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Modeling of atmospheric air quality in the Tomsk using WRF/CAMx complex

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ABSTRACT

The results of numerical modeling of meteorological parameters and concentrations of small components of atmospheric air Tomsk city obtained using the Weather Research & Forecasting (WRF) and Comprehensive Air quality Model with eXtensions (CAMx) models are presented. Several periods were selected when increased concentrations of pollutants were observed with the TOR-station of the IAO SB RAS to estimate the level of atmospheric air quality in the city based on numerical modeling. For these periods, the values of the Air Quality Index were calculated using the WRF/CAMx complex with using US Environment Protection Agency (EPA) recommendations. The obtained results of the numerical forecast show the possibility of the formation of a high level of air pollution under certine meteorological conditions in the city.

Keywords: Numerical modeling, urban atmosphere pollution, air quality, WRF, CAMx

1. INTRODUCTION

Air quality is a measure of the suitability and safety of the air for breathing. The amount of pollutants contained in the air is one of the objective characteristics of its quality. The World Health Organization regularly updates the air quality assessment guidelines[1]. It distinguishes four classes of pollutants: three gas impurities and aerosols. Gases include O_3, NO_2 and SO_2. The presence of certain aerosol pollutants in the atmosphere can lead to respiratory diseases and toxic poisoning, as well as can cause allergic diseases. Depending on the size, they enter different tissues of the body. The smallest micron and submicron particles PM 2.5 can penetrate the alveolar membrane into the blood and spread throughout the body. Particles slightly larger PM 10 are settled in the lungs and also cause inflammatory reactions.

In general, the level of air pollution in Russian cities depends on a combination of various factors, among which both anthropogenic and natural phenomena are important. Tomsk is one of the cities with a high level of influence of internal anthropogenic sources of pollution. In the background, energy companies, transport, and least of all industry pollute the air in Tomsk, because industry located in the suburbs are represented in small quantities.

The potential for atmospheric pollution[2] (PAP) isn't related directly to the sources of emissions and is determined by the geographical and geological features of the area. If a city is located in a low-lying area with poor air circulation, the state of the atmosphere in it can be unsatisfying even with a small amount of emissions. The state of atmospheric air in such localities is unsatisfactory for a significant part of the year, even in the absence of any harmful industries. This is especially evident in winter during the heating season. Both natural atmospheric phenomena, such as calm conditions, and anthropogenic influences can contribute to the deterioration of air mass circulation. It can be attributed to the incorrect development of cities and suburbs with high-rise buildings[3]. The level of PAP is affected not only by the terrain, but also by geographical zoning. These phenomena are much stronger than in the western part of the country in the sharply continental climate of Siberia. And Tomsk is the Siberian city.

The deterioration of the atmosphere surface layer over large urban areas due to anthropogenic impact on the atmosphere can cause adverse environmental conditions and lead to a deterioration in the health of the population. Therefore, the issue of monitoring and forecasting the state of the atmosphere of overpopulated areas and their neighboring territories is relevant[4,5]. One of the ways to monitor and predict the quality of atmospheric air in the city is numerical modeling. To implement this method in specific cities, models of numerical weather forecasting and atmospheric air quality are currently being created and actively developed.

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The aim of this work is to use the complex of mesoscale models of numerical weather forecast WRF and atmospheric air quality CAMx to estimate the level of surface air pollution in Tomsk city.

2. MATERIALS AND METHODS

The WRF mesoscale meteorological model[6] is one of the publicly available models that can be used for any territory and therefore allows to choose different parameterizations of physical processes and set them up in accordance with specific conditions. Earlier [7,8] for Tomsk city, forecasts of the state of the atmosphere for individual seasons and weather conditions were made for different parameterizations using the WRF model[6] version 3. Satisfactory results of using in the conditions of the Siberian region were obtained and shortcomings concerning the accuracy of the forecast of individual meteorological values were identified.

The CAMx model[9] with open source is computationally efficient and adapts well to any input data formats. Weather data is fed to CAMx from separate numerical weather forecast models (in particular, WRF, MM5, and RAMS are supported). The input emissions data comes from external preprocessing systems (for example, SMOKE and EPS3) or is included in the model using user preprocessor programs[9]. The WRF/CAMx complex is widely used to predict air quality[10-12].

The available instrumentation of the IAO SB RAS is used to estimate the quality of the level of surface air pollution and meteorological parameters modeling.

The TOR-Station instrumentation complex of the IAO SB RAS (56,478° N and 85,054° E) consists of several units: aerosol, gas-analytical, meteorological, radiation, and the control unit for data collection and transmission[13]. The authors have at their disposal the results of measurements of aerosol concentrations of different diameters (from 0.25 microns to 32 microns) from the aerosol block and the number of gases from the gas-analysis block: CO, O_3, SO_2, NO, NO_2, measured at the observation point TOR-station of the IAO SB RAS from January 1 to October 31, 2020. During the specified period, there are the number of omissions in the measurements due to technical reasons and there are problems with the measurement of NO and NO_2, so they are not taken into account in the analysis.

Also to control and compare observations of the TOR-station and WRF calculations with air temperature and wind speed, information from the Tomsk Meteo Station[14] (MS) located in the southern part of the city of Tomsk (56.4666° N and 84.9666° E) is used.

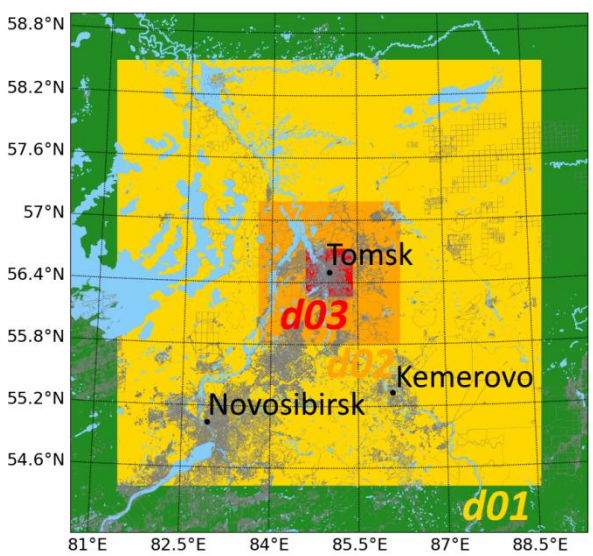

Figure 1. Areas of modeling: center in Tomsk (56,5° N and 85° E) dimension d01 450x450 km with grid step 9 km, dimension d02 150x150 km with grid step 3 km, dimension d03 50x50 km with grid step 1 km.

The WRF model version 4.2[15] was used when calculating meteorological parameters. Based on the reanalysis data of the National Center for Environmental Forecasting NCEP GFS 0.25 Degree Global Forecast Grids Historical Archive (ds083.3), using the programs of the WPS model preprocessing system, initial and boundary conditions and geodetic parameters were obtained on the calculated grid covering the study area. The simulation area has dimensions of 450x450 km (geographical coordinates of the center of the area are 56.5°N, 85°E, they coincide with the city center) and includes two nested subdomains with dimensions of 150x150 - d02 and 50x50 km - d03 which using in the CAMx model (Fig. 1). The grids step are 9, 3 and 1 km, respectively. 41 calculated levels were considered in the vertical direction. The calculations were performed for a time period of three days, the spin up of the WRF model was 24 hours, and this period was not taken into account in the analysis. Table 1 shows the set of parameterizations used in the calculations.

Table 1. Parameterizations used in calculations by the WRF model.

Parameterizations	Name	Choice for the areas
Moisture microphysics	mp_physics	WSM6
Long-wave radiation	ra_lw_physics	RRTMG
Short-wave radiation	ra_sw_physics	Dudhia
Surface layer	sf_sfclay_physics	Eta
Earth's surface	sf_surface_physics	Noah LSM
Planetary boundary layer	bl_pbl_physics	Mellor-Yamada-Janjic
Cumulus cloudiness	cu_physics	Kain-Fritsch/none/none
Urban surface	sf_urban_physics	None/none/none

The detailed description of the methods for parameterizations subgrid processes (Table 1) is given in the User Manual[15].

The CAMx model version 6.30[9] was run on nested grids based on meteorological fields calculated using the WRF modeling system for the areas d03 and d02, in the center of which Tomsk city was located. The grid sizes were 3 and 1 km. Carbon Bond 6 with modeling of aerosol particle formation, which includes 216 different reactions of chemistry and photolysis of gases, was chosen as the chemical mechanism in CAMx. Information about the general atmospheric ozone layer is taken from open sources[16]. The measurements of the TOR station are taken into account as background concentrations of pollutants, when the incoming air flows come from areas with a low anthropogenic load. Background concentrations are obtained from the average daily observations with a weak wind.

Table 2. Background concentration values used in calculations.

CO, ppm	SO_2, ppm	NO_2, ppm	O_3, ppm	NO, ppm	PM 10, μg/m^3
0.35	0.005	0.02	0.02	0.0001	0.0

The CAMx model takes into account the physical processes in which aerosols are formed or participate: gas-phase chemistry, aerosol chemistry, dry and wet deposition [9]. The CF scheme was used as available option for aerosol chemistry. This scheme distributes aerosols statistically in two types. Primary aerosols are modeled as fine (up to 2.5 microns) and coarse (up to 10 microns) particles while secondary (chemically formed) ones are modeled only as fine particles. The aerosols used in CAMx are divided into the following types: sulfates (PSO_4), particulate nitrates (PNO_3), ammonium (PNH_4), secondary organic aerosols (SOA), particulate mercury (HgP), elemental carbon (PEC), primary organic aerosols (POA), coarse (CCRS) and fine (FCRS) crystals and other coarse (CPRM), such as soot, and fine (FPRM) particles. Secondary organic aerosols (SOA) include the sum of all aerosols that differ in molar mass, non-volatile oxidation products, and secondary organic aerosol polymers: biogenic and anthropogenic.

Due to the absence of observations with components for aerosol, as well as for other small components of atmospheric air pollutants, their background concentrations are set to zero. It is assumed that the aggregate aerosol of the CAMx calculation is the PM 10 formed inside the city without external sources.

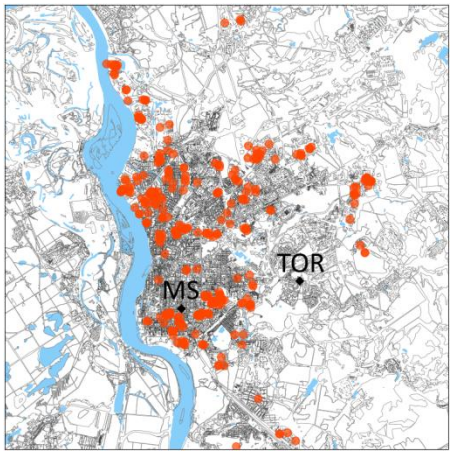

Figure 2. Stationary sources of atmospheric pollution in Tomsk and its suburb and the location of the TOR-station and Meteo Station.

The intensity of the grid anthropogenic sources of emissions varies during the day with a maximum in the daytime period, which corresponds to road traffic. The parameters of emissions from large industrial chimneys are used when modeling the influence of point sources which are marked with icons in Figure 2. The aggregate daily values of road transport emissions and point sources for the city were estimated from the report of the Department of Environmental Protection of the Tomsk Region[17].

3. RESULTS

The analysis of the available observations of the TOR-station for the gas and aerosol composition of ground air on the eastern edge city was carried out to select the dates of 2020 for estimation the quality of atmospheric air in Tomsk. Figure 3 shows the CO, O_3 and PM 10 daily average concentrations for January, February and July, 2020. The figure shows that in winter, the highest values were January 11-12 and February 16-17. In these days, in a relatively environmentally friendly area of the city, where the TOR-station is located, the concentration of carbon monoxide reached 0.45 ppm, ozone - ppm and PM 10 particles - 35-60 µg/m3. During the summer period under review, the period July 25-26 was selected. Observed meteorological conditions were close to calm during the night and morning hours of this period. The concentrations of CO, O_3 and PM 10 in the area of the TOR-station reached values of 0.3, 0.015 ppm and 9 µg/m3, respectively (Fig .3).

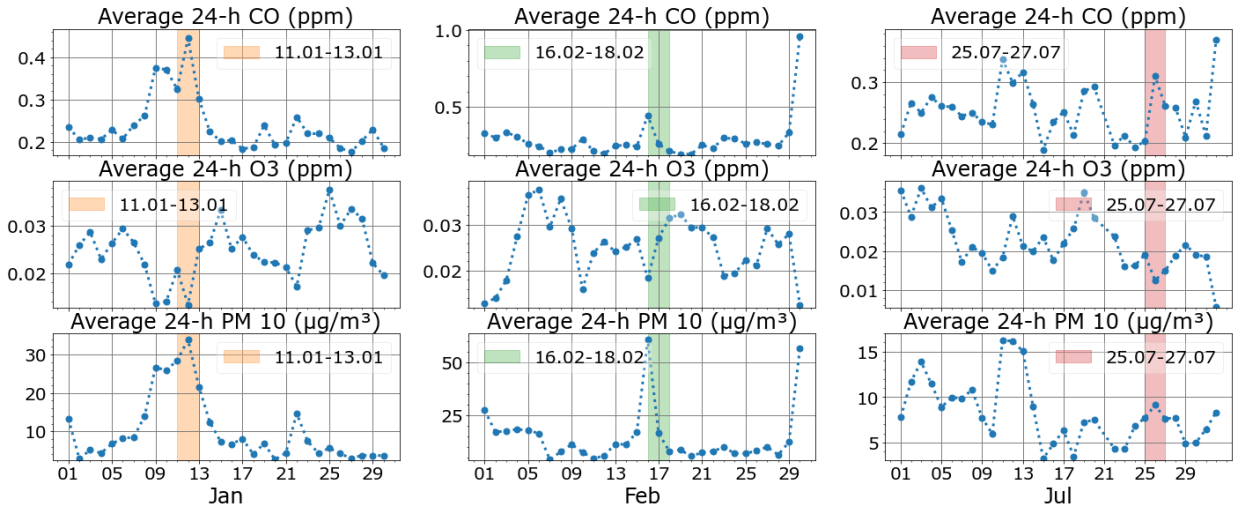

Figure 3. Average daily concentrations of pollutants CO, O_3 and PM 10 in the area of the TOR-station for January, February and July, 2020, with selected calculation periods allocated to them.

The enumerated periods were selected from the available observations because the average daily concentrations of CO (for all periods), O_3 (25.07 - 26.07) and PM 10 (for 11.01-12.01 and 16.02 – 17.02) stand out strongly from the rest of the average daily concentrations.

The description of the actual weather observed on the selected days can be obtained from the website http://rp5.ru openly providing data recorded with the help of instruments of the meteo station of Tomsk city.

The time period January 11-12, 2020 was characterized by changing of wind speed from 1 to 5 m/s. The wind direction for almost the entire observed period was south with the exception of the period from 18 hours on January 11 to 12 hours on January 12 when the direction was southeast. The air temperature increased from - 18 to - 14 degrees with small variations depending on the time of day. On January 11, it was cloudy with light continuous snow, and, on January 12, it was clear and little cloudy.

The time period February 16-17, 2020 was characterized by the wind speed variations from 1 to 3.5 m/s, and the wind direction was extremely variable and changed from southeast to northwest and further from northeast to south. The temperature dropped from - 8 to - 14 degrees and then ranged from - 10 to - 4 degrees depending on the time of day. 100% cloud cover was observed for the entire period with the exception of the periods from 1 to 4 and from 13 to 19 hours on February 16. Since 13 hours on February 17 there was the continuous light snow.

The weather July 25-26, 2020 was characterized by a calm wind (1m/s). The wind direction during this period was variable. The air temperature ranged from 12 to 15 degrees in the morning and from 18 to 21 degrees in the afternoon. At night, the sky was clear, the other parts of time the sky was cloudy, clear at times. From 7 to 13 hours local time on July 26 there was fog.

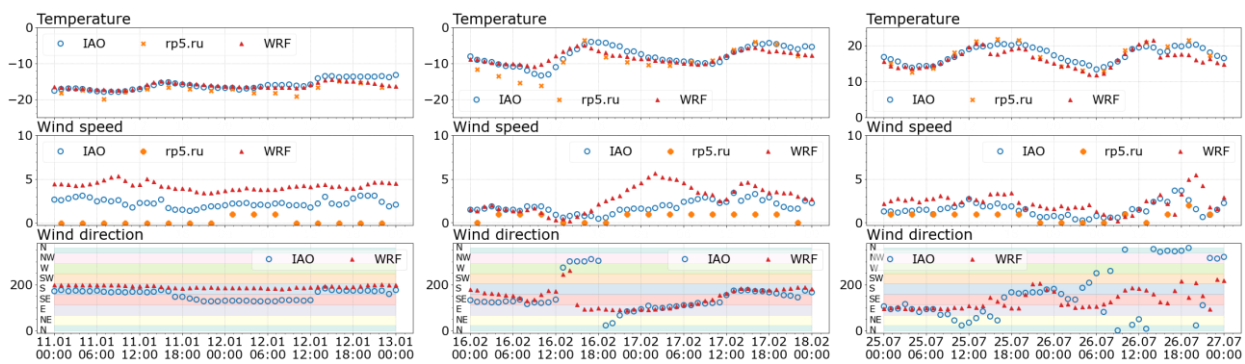

Figure 4. Temperature, speed of surface wind and wind direction calculated with WRF and measured for the time periods from January 11 to 12, from February 16 to 17 and from 25 to 26 July, 2020.

Figure 4 shows the values of air temperature on a height of 2 m, wind speed and direction on a height of 10 m calculated for the selected time periods using the WRF model, and the measured values of air temperature, speed and direction using the instrument base described above. The figure shows that the best coincidence of calculations and observations in the winter period takes place for the surface air temperature. As for the period January 11-12, 2020, it can be noted that the WRF model predicts more significant levels of surface wind speed in the city than is observed with the instruments of the city's meteo stations and the scientific institute. Also, in these days, the WRF calculations for the wind direction don't agree very well with the observations with the IAO SB RAS weather station. In the period February 16-17, 2020, the comparison of characteristics of the surface wind calculations and observations looks better. Only in the evening and night hours February 16-17, 2020, the WRF model predicted a significant increase in wind speed in the city to 5 m/s, while on weather devices this parameter didn't exceed 3 m/s.

In the summer period July 25-26, 2020, the WRF model predicted quite well the change in the surface temperature in the city and its amplitude. The dynamics of the wind speed during the two days under consideration was calculated quite satisfactorily. But with a little overestimation of the speed values compared to the observed ones. On July 26, the WRF model unsatisfactorily predicted the direction of the wind speed, it is significantly different from that observed with the IAO SB RAS weather station, although the surface wind speed at this time was more than 2m/s.

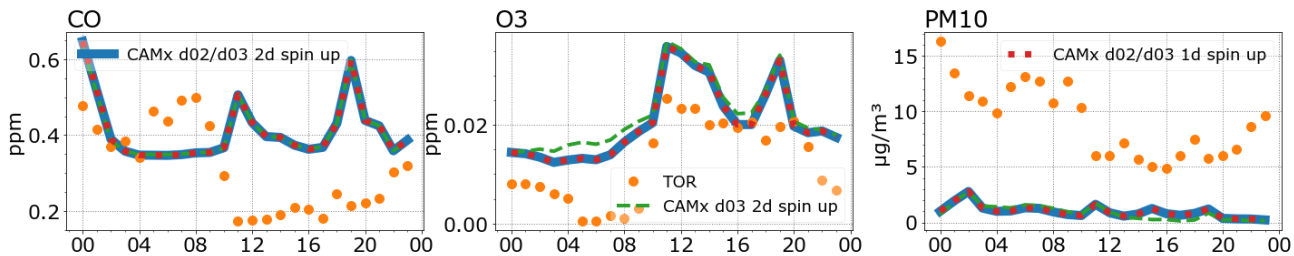

Figure 5. Calculated and observed surface concentrations of carbon monoxide, ozone and PM 10 particles on July 26, 2020. Calculations are given for different launch conditions of the CAMx model: d02/d03 2d spin up - two nested areas and 2 days for a spin up, d02/d03 1d spin up - two nested areas and 1 day for a spin up, d03 2d spin up - one area and 2 days for a spin up.

Some tuning runs of the CAMx program were performed before applying the CAMx air quality model. Two issues were considered: the necessity to perform impurity transfer calculations in two nested areas, and the necessity to use a one or two day spin up for the CAMx model. Figure 5 shows the calculated profiles of the concentrations of carbon monoxide, ozone and PM10 particles in comparison with the values observed with the TOR-station IAO SB RAS. The figure shows that, in principle, for the case under consideration, the CAMx model doesn't show large differences in the calculations between taking into account a two or one day spin up and using two nested instead of one nested areas. However, there is a tendency that for chemically more active substances (for example, O_3) calculations show sharper changes in concentrations during the day when two nested calculation regions are used which seems to provide more realistic boundary conditions for the internal modeling area with the grid step of 1 km.

Calculations were performed using the CAMx model for two nested areas to estimate the level of atmospheric air quality in Tomsk city for the three selected time periods. For each period, one day was used to spin up the air quality model, and the other two were used to estimate air quality from the numerical forecast results. The estimation of the surface air quality was carried out based on the results of the numerical forecast for the nested area dimension of 44x44 km in the center of which the Tomsk city was located. The Air Quality Index (AQI) was determined based on the results of calculations for two control days in accordance with the recommendations of the US Environment Protection Agency[18] (EPA). Table 3 shows the rules for calculating the AQI for the three averaged concentrations:

$$AQI = \max\left\{ \max_{\substack{time\ average,\\ d03}} (AQI_{CO}),\ \max_{\substack{time\ average,\\ d03}} \left(AQI_{O_3}\right),\ \max_{\substack{time\ average,\\ d03}} (AQI_{PM10}) \right\}$$

Table 3. Breakpoint EPA to estimate the results of the CAMx calculation in Tomsk city.

O_3 (ppb)	**PM 10 (μg/m^3)**	**CO (ppm)**	**AQI**	
$C_{low} - C_{hight}$ (avg)	$C_{low} - C_{hight}$ (avg)	$C_{low} - C_{hight}$ (avg)	$I_{low} - I_{hight}$	Category
0–54 (8-hr)	0–54 (24-hr)	0.0–4.4 (8-hr)	0–50	Good
55–70 (8-hr)	55–154 (24-hr)	4.5–9.4 (8-hr)	51–100	Moderate
71–85 (8-hr)	155–254 (24-hr)	9.5–12.4 (8-hr)	101–150	Unhealthy for Sensitive Groups
86–105 (8-hr)	255–354 (24-hr)	12.5–15.4 (8-hr)	151–200	Unhealthy
106–200 (8-hr)	355–424 (24-hr)	15.5–30.4 (8-hr)	201–300	Very Unhealthy

AQI for CO, O_3 and PM 10 are calculated using the following formula:

$$AQI_* = \frac{I_{high} - I_{low}}{C_{high} - C_{low}}(C - C_{low}) + I_{low},$$

where AQI_* – air quality index, * - the component for CO, O_3 or PM 10, C - the averaged pollutant concentration, C_{low} - the concentration breakpoint that is $\leq C$, C_{high} - the concentration breakpoint that is $\geq C$, I_{low} - the index breakpoint corresponding to C_{low}, I_{high} - the index breakpoint corresponding to C_{high}.

Table 4. The maximum AQI for the entire time period under review in accordance with the averaging.

Time period	AQI_{CO}	AQI_{O3}	AQI_{PM10}	AQI
January 11-12	9	23	4	23
February 16-17	24	201	17	201
July 25-26	15	47	31	47

Table 4 shows the maximum values of the Air Quality Index for the two days considered for the components of the impurity CO, O3 and PM 10. The table shows that good values for air quality are obtained for the periods January 11-12, 2020, and July 25-26, 2020, (according to the criteria in Table 3). In the winter period February 16-17, calculations for the WRF/CAMx complex showed the sharp deterioration in air quality in the city due to the increase in ozone concentration. Again, the main "role" in the deterioration of air quality belongs to ozone. Note that in all three time periods considered, the measured values of ozone concentrations were in the "good" zone in accordance with Table 3. The results indicate the necessity to increase the number of measuring stations monitoring air quality in Tomsk city, or the constant use of numerical monitoring of air quality in the city in conjunction with mobile measuring stations.

4. CONCLUSION

The results of numerical modeling of the meteorological situation and atmospheric air quality in Tomsk city for two-day time periods: January 11-12, February 16-17, and July 25-26, 2020, are presented. Their selection was made on the basis of measuring instruments of the TOR-station of the IAO SB RAS. Their results showed the increase in the concentrations of carbon monoxide, ozone and PM 10 particles on the days under consideration.

The WRF and CAMx models are binding to the selected territory, grid and point sources are presented, and boundary conditions are set. The necessity of using an additional spin up for models, as well as the use of nested areas for calculating concentrations, was evaluated.

Based on the calculations carried out using the WRF/CAMx complex for the considered historical dates, it was found that February 16-17, 2020, the deterioration of air quality in the city was numerically predicted, and this is due to the increase in the concentration of ozone.

AQI US EPA was used as the quality assessment criteria.

ACKNOWLEDGEMENTS

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