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Numerical modeling of aerosol pollution for the observatory Fonovaya IAO SB RAS

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ABSTRACT

The paper compares the results of numerical modeling of the calculated concentration of aerosol with the results of measurements performed on the territory of the Fonovaya(Background) Observatory.

Keywords: atmospheric aerosol, modeling, WRF-Chem

1. INTRODUCTION

Monitoring the air pollution of small gas and aerosol components of the atmosphere is an important task because of their negative impact on the biosphere in general and human health in particular. From this point of view, it is important not only to conduct monitoring but also to be able to predict the level of pollution. Currently, mesoscale chemical transport models (WRF-Chem [1], TSUNM3 [2]) are actively used to predict pollution levels. The main problem with their use is setting the initial and boundary conditions for chemicals. The aim of this work is to assess the reproducibility of the aerosol composition of air using the WRF-Chem v.4.1.2 model for the background region of Western Siberia. To set the initial and boundary conditions for chemicals, we used the calculations of two global chemical transport models MOZART-4 (Model for Ozone and Related chemical Tracers, version 4) and WACCM (Whole Atmosphere Community Climate Model).

2. MODEL AND MEASUREMENT DATA

Modeling was carried out WRF-Chem v 4.12. For the numerical simulation, one domain in the Lambert projection was used, limited horizontally by coordinates 56.1-57.8°N and 83'-86°East and height level of 100 hPa. The number of nodes in the computational domain is 52x50x30 in longitude, latitude, and height, respectively. The horizontal grid spacing was 4 km, a variable time modeling step was used in the range from 24 to 200 s for meteorological parameters and 6 s for chemical reactions, the grid step-in height was given by the ETA coordinate, taking into account the orographic surface, and increased with increasing height. The height of the lower level was 50 m, the relief data was set with a resolution of 30". Computational experiments were carried out for August 2013 and April 2020.

As the initial fields of meteorological values, we used the data of the FNL (NCEP) model [3] with a 6-hour time resolution. Fields of initial FNL meteorological data were obtained on the basis of GFS data using an increased volume of observational data. The source of anthropogenic emissions HTAP-2 [4] was used to specify the emission sources, methane emissions were supplemented from the EDGAR V. 4.3.2 database [5] with a spatial resolution of 0.1x0.1°and a time resolution of 1 month. The power of the sources was set constant without taking into account the intraday and weekly dynamics of emissions. Emission sources were specified in the surface layer.

Biogenic emissions were set using the MEGAN2.04 model [6], and emissions from fires were FINN v1.5 [7]. Emissions from swamps were set with constant values, using the results of MACC II inverse modeling for 2012 [8]. The initial and boundary conditions for chemicals were set using the global Mozart4 model for 2013 and the WACCM model for 2020. The parameterizations used in the Wrf-Chem model are: microphysics - Morrison; long-wave radiation - RRTM; shortwave radiation - Dudhia; surface layer - Rev. MM5; surface model - Noah;

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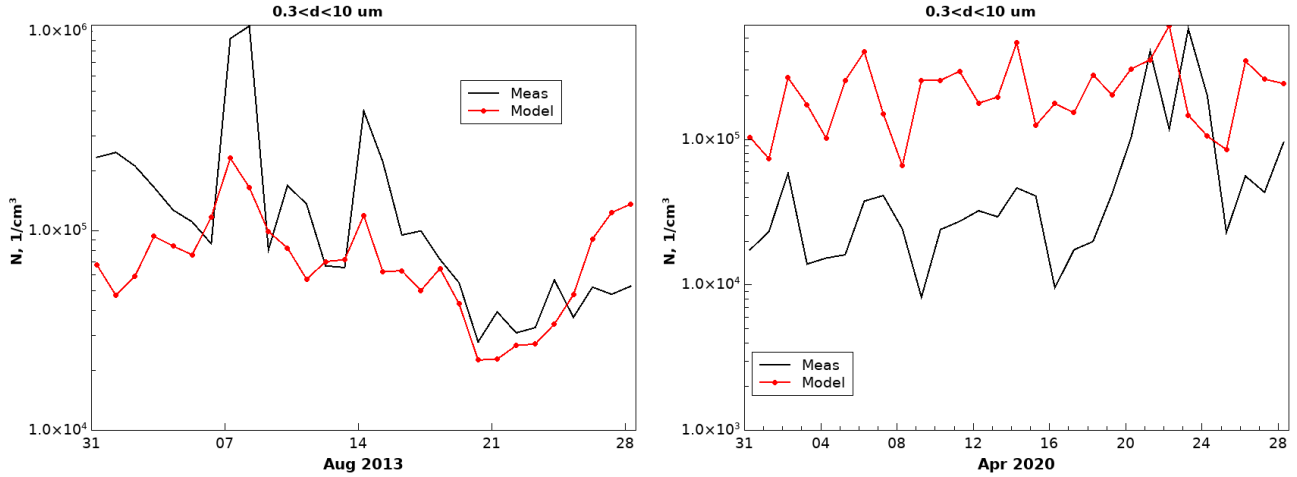
boundary planetary layer - Yonsei Univ .; cloud parameterization - Grell 3D. The WRF-Chem emission module code has been upgraded to allow methane emissions from fires and bioemissions to be read. In the calculations, the chemical mechanism MOZART-4 [9] was used together with the aerosol mechanism MOZAIC [10]. The chemical block of the model uses 85 substances, 157 reactions, and 39 - photochemical ones. The aerosol block allows calculations for 4 size ranges, with median diameters of 0.078125, 0.3125, 1.25, 5 μm.

To verify the simulation results, we used the results of measurements of the concentration of aerosol and meteorological parameters performed at the Fonovaya Observatory of the IOA SB RAS, which is located in the background region of the Tomsk Region (56°25' N, 84°04' E, 80 m. above the sea level, http://lop.iao.ru [11]). The aerosol was measured with a GRIMM 1.108 counter. To verify the results, the data obtained in August 2013 and April 2020 were used.

To compare the simulation results with the measurement data, the nearest network node to the station was selected. The temporary output of the model is organized in GMT, so the time was transferred to local (GMT + 7). For analysis, the calculated concentration of aerosol was used, which for convenience was recalculated into dN/dlog(di) (di - diameter) in the work.

3. RESULTS

We begin our consideration with the results of modeling the average daily concentration of aerosol components. Let us consider separately the calculated concentration of aerosol particles for each median diameter. Figure 1a presents the simulation results for the total number concentration of aerosol with diameters from 0.3 to 10 μm.



a) b)

Figure 1. The average daily aerosol concentration is 0.3< di <10 μm for 20130 (a) and 2020 (b). Measured values (black line), model (red).

From the data presented in the figure, it follows that the model reproduces the aerosol concentration. However, for August 7 and 14, 2013. the model showed an increase in concentration, but the values are underestimated. The correlation coefficient (r) was 0.72, and the mean square error (RMSE) was 2.3e5 $1/cm^3$. For April 2020, the picture is different. The model restores behavior over time but gives overestimated values. If we compare the monthly average values, they will be 2.28±1.24e5 and 2.25e5 ±1.24e5 $1/cm^3$ for the model and measured values, respectively. The correlation coefficient is 0.4 and 0.74, respectively. The low correlation value was due to the fact that the model was not able to reproduce the two peaks observed from April 20-24.

We continue consideration separately for three ranges of diameters: 0.3< di <0.625 m, 0.625< di <2 μm and 2< di <10 (fig.2).

For the range of aerosol diameters from 0.03 to 0.625 m (fig.2a,b), the patterns are preserved as for the figure. For the next range of sizes (fig.2c,d) for August 2013, the model values can be seen that reproduced the average values, but could not show the maxima observed on August 8, 11 and 15. But for April 2020, the

model gives peaks of concentration 6 and 14 which are not observed in the measurements. also fixes the presence of concentration peaks that are not observed in the measurements. Note that the model restores the average concentration value. For a coarse aerosol (fig.2e, f), the model restores the average values. The model also fixes the presence of concentration peaks that are not observed in the measurements.

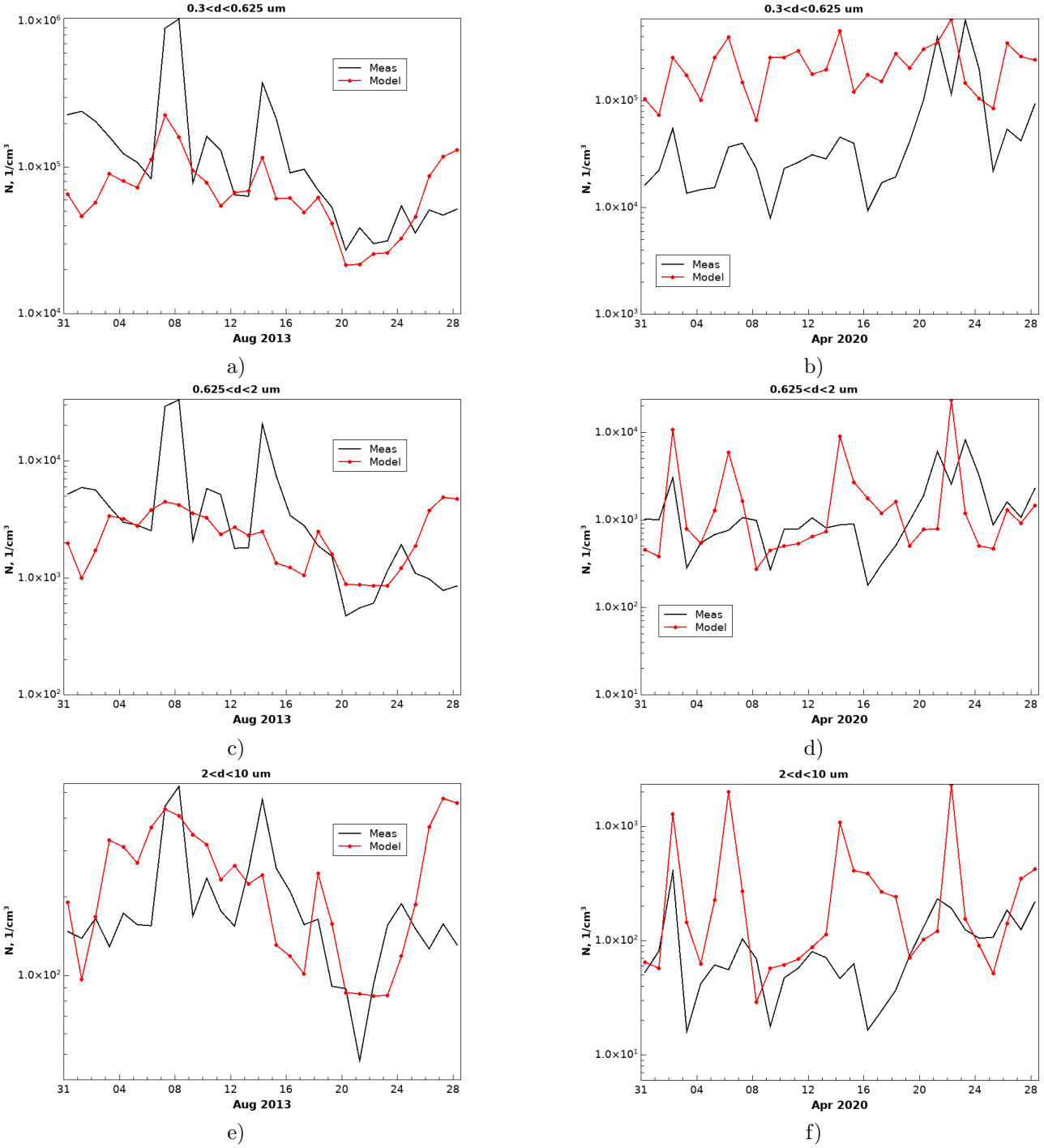
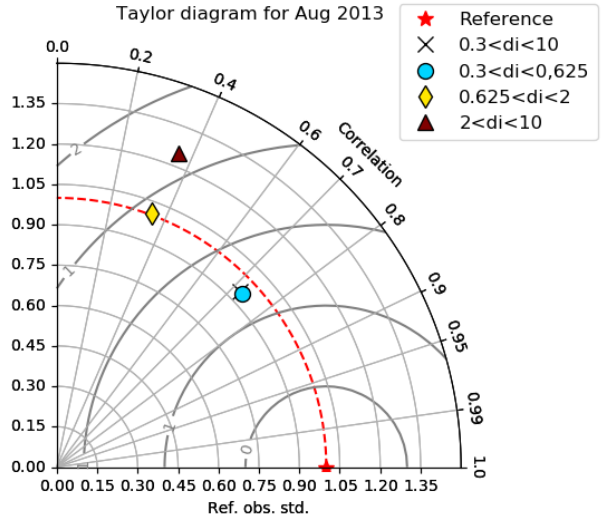
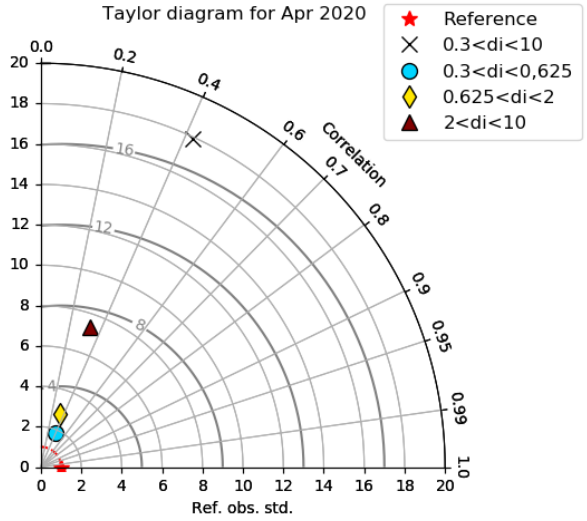


Figure 2. The average daily aerosol concentration is 0.3< di <0.625 μm - (a,b), 0.625< di <2 μm (c,d) and 2< di <10 μm (e,f). Measured values (black line), model (red).

To complete the picture, we present Taylor diagrams. From the data rearranged in Figure 3, it follows that for August 2013, the model as a whole restores the variance of a number of measurements. For coarse aerosol she overestimates it. The correlation coefficients of the calculated aerosol concentration range from 0.4 to 0.8. For April 2020, the picture is different. The model gives a very high dispersion and an average value of the concentration of aerosol. The correlation coefficients range from 0.2 to 0.4.



a)



b)

Figure 3. Taylor diagrams for August 2013 (a) and April 2020 (b)

4. CONCLUSION

As a result of the study, it was shown that when modeling using the WRF-Chem model and the selected set of emissions, it was possible to reconstruct the aerosol concentration for the diameter ranges 0.3-0.625 μm and partly for 0.625-2.5 μm. The probable causes of the discrepancies may be inaccuracies in setting the power

of emission sources and features associated with the implementation of aerosol cycle simulations. Our further research will be aimed at a detailed study of the reasons for the discrepancies and refinement of the used databases of emission sources using the approach used in [12,13].

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