¹ and the maximum is 574.2 and 541.9 μ g m⁻² h⁻¹ for BASE and OBSNUD, respectively. For most of the stations (nine out of eleven), the BASE emission is higher than OBSNUD. The difference for individual stations does not exceed 8%. The highest is for Opole – about 8% lower for OBSNUD compared to BASE. The mean correlation coefficient between BASE and OBSNUD emissions is 0.92,



Relative humidity

Fig. 3. Spatial distribution of MB and IOA for the BASE (upper) and OBSNUD (lower) simulation for RH for 1 March-31 May 2019. In the background - seasonal mean RH for the BASE (upper) and OBSNUD (lower) simulation.

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Fig. 4. Spatial distribution of MB and IOA for the BASE (upper) and OBSNUD (lower) simulation for WS for 1 March-31 May 2019. In the background - seasonal mean WS for the BASE (upper) and OBSNUD (lower) simulation.

and varies from 0.88 for Kraków to above 0.95 for Łódź, Bydgoszcz, and Zielona Góra.

The time series of BASE and OBSNUD emissions are presented in Fig. 6. It is worth pointing out that for some stations (Warszawa, Białystok, Bydgoszcz), OBSNUD gives higher emissions for the first days of the season compared to BASE but are simultaneously lower in the last days of the season, which is probably a consequence of an open pocket method used in the calculation of emissions.

3.3. Impact of data assimilation on the WRF-Chem model performance for birch pollen concentrations

Both modelled (BASE and OBSNUD) and observed characteristics (season start, end, and SPIn) of the birch pollen season in Poland in 2019 are summarised in Table 5. According to observations, the 2019 birch pollen season started from April 4 (western Poland) to April 18 (north-eastern Poland). Both model runs (BASE and OBSNUD) indicate a season start earlier than observations at all stations. The mean difference between model and observations is about 8–9 days for both

Table 3Mean statistics for HDD based on daily T2 from WRF model (BASE and OBSNUD) and observations for the period March 1–April 10, 2019.

	MB	NMB	MGE	NMGE	R
HDD BASE	-1.55	-0.03	8.23	0.14	0.97
HDD OBSNUD	0.71	0.01	7.53	0.13	0.97

For MB and MGE the units are °C. NMB, NMGE and IOA are unitless.

model runs. The start of the season did not change for OBSNUD compared to BASE at 8 stations and improved at 2 stations. For Wrocław and Opole, both located in south-western Poland, the difference in the number of days between the model and observations for the start day decreased by two days and one day, respectively. There is one station (Białystok, north-east Poland) for which the difference increased by one day.

At all stations, the BASE and OBSNUD runs indicate a later end of the season than observations, and the mean difference between the models and observations is 7–8 days. The date of the season's end did not change between the BASE and OBSNUD model run at 10 stations and worsened for Szczecin in north-west Poland. Both simulations highly overestimated the observed SPIn. The modelled SPIn is usually 3–4 higher than observations for the BASE run and 4–5 times higher for the OBSNUD run.

A comparison of the main pollen season's characteristics for two model runs shows that at most of the stations (8 out of 11), the day of start and end of the season did not change between BASE and OBSNUD, whereas there was improvement in stations located in southern Poland.

Table 4

Mean statistics for HDD based on daily T2 from WRF model (BASE and OBSNUD) and observations for the period April 4-April 10, 2019.

	MB	NMB	MGE	NMGE	R
HDD BASE	4.65	0.04	14.29	0.11	0.89
HDD OBSNUD	6.67	0.05	14.25	0.11	0.89

For MB and MGE the units are °C. NMB, NMGE and IOA are unitless.

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Fig. 5. Time series of heating degree days (daily temperature above 3.5 °C from March 1st) for example stations in northern (Borucino, Olecko), central (Legionowo, Jarocin, Jastrzębia) and southern (Tarnów) Poland. Black horizontal line (HDD = 85) shows mean HDD threshold (value for which birch pollen emission starts) for Poland.

Modelled (BASE & OBSNUD) and observed time series of birch pollen concentrations are shown in Fig. 7. The WRF-Chem model represents the main peaks but highly overestimates the measured birch pollen concentrations, especially for stations in northern Poland (Bydgoszcz, Białystok).

3.4. Impact of SPIn factor for emissions on the WRF-Chem model's performance for birch pollen concentrations

The application of the scaling factor for the emissions (BASE and OBSNUD) had a great impact on SPIn calculated from the WRF-Chem model. The overestimation of birch pollen concentrations was significantly reduced. The mean for all stations' ratio between SPIn from OBSNUD_SPI and observations is close to 1, and for most of the stations it is between 0.7 and 1.1, which is much better compared to the OBSUND run (SPIn was overestimated by 4-5 times for most stations, Table 5). This mean ratio for the SPIn value is equal to 0.9 and 6.9 for the BASE_SPI and BASE simulation, respectively. Simultaneously, the application of the scaling factor for emissions increased the distance between the modelled and observed start of the season - for instance for half of the stations, the start was calculated 1-2 days earlier for the OBSNUD_SPI compared to the OBSNUD run. The end of the season only changed at one station for BASE_SPI and OBSNUD_SPI compared to the runs without the SPI factor. The time series of birch pollen concentrations for the BASE_SPI and OBSNUD_SPI run are much closer to the measured values compared to the BASE and OBSNUD simulation; however, the main peak in the season is lower than that observed at most of the stations, although these are usually resolved (Fig. 7).

The Taylor diagram (Fig. 8) indicates higher correlation coefficient (R at a level of 0.5) for the simulations with SPI factor included,

compared to the BASE and OBSNUD run (R at a level of 0.4). It also shows that the variance of the modelled birch pollen concentrations for the BASE_SPI and OBSNUD_SPI is closer to the observed variance, compared to the simulations without SPI factor.

4. Discussion

The meteorological WRF model results show that the model has a tendency to overestimate observed temperature (MB at 0.80 °C for BASE) and wind speed (MB at 1.83 m s⁻¹ for BASE) for Poland for the period March–May 2019. This accords with long-term high-resolution WRF simulations for Poland, covering the years 1981–2010. The simulations have shown that the model overestimates temperature for the warm season (April–October), and underestimates it for winter (December, January, February). March and November have shown a mean error close to zero (Kryza et al., 2017).

The quality of WRF-simulated temperature over north and Central Europe in the context of its impact on the uncertainty of biological models has been evaluated by Skjoth et al. (2015). They have found that the bias in temperature is statistically grouped in two areas: continental- and marine-influenced. The best results have been obtained in areas that are influenced by a maritime climate (e.g. UK, parts of France, Germany) for the period of January–June, while a significant positive bias in Central Europe (exceeding 2.0 °C) has been found. They have also indicated some improvement due to an increase in grid resolution from 36 to 12 km while emphasizing the unresolved issues in the surface processes, such that the applications of temperature data in biological models require the post-processing of the simulated temperature fields. We refer to this issue in our study, not by the post-processing of simulated fields but by the assimilation of observational data to the model with the aim of also bringing the model closer to

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measurements. The abovementioned studies have also shown that a meteorological model has to be tested and verified for a study area, as the results can vary for different geographic areas, even with the same model setups and parameterisations.

Bias in modelled temperature will affect pollen modelling. Many studies indicate that meteorology is the main factor influencing pollen seasons. The impact of meteorological data and other environmental parameters on a pollen season characteristic has recently been summarised by (Robichaud and Comtois, 2021; Schramm et al., 2021). Their general conclusions are that warmer temperatures contribute to an earlier start of the pollen season, lengthen the pollen season, augment the quantity of emitted pollen, and increase pollen allergenicity.



Fig. 6. Time series of modelled emissions [µg m⁻²] for the BASE and OBSND simulations for the locations of pollen observational stations for the season 2019. Please notice different scales for y-axis.

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Fig. 6 (continued).

However, a study by Schramm et al. (2021), which was based on an analysis of more than 90 pollen papers, emphasized that different relations between meteorology and pollen are found when considering different stations. For instance, they found that the start date of the main pollen season was the indicator with the most frequent correlation with temperature. A majority of the analysed papers found significant negative correlations between the main pollen season's start date and temperature (78 of 122 analyses), indicating that earlier pollen seasons were correlated with warmer temperatures. However, it simultaneously shows that for 44 studies (out of 122) the dependence was opposite. They also reported that a majority of these papers found a positive correlation between temperature and average daily pollen concentrations, which suggests that higher daily pollen concentrations occur with warmer temperatures.

Our analysis shows that assimilation of meteorological observations to the WRF model improves modelled meteorological parameters, especially for air temperature. The mean bias was reduced from 0.80 °C (BASE) to 0.48 °C (OBSNUD) and mean gross error from 1.85 (BASE) to 1.38 (OBSNUD). The spatial distribution of errors for air temperature indicates that the improvement concerns most of the stations in northern and central Poland, while in total the improvement concerns 80% of all stations. An increased value in the mean error (poorer results) for air temperature after data assimilation appears in southern Poland in the mountainous region. It concerns area for which we have stations with over- and under-estimations by the model in a close distance to each other. A similar situation has been reported by Werner et al. (2019) for the assimilation of air pollution observations in WRF-Chem. They have shown that a local decrease in model performance for PM2.5 concentrations can appear when a station with a mean bias close to zero is surrounded by stations with relatively high underestimations of measured PM2.5 concentrations.

The consequence of changes in meteorological parameters is changes in birch pollen emissions. The accumulated value of air temperature directly affects the moment of the emission start for an individual grid. When emission starts, air temperature then affects the number of pollen grains that is emitted into the atmosphere. Other parameters, Science of the Total Environment xxx (xxxx) xxx

such as wind speed, relative humidity and rainfall, are also used in the emission calculations but they contribute as threshold values, above/ below which the emission is higher/lower or is stopped (Sofiev et al., 2013). For instance, the threshold values for relative humidity are 50% and 80%. Until these thresholds are reached, this variable neither affects nor promotes the release, whereas near the threshold, the piecewise linearly decreasing transition function is used. Therefore, data assimilation for relative humidity or wind speed might have a lower impact on pollen emission compared to air temperature.

The results also show that a relatively small bias in air temperature from the model leads to significant differences in the value of heating degree days. This causes the HDD threshold to be reached several days earlier than indicated from observational data which has a further impact on the start of pollen emission.

A reduction in air temperature bias through data assimilation directly affects the total amount of pollen released as well as the temporal distribution of emission. The highest difference in mean emissions for individual stations between OBSNUD and BASE reaches 8%. For most of the stations, BASE emission is higher than that for OBSUND which is probably related to a higher air temperature for the BASE run.

As we cannot directly evaluate the emission results (no emission measurements available), we use the WRF-Chem chemical transport model and compare modelled pollen concentrations with observations. This is a standard procedure used, e.g. for the assessment of anthropogenic emission databases in air pollution modelling (e.g. Denier Van Der Gon et al., 2015; Kryza et al., 2020). The WRF-Chem results show that the BASE run indicates an earlier start of the season than observations with a mean difference of 8-9 days for the year 2019. Even though the bias for air temperature was reduced for OBSNUD, the model indicates a too-early start of the birch pollen season compared to observations. The start date of the pollen season was improved at two stations in south-western Poland. Meteorological stations located close to this area indicate one of the highest reductions of MB for T2 for the OBSNUD compared to the BASE simulation. MB decreased there by about 0.5 °C, whereas the average reduction of MB for all stations was about 0.3 °C. This indicates that further reduction of T2 bias might improve the pollen modelling results. Assimilation of data from a bigger number of surface stations (in this study we used one set of stations for assimilation and second for validation) or application of satellite data might be one of the ways for the further improvement of modelled T2.

Our results for the year 2019 shows that the model (without SPIn factor for emissions) has a tendency to overestimate measured birch pollen concentrations despite the fact that the year 2019 characterised with relatively high observed birch pollen concentrations. On the other hand, the modelled birch pollen concentrations reached the observed level of concentrations after application of SPIn emission, which confirms the role incorporation of pollen data in source maps as proposed by Kurganskiy et al. (2020). Simultaneously, however, we have to say that the application of the scaling factor worsens prediction

Table 5

Modelled and observed date	of start end	and SPIn of the birch	pollen season for th	e vear 2019
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City	Start of the pollen season					End of	End of the pollen season				SPIn				
	OBS	BASE	OBSNUD	BASE_SPI	OBSNUD_SPI	OBS	BASE	OBSNUD	BASE_SPI	OBSNUD_SPI	OBS	BASE	OBSNUD	BASE_SPI	OBSNUD_SPI
Bialystok	18.04	02.04	01.04	31.03	31.03	6.05	22.04	20.04	23.04	21.04	7348	206,932	275,786	14,957	22,267
Bydgoszcz	9.04	30.03	30.03	30.03	30.03	2.05	22.04	22.04	22.04	22.04	22,555	109,413	141,264	16,369	20,290
Kraków	5.04	29.03	29.03	28.03	28.03	27.04	26.04	26.04	26.04	26.04	16,649	66,371	70,545	10,983	11,422
Łódź	8.04	30.03	30.03	29.03	29.03	30.04	21.04	21.04	21.04	21.04	30,080	110,898	122,909	18,091	19,108
Lublin	9.04	31.03	31.03	31.03	31.03	29.04	21.04	21.04	21.04	24.04	26,919	139,161	145,617	18,661	20,086
Opole	5.04	27.03	29.03	25.03	25.03	28.04	22.04	22.04	22.04	22.04	20,392	99,684	102,791	17,884	18,122
Sosnowiec	9.04	28.03	28.03	27.03	27.03	1.05	22.04	22.04	22.04	22.04	15,864	105,122	109,266	17,039	17,444
Szczecin	4.04	30.03	30.03	30.03	30.03	29.04	29.04	22.04	26.04	22.04	17,527	116,211	124,897	18,606	19,582
Warszawa	8.04	30.03	30.03	30.03	30.03	1.05	21.04	21.04	21.04	21.04	31,103	135,291	163,392	19,017	22,058
Wrocław	4.04	27.03	28.03	25.03	27.03	30.04	22.04	22.04	22.04	22.04	21,609	84,062	93,843	15,453	16,473
Zielona Góra	4.04	29.03	29.03	29.03	29.03	30.04	22.04	22.04	22.04	25.04	26,568	97,205	103,587	19,257	19,745



Date

Fig. 7. Time series of modelled and measured daily birch pollen concentrations for Poland for the season 2019. Please notice different y-scale for Warszawa, Białystok and Bydgoszcz.



Fig. 8. Taylor plot for daily birch pollen concentrations for Poland for the season 2019.

results for the start of the season – for instance the difference between the model and observations increased by 1–2 days for 6 stations for OBSNUD_SPI compared to the OBSNUD run.

Previous studies have shown that a model performance can vary a lot for different stations as well as different years of simulations (Sofiev et al., 2015a; Werner et al., 2020). Therefore it is not straightforward to compare results from different model runs. Validation of chemical transport models for birch pollen over Europe for the year 2013 has been done by Sofiev et al. (2015a). They showed the results for six individual models and for the ensemble approach based on comparison of the modelled concentrations with observations from 11 European countries (mainly western Europe and some stations in north-eastern Europe). The correlation coefficient (mean for all stations) for individual models varied from 0.28 to 0.41, while the mean from all models was equal to 0.38, which is comparable to our results for the BASE and OBSNUD run (correlation around 0.4) and lower compared to the BASE_SPI and OBSNUD_SPI (correlation around 0.5). Study of Kurganskiy et al. (2020) with Enviro-HIRLAM model over Europe for 2006 (comparison for stations in Finland, Russia, and Denmark) indicated correlation coefficient varied from 0.42 to 0.71 depending on the source map used in the simulations and the correlation was higher for simulations with SPI scaling factor applied. Their analysis has not revealed a significant dependency of the start/end of the birch pollen season on the underlying pollen source map, which is also confirmed by our results. We also have to emphasize that there are other parameters, besides meteorology, that influence the amount of pollen as well as the model-measurement performance. Maya-Manzano et al. (2020) showed that for Ireland, an increase in the amount of birch pollen in recent years is related to an increase in forest surface occupied by broadleaved forests as well as the ornamental use of birch in urban areas. A huge potential for mapping forest type and tree species is the application of satellite data. Currently, these data are successfully used to determine the presence of specific species in an analysed area, (e.g. Hościło and Lewandowska, 2019). Further studies will hopefully develop methods that can quantitatively estimate the number of trees (spatial cover) in a grid. Development of new satellite sensors and availability of these data at a high temporal frequency provides also the opportunity to estimate vegetation phenological variables that can be used to characterize the stages of vegetation development during the growing season. The latter can be linked to the flowering phenophase related to pollen release. The success application of satellite data to predict the start and peak of birch pollen season over Europe has been described by Khwarahm et al. (2017) and Bogawski et al. (2019b) and it will be a step forward to incorporate these methods into daily pollen forecasting systems.

5. Summary and conclusions

We used three main modelling tools in this study: 1) meteorological WRF model; 2) emissions model based on meteorology from the WRF model; 3) chemical transport model WRF-Chem. Our first aim was to analyse the impact of the assimilation of surface meteorological data to the WRF model on meteorological variables used in pollen emission calculations and in consequences on birch pollen emissions and concentrations. Finally, we used a scaling factor for the BASE (based on meteorology without data assimilation) and OBSUND (based on meteorology with data assimilation) emissions based on the ratio between simulated and observed seasonal pollen integral, and then analysed its impact on modelled birch pollen concentrations. The study was carried out over Central Europe, Poland for the 2019 pollen season. The results show that:

- The WRF model without data assimilation (BASE) overestimates the air temperature with a mean bias of 0.80 °C. The model well reproduces the relative humidity with MB at 0.99% and IOA at 0.84 while overestimating the wind speed on average by 1.91 m s⁻¹.
- The assimilation of observational data significantly reduces model overestimation of air temperature (MB is reduced to 0.48), which is the main parameter responsible for the start of the birch pollen emission and amount of pollen released during the pollen season. The MB for air temperature was improved for stations in northern Poland and also partially for those in central Poland, an improvement that

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concerned 80% of all stations. The impact of data assimilation on other meteorological parameters, i.e. relative humidity and wind speed, is smaller although simultaneously such parameters have a potentially lower impact on emission modelling (used as the threshold value in the emission model).

- Data assimilation to the meteorological model modifies the temporal distribution of emissions and the total amount of released pollen. The changes in mean seasonal emissions for the individual stations do not exceed 8%. The results show that if the emission model calculates a higher emission at the beginning of the season, then the emissions will be lower in the last days of the season for the same run, probably due to the open pocket method used in the calculation of emissions.
- Even though the bias for air temperature was reduced for OBSNUD, the model indicates a too-early start of the birch pollen season compared to observations. The start date of the pollen season was improved at two out of 11 stations in Poland. Data assimilation has had no significant impact on the calculations of the end of the season or SPIn value.
- The application of the SPIn factor for the emission causes that modelled birch pollen concentrations are much closer to observed values for all pollen stations. However, it does not improve calculations of the start or end of the pollen season.

The results show that a relatively small bias in the modelled air temperature leads to significant differences in the value of heating degree days, which causes the HDD threshold to be reached several days earlier than indicated from observations, thereby leading to a too-early start of the emissions. The post-processing of the modelled meteorological fields, e.g. as suggested by Skjoth et al. (2015) by the application of bias correction, can be considered as a way to further improve the pollen emission modelling.

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CRediT authorship contribution statement

Małgorzata Werner: Conceptualization, Methodology, Software, Investigation, Writing – original draft, Project administration. Daria Bilińska-Prałat: Formal analysis, Investigation, Visualization, Writing – original draft. Maciej Kryza: Methodology, Investigation, Writing – original draft. Jakub Guzikowski: Software. Małgorzata Malkiewicz: Investigation, Writing – review & editing. Piotr Rapiejko: Investigation. Kazimiera Chłopek: Investigation. Katarzyna Dąbrowska-Zapart: Investigation. Agnieszka Lipiec: Investigation. Dariusz Jurkiewicz: Investigation. Ewa Kalinowska: Investigation. Barbara Majkowska-Wojciechowska: Investigation. Dorota Myszkowska: Investigation, Writing – review & editing. Krystyna Piotrowska-Weryszko: Investigation. Małgorzata Puc: Investigation. Anna Rapiejko: Investigation. Grzegorz Siergiejko: Investigation. Elżbieta Weryszko-Chmielewska: Investigation. Andrzej Wieczorkiewicz: Investigation. Monika Ziemianin: Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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