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# Validation of Atmospheric Numerical Models Based on Satellite Measurements of Ozone Columns

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**Abstract**—The time series of ozone columns measured with the SBUV satellite instrument over three subarctic stations (Saint Petersburg, Harestua, and Kiruna) are analyzed. The daily and monthly mean ozone values in the layers of 0–25, 25–60, and 0–60 km are compared with the results of simulations with RSHU and EMAC numerical models for the period of 2000–2015. Model data are in good agreement with satellite data both in general and in the cases of rapid short-term ozone loss. However, there are some differences between the models and measurements as well as between the two considered models. These differences require the more detailed analysis in order to modify model parameters. Experimental data demonstrate the increase in ozone columns in the layer of 25–60 km which amounts to 2.1 ± 0.7, 2.4 ± 0.7, and 1.5 ± 0.8% per decade for Saint Petersburg, Harestua, and Kiruna stations, respectively. The results of numerical simulations do not contradict these estimates.

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## INTRODUCTION

The comparison of the results of simulation of spatiotemporal variations in ozone columns (OC) with measurement data allows assessing the model performance and modifying it if needed. The improved models are subsequently used for producing reliable forecasts of ozone variations under different scenarios of anthropogenic and natural impacts on the ozonosphere. The early forecasts of ozone anomalies are important, because the decrease in total ozone column (TOC) leads to the increase in the level of surface UV irradiation. This problem has recently become urgent both for the Southern and Northern hemispheres. For example, the formation of ozone mini-holes was observed over Russia in the winter of 2015/2016 [2, 3].

The comparison of simulation results with TOC measurement data was carried out many times [1, 7, 8, 10, 15, 16]. However, the exclusive consideration of TOC measurement data does not enable the objective identification of photochemical and dynamic factors defining the observed seasonal and interannual variability of ozone. The more informative way is the comparison of ozone values in separate atmospheric layers, because different processes of ozone formation and transformation dominate at different heights [4].

To validate the models, the present study utilizes the satellite measurements of ozone values in different atmospheric layers with the Solar Backscatter Ultraviolet Instrument (SBUV) over three subarctic stations for the period from January 1, 2000 till December 31, 2015. The SBUV instruments provide the nadir measurements of the spectra of reflected and scattered radiation in the band of 250–340 nm with the horizontal resolution of about 200 × 200 km. The description of the instrument, the interpretation algorithm, and the analysis of measurement errors can be found in [5]. The accuracy of satellite measurements of ozone values in separate atmospheric layers is ~5–15%. The analyzed SBUV data are the certain averaged daily mean values (Merged Ozone Data) interpolated to the coordinates of the following ground-based stations: Kiruna (67.8° N, 20.4° E), Harestua (60.2° N, 10.8° E), and Saint Petersburg (59.9° N, 29.8° E).

**Table 1.** Statistical characteristics of the results of comparison between the data of measurements and model simulations by EMAC and RSHU

| Model | Layer, km 0–60 | | 0–25 | | 25–60 | |
|---|---|---|---|---|---|---|
| | | K | | K | | K |
| **Saint Petersburg** | | | | | | |
| EMAC | 8 15 | 0.950 0.001 | 10 15 | 0.942 0.001 | –1.9 3.9 | 0.955 0.001 |
| | 2.5 4.7 | | 4 6 | | –1.9 3.8 | |
| RSHU | 0 22 | 0.901 0.002 | 3 19 | 0.891 0.003 | –2.5 7.6 | 0.836 0.004 |
| | 0 7 | | 1 8 | | –2.4 7.4 | |
| **Harestua** | | | | | | |
| EMAC | 8 16 | 0.947 0.001 | 11 15 | 0.936 0.002 | –2.7 3.8 | 0.956 0.001 |
| | 2.4 4.8 | | 5 7 | | –2.7 3.7 | |
| RSHU | 3 23 | 0.891 0.003 | 6 20 | 0.879 0.003 | –3 8 | 0.817 0.004 |
| | 7 7 | | 3 9 | | –3 8 | |
| **Kiruna** | | | | | | |
| EMAC | 10 15 | 0.964 0.001 | 12 14 | 0.960 0.001 | –1.5 3.9 | 0.944 0.002 |
| | 3 4 | | 5 6 | | –1.6 4.0 | |
| RSHU | 4 23 | 0.916 0.002 | 10 20 | 0.908 0.003 | –6 9 | 0.783 0.006 |
| | 1 7 | | 4 8 | | –6 9 | |

Note: is disagreement (the average difference "measurements minus model" root-mean-square deviation ; the numerator is Dobson units; the denominator is percentage). *K* is the correlation coefficient.

The experimental data are compared with the results of simulation with the chemical transport model of the lower and middle atmosphere composition developed at Russian State Hydrometeorological University (RSHU) [4] and EMAC chemistry climate model (ECHAM/MESSy Atmospheric Chemistry model) [9]. The main difference between these models is that in EMAC the variability of dynamic parameters was computed using the assimilation of ERA-Interim reanalysis data [6], and the RSHU model directly used the MERRA reanalysis data [11] as dynamic parameters. The detailed description of the models and the examples of their application results are presented in [1, 4, 12]. As the measurements for each station are usually conducted approximately at the same certain time during one–two hours, the results of EMAC simulations were averaged over the period of 2 hours from the measurement time period for the comparison with satellite data; for the RSHU model, average daily data were taken.

The analysis was performed both for TOC and for the ozone values in the layers of 0–25 and 25–60 km. The above division is substantiated by the fact that in the layer of 25–60 km ozone values are basically defined by photochemical processes, whereas in the layer of 0–25 km ozone values are mainly controlled by dynamic processes in the atmosphere. Thus, the objective of the present study is to verify the quality of simulation of short- and long-period variations both in TOC and in OC in the layers where the variability of ozone content is caused by different physical factors.

## GENERAL DESCRIPTION OF COMPARISON RESULTS

Table 1 presents the statistical characteristics of the results of comparison (average differences and root-mean-square deviations ) between the data of measurements and simulations of TOC and OC in two layers (0–25 and 25–60 km) for three ground-based stations. The table data on the values of the correlation coefficient *K* and demonstrate that EMAC describes ozone variability more accurately than RSHU. At the same time, EMAC underestimates TOC and OC in the layer of 0–25 km more significantly than RSHU. The smallest values of the difference for RSHU are observed for Saint Petersburg; the highest values were obtained for Kiruna station, especially for the layer of 25–60 km, where RSHU overestimates ozone

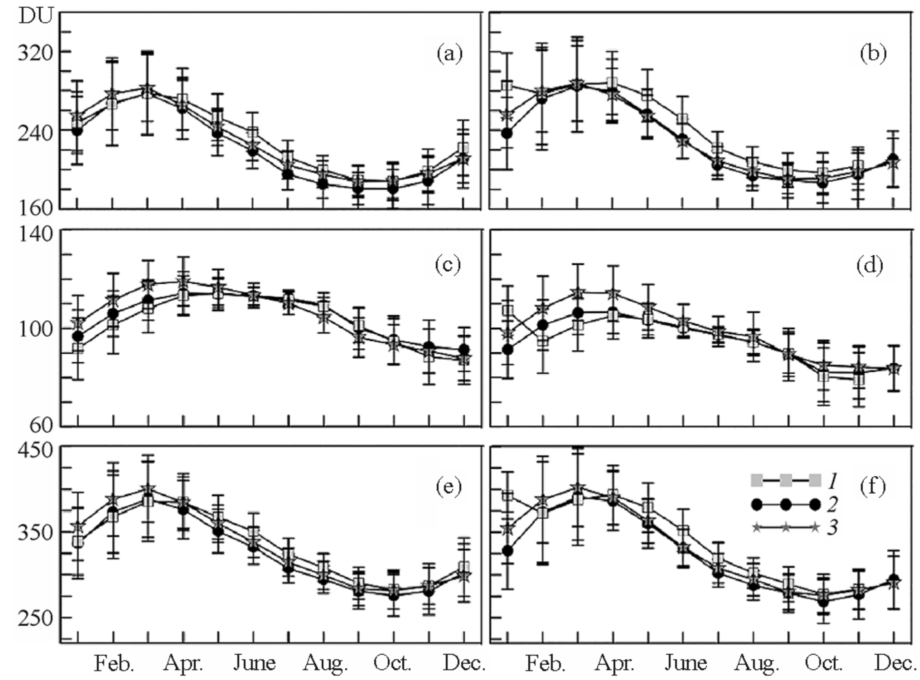


**Fig. 1.** The seasonal variations in monthly mean ozone values ((*1*) SBUV, (*2*) EMAC, (*3*) RSHU) for the layers of (a, b) 0–25, (c, d) 25–60, and (e, f) 0–60 km at (a, c, e) Saint Petersburg and (b, d, f) Kiruna stations.

values by 3%. However, the change in the sign of  for different layers may also be associated with different vertical ozone distribution in the model and measurement data.

Figure 1 presents seasonal variations in monthly mean ozone values calculated for the whole period of 2000–2015 which were obtained from the data of two models and measurements for Saint Petersburg and Kiruna stations. Harestua station located at the same latitude as Saint Petersburg is characterized by the same basic features of temporal OC variations; therefore, the figure is not presented. The data are presented both for TOC (Figs. 1e and 1f) and for OC in different layers.

Both models underestimate TOC and OC in the layer of 0–25 km containing the most of ozone in April to October inclusive for all three stations. This means that the models predict the more rapid OC decrease than that observed from SBUV data. In December and January there are almost no SBUV measurements over Kiruna station; therefore, conclusions for these months were not made. In the other months the model simulations of TOC agree well with measurements at all stations.

In the layer of 25–60 km (Figs. 1c and 1d), where ozone values are basically controlled by photochemical reactions, the RSHU model data exceed both the EMAC data and satellite data in January–May. The EMAC model also overestimates OC (to a lesser extent though) in this layer during the first four months of the year.

## PERIODS OF RAPID VARIATIONS IN TOC

The reproducibility of the rapid and significant decrease in TOC is essential for forecasting the surface UV irradiance increase. The analysis of experimental (SBUV) data revealed several cases over the considered 15 years when TOC decreased by 20% and more per day near the analyzed ground-based stations. The number of such cases during the analyzed period over the considered stations is rather small and amounts from 5 (Saint Petersburg) to 13 (Harestua).

Figure 2 presents the difference between measurement data and simulation results for these cases. As a rule, for all stations for EMAC (about 5 DU on average) this difference is smaller than for RSHU (about 30 DU on average), i.e., RSHU underestimates ozone loss more significantly. At the same time, for example, for Saint Petersburg station at the end of 2011 (Fig. 2a), EMAC underestimated the TOC decline more strongly than RSHU. The EMAC model rather often overestimates the TOC decrease for all stations that generally makes its estimates closer to measurement data. Even for such small ensemble, the

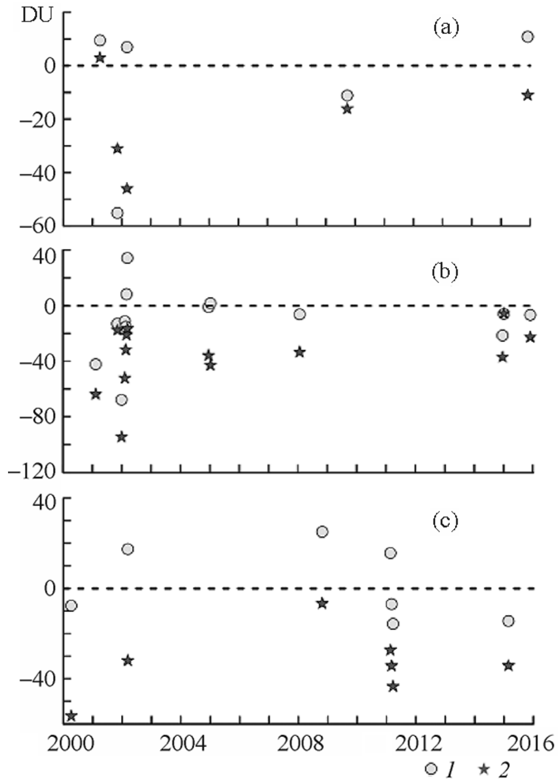


**Fig. 2.** The difference between the SBUV measurement data and model simulation results ((*1*) EMAC, (*2*) RSHU) on the days with TOC decrease by 20% at (a) Saint Petersburg, (b) Harestua, and (c) Kiruna stations.

coefficients of correlation between the observation and model data are rather high (close to 1). This means that both models correctly describe dramatic variations in TOC, i.e., they are sensitive to the rapid TOC decline in the subarctic atmosphere.

Figure 3 presents the example of separate short periods with the duration of several weeks during which TOC varied significantly over three stations. It is noteworthy that there are cases when model simulations lag behind the real ozone loss for some time (the example for Saint Petersburg station); it happens that both models incorrectly describe the peaks in temporal TOC variations or systematically overestimate them (the example for Harestua station) or both models describe ozone variability rather well (the example for Kiruna station). In the overwhelming majority of cases, both models correctly respond to TOC variations.

## LONG-TERM OZONE TRENDS

The relatively long period of analysis (15 years) allows assessing long-term variations in ozone values. Such estimates were provided with the simple model of linear approximation for TOC and OC in the layers of 0–25 and 25–60 km for all time series (Table 2).

It is noteworthy that the trends are close to zero for all analyzed cases and are often smaller than the errors of their calculation. The SBUV data reveal an insignificant negative trend in the layer of 0–25 km (1.68% per decade) at Saint Petersburg station and a small positive trend (2.1% per decade) for the layer of 25–60 km. It should be noted that satellite data reveal a small positive trend in OC in this layer for all stations (minimum for Kiruna and maximum for Harestua). At the same time, the models also detect the statistically significant positive trend in this layer only for Harestua station; however, its value is much smaller than the value derived from satellite data. All trend estimates for TOC are statistically insignificant. Taking into account the values of trend calculation errors, it can be concluded that both measurements and simulations generally indicate very small trends in ozone values in the area of the analyzed ground-based subarctic stations during 2000–2015. The authors of [14] provided the analysis of ground-based measurements of ozone values performed with Bruker Fourier spectrometers; it demonstrated that no significant

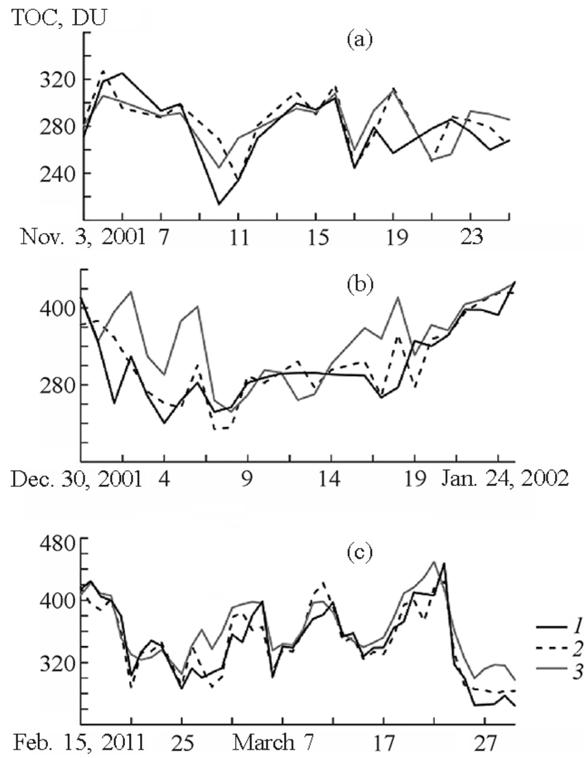


**Fig. 3.** The temporal variations in TOC from the data of (*1*) SBUV measurements and (*2*) EMAC and (*3*) RSHU models during the periods of significant TOC variations at (a) Saint Petersburg, (b) Harestua, and (c) Kiruna stations.

**Table 2.** Quantitative characteristics of trends in daily mean ozone values measured with the SBUV satellite instrument over different ground-based stations for the period of 2000–2015 as well as the uncertainty of trends for the confidence interval of 95%

| Station | Layer, km | | | | | |
|---|---|---|---|---|---|---|
| | 0–25 | | 25–60 | | 0–60 | |
| | DU/year | %/decade | DU/year | %/decade | DU/year | %/decade |
| Saint Petersburg | **–0.39 0.24** | **–1.68 1.03** | **0.22 0.07** | **2.1 0.7** | –0.17 0.27 | –0.51 0.81 |
| Harestua | –0.02 0.23 | –0.07 1.02 | **0.25 0.07** | **2.4 0.7** | 0.23 0.27 | 0.7 0.80 |
| Kiruna | –0.20 0.30 | –0.82 1.25 | **0.14 0.08** | **1.48 0.78** | –0.06 0.35 | –0.17 1.04 |

Note: The statistically significant estimates are bolded.

TOC trends are observed for Harestua station in 1995–2012 and for Kiruna station in 1996–2012. TOC measurements with the Bruker 125HR Fourier spectrometer have also been conducted since 2009 at Petergof station in the neighborhood of Saint Petersburg [1, 13]. The estimates for the period of 2009–2016 based on ground-based measurements at this station also revealed the absence of statistically significant TOC trends.

## BASIC RESULTS AND CONCLUSIONS

The temporal variations in ozone values in two layers (0–25 and 25–60 km) and in TOC over three subarctic observation stations (Saint Petersburg, Harestua, and Kiruna) were studied for the period of 2000–2015 using the SBUV measurement data and RSHU and EMAC model simulations.

In general, the results of numerical simulations are in good agreement with satellite data on ozone columns. The correlation between the data of measurements and simulations is 0.95–0.96 for EMAC and 0.78–0.84 for RSHU. At the same time, EMAC underestimates TOC and OC in the layer of 0–25 km more significantly (by 2.5–5%) than RSHU (by 0–4%). The absolute values of the difference between the SBUV data and RSHU simulation results are the smallest for Saint Petersburg (0–3 DU) and the highest for Kiruna (4–10 DU). For EMAC this difference is also minimum for Saint Petersburg (2–10 DU).

The analysis of monthly mean ozone values revealed that both models underestimate TOC and OC in the layer of 0–25 km by 5–10 DU during the period from April to October inclusive. In the other months the TOC simulations based on EMAC agree well with measurements at all three stations. At the same time, in January–March the RSHU model data on TOC exceed both the EMAC data (by 10–20 DU) and satellite data (by 10–15 DU). In the layer of 25–60 km, where ozone values are mainly regulated by photochemical reactions, the model values of OC overestimate experimental data during the first four months of the year: by 1–4 DU for EMAC and by 7–10 DU for RSHU.

Both models describe the cases of rapid TOC decline rather well that is important for the prediction of surface UV irradiance. The RSHU model often underestimates the TOC decrease (sometimes up to 35 DU). For EMAC this underestimation is 10 DU on average (Saint Petersburg and Harestua); at Kiruna station, EMAC even overestimates the TOC loss.

The estimates of long-term ozone trends for the period of 2000–2015 demonstrated that, with account of trend calculation errors, both model and experimental data indicate very small changes in OC over the analyzed subarctic stations. The reliable estimates include ozone loss in the layer of 0–25 km (–1.68  1.03% per decade) and the OC increase (2.1  0.7% per decade) in the layer of 25–60 km from SBUV data in Saint Petersburg. The OC increase in the layer of 25–60 km is also observed from measurement data for Harestua and Kiruna stations: by 2.4  0.7% and 1.5  0.8% per decade, respectively. The model results do not contradict these estimates.

Thus, both models may be used for the prediction, analysis, and assessment of short- and long-period variations in ozone values in subarctic latitudes.

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