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Numerical modeling of nitrogen dioxide for the Fonovaya Observatory and TOR-station

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ABSTRACT

The study presents the results of numerical modeling of ground-level nitrogen dioxide concentration for the Fonovaya Observatory and TOR station. The calculations were carried out for February 2023, when favorable conditions for the accumulation of pollutants in the surface layer were observed in the study area. As a result of the study, it can be concluded that the nitrogen dioxide emission rates provided in the EDGAR database for the study area are underestimated and need to be increased by a factor of 3 to 5.

Keywords: atmospheric gases, modeling, WRF-Chem

1. INTRODUCTION

Air pollution by nitrogen dioxide is one of the significant environmental problems worldwide. Urban populations face constantly increasing levels of pollution, which can lead to serious consequences for human health and the environment. Therefore, modeling air pollution levels is critically important for understanding its dynamics and taking measures to improve its quality.

Modeling allows for the assessment of the spread of air pollution over time and space, identification of sources of pollution, and evaluation of the impact on the environment and human health. This can help make informed decisions when developing strategies to reduce air pollution and monitoring air quality. Recently, chemical transport models (CTMs) [**?**] have been actively used for studying and predicting air pollution levels. However, to obtain a quality prediction of pollution, reliable information on the sources of emissions of pollutants is necessary, as well as verification of the modeling results with measurement data. This study compared modeling results with measurement data obtained at the atmospheric composition monitoring station of the "Fonovaya" observatory of the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences, to refine the databases of pollution sources used in the calculations.

2. MODEL AND MEASUREMENT DATA

Numerical modeling of air pollution levels was performed using the regional CTM WRF-Chem v.4.2 [1]. To do this, a rectangular domain was created with boundaries of 55.4-57.5°N and 82.8-86.1°E, with a horizontal grid spacing of 4 km. To eliminate edge effects, the "Fonovaya" observatory of the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences was located at the center of the domain.

The RACM [3] set of reactions was used as the chemical mechanism in the work, which included 77 substances and 237 reactions, 23 of which were photolytic. The MADE/SOGRAM (VBS) [4, 5] model was chosen for the aerosol mechanism, which allows obtaining the number concentration of aerosol for the nucleation, accumulation, and coarse mode.

To run the WRF-Chem model, initial and boundary conditions for the chemical composition of the air were set using data from the WACCM [6] global model calculations [3]. The EDGAR 4.3.2 [7] database was used to set anthropogenic emissions, and the distribution of biogenic sources was obtained using the MEGAN2

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model [8]. FNL [9] data with a resolution of 0.25x0.25° were used to set meteorological parameters. Various parameterization schemes were used in the calculations, such as: microphysics - Morrison; long-wave radiation - RRTMG; short-wave radiation - RRTMG; surface model - Noah; planetary boundary layer - Mellor-Yamada-Janjic; cloud parameterization - Grell 3D.

For verification of the modeling results, gas composition measurements conducted at the "Fonovaya" Observatory of the Institute of Atmospheric Optics of the Siberian Branch of the Russian Academy of Sciences, located in the background area of the Tomsk region (56°25' N, 84°04' E, 80m above sea level, http://lop.iao.ru)[10], and the TOR station [4] were used. The TOR station is located on the northeastern outskirts of Akademgorodok, Tomsk (56°28' N, 85°03' E) [11]. The measurement period was chosen from February 1 to February 20, 2023. The results of numerical modeling and measurement data were brought to the same units for convenience of comparison (μg/m3) and were synchronized in time. Daily average values of measured gas concentrations were used for verification.

3. RESULTS

The results of the calculations are presented in Figures 1-3. From the obtained modeling data, it follows that when using the database of anthropogenic emissions witl emission power values, the concentration and temporal dynamics of nitrogen dioxide are not reproduced (Fig. 1). On average, the daily average concentrations are underestimated by a factor of 3 for the "Fonovayh the originaa" observatory and the TOR station.

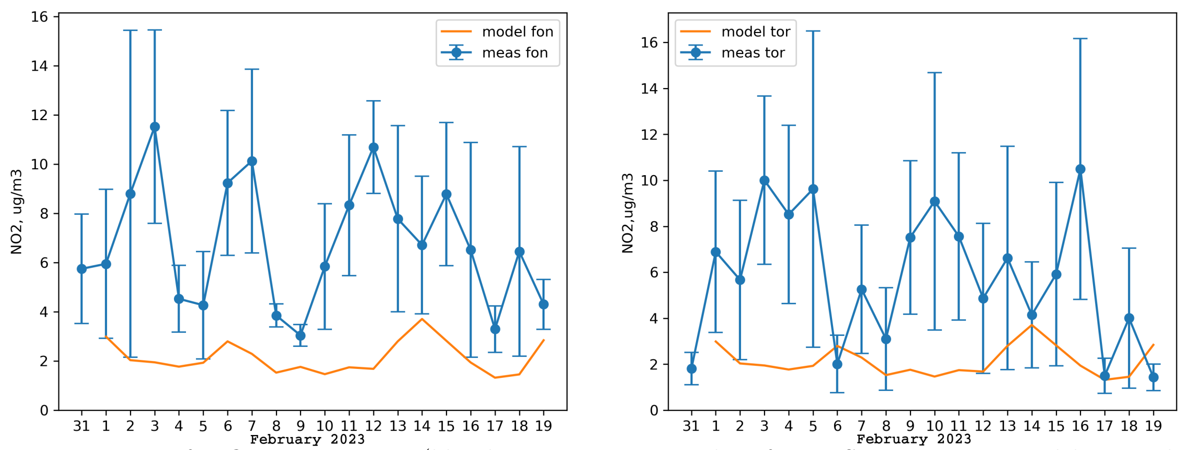

Figure 1. Dynamics of NO_2 concentration (blue line - measurement data from RSME, orange - modeling results) for original emissions. Left panel - "Fonovaya" observatory, right - TOR station.

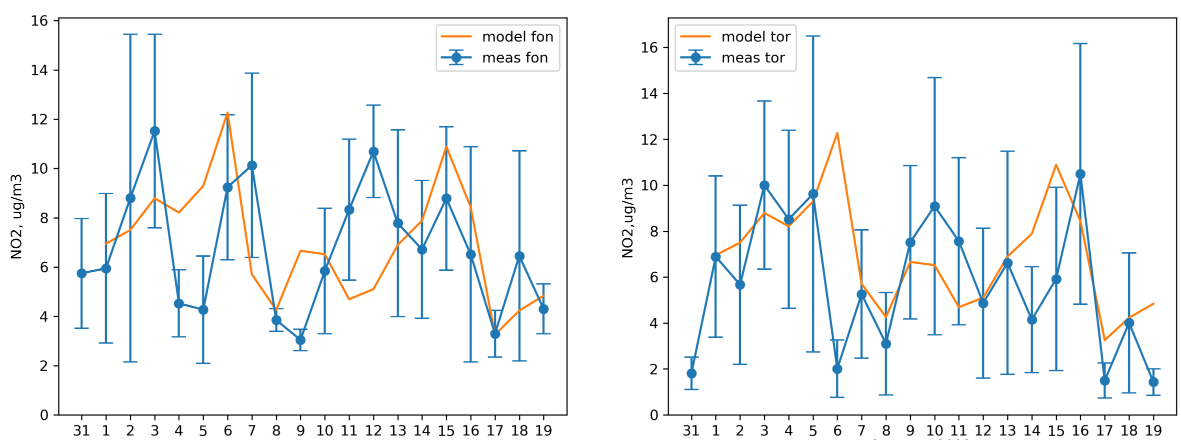

Figure 2. Dynamics of NO_2 concentration (blue line - measurement data from RSME, orange - modeling results) for emissions increased by 5 times. Left panel - "Fonovaya" observatory, right - TOR station.

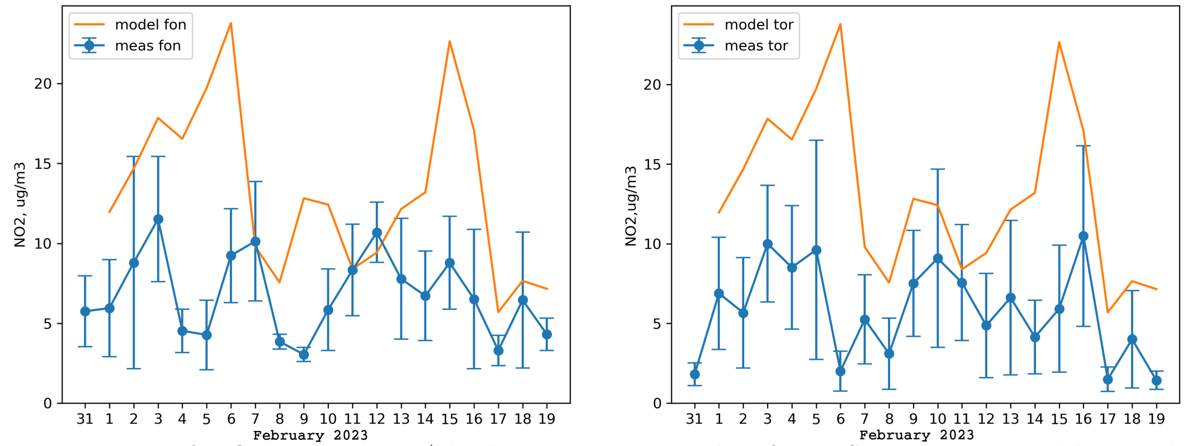

Figure 3. Dynamics of NO_2 concentration (blue line - measurement data from RSME, orange - modeling results) for emissions increased by 10 times.Left panel - "Fonovaya" observatory, right - TOR station.

Based on the analysis of the temporal trend, it can be observed that there is an out-of-phase relationship between the observation data and the model results for the TOR station. The correlation coefficient was 0.21 and -0.22 for the "Fonovaya" observatory and the TOR station, respectively. These differences between the modeling results and measurements indicate that the emission values used in the model are underestimated. Given the measurement period (winter), it is likely that the anthropogenic emissions are the ones that are underestimated. Therefore, to test this hypothesis, a series of numerical experiments were conducted by adjusting the emission values.

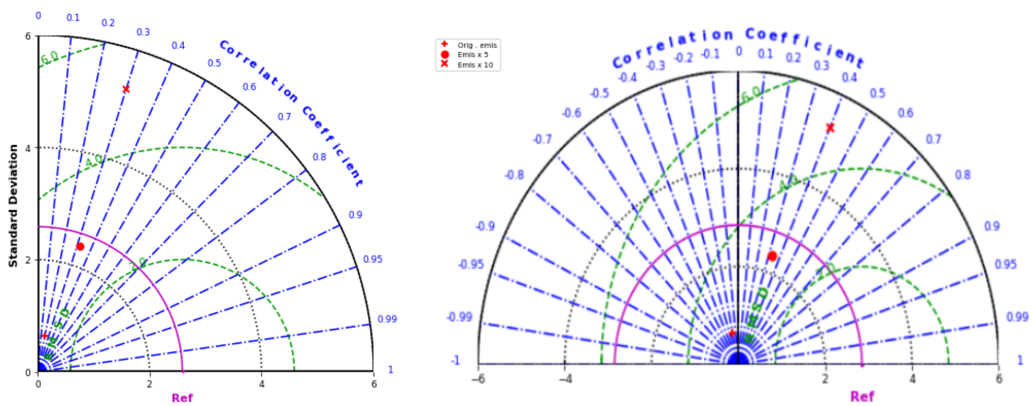

Figure 4. Taylor diagram for different levels of emissions. Left panel - "Fonovaya" observatory, right - TOR station.

Figure 2-3 shows the results of the calculations with an increase in nitrogen dioxide emissions by a factor of 5 and 10, respectively. When emissions were increased by a factor of 5, the modeling results showed a better reproduction of the temporal trend of the daily average NO_2 values for both monitoring stations (Fig. 4). The root mean square error of modeling the daily average values was 2.82 and 3.12 (μg/m3) for the "Fonovaya" observatory and the TOR station, respectively. The correlation coefficient also increased for both stations, reaching 0.35. However, when emissions were increased by a factor of 10 relative to the original values, the modeling results showed a dynamic trend, but the obtained concentration values were significantly overestimated.

4. CONCLUSION

Based on the findings, it can be concluded that the nitrogen dioxide emission values obtained from the EDGAR database for the study area are underestimated and require an increase by a factor of 3-5. [12, 13]

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