
STYDYING SEAS AND OCEANS
FROM SPACE

Study of Ozone Layer Variability near St. Petersburg on the Basis of SBUV Satellite Measurements and Numerical Simulation (2000–2014)

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Abstract—A comparison between the numerical simulation results of ozone fields with different experimental data makes it possible to estimate the quality of models for their further use in reliable forecasts of ozone layer evolution. We analyze time series of satellite (SBUV) measurements of the total ozone column (TOC) and the ozone partial columns in two atmospheric layers (0–25 and 25–60 km) and compare them with the results of numerical simulation in the chemistry transport model (CTM) for the low and middle atmosphere and the chemistry climate model EMAC. The daily and monthly average ozone values, short-term periods of ozone depletion, and long-term trends of ozone columns are considered; all data sets relate to St. Petersburg and the period between 2000 and 2014. The statistical parameters (means, standard deviations, variations, medians, asymmetry parameter, etc.) of the ozone time series are quite similar for all datasets. However, the EMAC model systematically underestimates the ozone columns in all layers considered. The corresponding differences between satellite measurements and EMAC numerical simulations are $(5 \pm 5)\%$ and $(7 \pm 7)\%$ and $(1 \pm 4)\%$ for the ozone column in the 0–25 and 25–60 km layers, respectively. The correspondent differences between SBUV measurements and CTM results amount to $(0 \pm 7)\%$, $(1 \pm 9)\%$, and $(-2 \pm 8)\%$. Both models describe the sudden episodes of the ozone minimum well, but the EMAC accuracy is much higher than that of the CTM, which often underestimates the ozone minima. Assessments of the long-term linear trends show that they are close to zero for all datasets for the period under study.

Keywords: atmospheric ozone, numerical simulation, satellite measurements

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INTRODUCTION

A comparison between the simulation results of spatiotemporal variations in the ozone column in a model and data of different measurements allows estimating the model quality and, if necessary, its refinement, which allows the use of the models for reliable forecasts of the ozone variations under different scenarios of anthropogenic and natural impacts on the ozone-sphere. The forecasts of a significant decrease in the total ozone column (TOC) are particularly important near megacities due to the increase in the UV illumination of the surface with the appearance of ozone “mini-holes.” The simulation results were compared with TOC measurements repeatedly (Wiel et al., 1998; WMO, 2003, 2007; Egorova et al., 2005; Eyring et al., 2005; 2006; Virolainen et al., 2016; Pendlebury et al. 2015).

However, considering only the TOC measurement data does not allow discriminating all the altitude features of the ozone-column variability or objectively

identifying the photochemical and dynamic factors that determine the seasonal and interannual variability that is observed. Comparisons for individual atmospheric layers are of a higher information content, since different processes of ozone formation and transformation prevail at different altitudes (Smyshlyaev et al., 2017). Note that the validation of different models is carried out regularly using various ground-based and satellite measurements. Special sites have been created for validation (e.g., <http://gmes-atmosphere.eu/d/services/gac/verif/grg/gaw> and (Eyring et al., 2016)).

Climatological (monthly average) characteristics of key atmospheric parameters are usually compared during the validation, i.e., temperature, wind field, humidity, ozone column, etc., for different periods of analysis. The comparisons are often carried out for different latitudinal zones and with certain characteristics (e.g., systematic and random deviations). In this work, we compare satellite measurements of the ozone

Table 1. Statistical parameters of the data ensembles under study

Layer, km	0–60			0–25			25–60		
	SBUV	EMAC	XTM	SBUV	EMAC	XTM	SBUV	EMAC	XTM
Parameter									
Mean, DU	333	317	333	230	215	228	103	102	105
SD, DU	48	50	51	42	45	42	13	12	14
Coefficient of variation, %	14	16	15	18	21	18	13	12	13
Median, DU	326	310	325	224	207	220	106	105	106
Asymmetry factor	0.55	0.70	0.56	0.73	0.84	0.71	–0.57	–0.44	–0.02
Kurtosis	0.00	0.32	–0.27	0.30	0.52	–0.04	–0.39	–0.38	–0.45

column in two atmospheric layers, 0–25 and 25–60 km, with data from two different models. The measurements and calculations refer to St. Petersburg in 2000–2014. The comparisons are made both for the daily and monthly averages values, which is relevant for climatological studies. Trends in the ozone columns are also compared.

OZONE-COLUMN MEASUREMENTS AND SIMULATION

The TOC is determined by different satellite methods, for example, from measurements of thermal radiation in the 9.6- μm ozone band (Uspensky et al., 1998; Polyakov et al., 2010). In the work (Virolainen et al., 2013), the TOC data from the OMI satellite instrument, which measures the spectra of outgoing (reflected and scattered) radiation in the 270–500 nm region, are compared with TOC measurements by a number of ground-based instruments.

In this work we use satellite measurements by the Solar Backscatter Ultraviolet Instrument (SBUV); they allow one to determine not only TOC, but also the ozone column in different altitude layers. The SBUV instruments perform nadir measurements of the spectra of reflected and scattered solar radiation in the 250–340 nm region with a horizontal resolution of about 200 \times 200 km. Descriptions of the instrument, interpretation algorithms, and an analysis of measurement errors can be found in the work (Bhartia et al., 2013). The accuracy of satellite measurements of ozone in thick atmospheric layers is 5–15%.

To study the altitude and temporal properties of the variability of the ozone column near St. Petersburg, the following two models were used:

(i) a chemical transport model (CTM) of the composition of the lower and middle atmosphere, which considers the variability of 74 trace atmospheric gases interacting in 174 chemical and 46 photo dissociation reactions and covers an altitude range from 0 to 60 km with a horizontal resolution of 300–400 km (Galín and other, 2007);

(ii) the EMAC (ECHAM/MESSy Atmospheric Chemistry model) chemical climate model, which simulates chemical and dynamic processes in the

atmosphere from 0 to 80 km with a horizontal resolution of 300 \times 300 km (Jöckel et al., 2006).

Unlike the EMAS model, the CTM uses MERRA data (Modern-Era Retrospective Analysis for Research and Applications) (Rienecker et al., 2011). The models and different results of their use are described in detail in the works (Virolainen et al., 2016; Smyshlyayev et al., 2005, 2010a, 2010b, 2017). In the present work, the comparisons are carried out for the period from January 2000 to June 2014, inclusively.

COMPARISON BETWEEN SIMULATION AND MEASUREMENT RESULTS

General Characterization of the Comparison

Table 1 shows the statistical characteristics of the three data ensembles under study (SBUV measurements and EMAS and CTM results on TOC and ozone column for two layers, 0–25 and 25–60 km): the mean distribution and its standard deviation (SD); the coefficient of variation, which determines the parameter dispersion; the distribution median which divides the distribution in half; the asymmetry factor, which characterizes the deviation in the parameter distribution in one or another direction; and the kurtosis, which determines the sharpness of the distribution peak. The boldface model parameters agree the best with satellite measurements.

Let us first of all note that both models (EMAS and CTM) reproduce the basic statistical parameter of the time series of ozone column derived from satellite data well. For the TOC (0–60 km), the CTM precisely predicts the means, slightly overestimates the SD, and very accurately reproduces the median of the distribution and the asymmetry factor. The kurtosis in this model, however, differs noticeably from the SBUV data. Most of the parameters of the TOC distribution in the CTM are in better agreement with the satellite measurements than in the EMAS model. For the 0–25 km layer, most of the statistical parameters for the CTM also agree better with the measurement data. The EMAS model slightly underestimates the means and the median of the ozone column and overestimates the SD, the coefficients of variation, the asymmetry factor, and the kurtosis (like for the TOC) in

Table 2. Statistical parameters of the comparison between different ensembles

Layer, km	0–60			0–25			25–60		
ensemble	discrepancy		CC	discrepancy		CC	discrepancy		CC
	DU	%		DU	%		DU	%	
SBUV–EMAC	16 ± 16	5 ± 5	0.946 ± 0.001	15 ± 15	7 ± 7	0.938 ± 0.002	1 ± 4	1 ± 4	0.959 ± 0.001
SBUV–XTM	0 ± 23	0 ± 7	0.893 ± 0.003	2 ± 20	1 ± 9	0.883 ± 0.003	–2 ± 8	–2 ± 8	0.820 ± 0.005

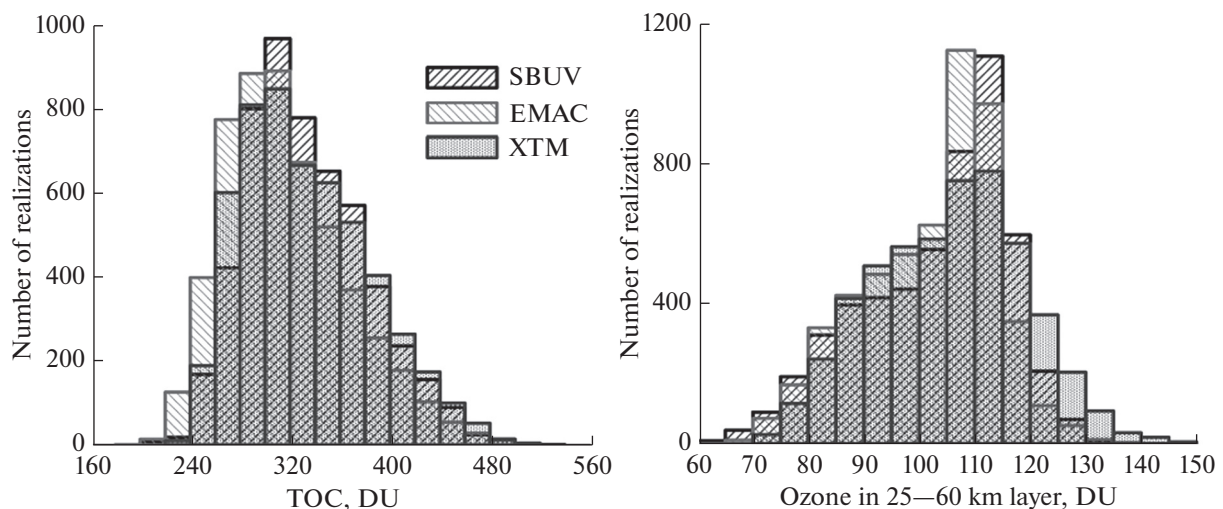
this layer. We can note that the EMAS model predicts the means, SD, asymmetry factor, and kurtosis better; the CTM predicts the coefficient of variation and the median better. Thus, for the 25–60 km layer, the distribution parameters in the EMAS model on the average agree better with the ozone-column distribution parameters from the satellite data than in CTM.

Numerical characteristics of the absolute and relative discrepancies between the two models (means and SD) and the satellite measurement data are given in Table. 2, as well as the coefficient of correlation (CC) between the ensembles. The EMAS model underestimates TOC (0–60 km) by 5%; the random component of the discrepancies is also 5%. For the CTM there are no systematic discrepancies, and the SD is 7%. The CC is maximal for the comparisons between EMAS and SBUV. For the 0–25 km layer, the EMAS model also underestimates the ozone column by 7% on average in comparison with satellite measurements, and the random component of the discrepancies between them is relatively small (7%). The same comparisons with the CTM data show very small systematic discrepancies (1.0%), but a large random component of them (9%). The CCs are maximal in the comparison between the time series of satellite measurements and EMAS results. For the 25–60 km layer, both absolute and relative discrepancies between the models and the

experimental data are small. Thus, the EMAS results differ from satellite data by 1%, the random discrepancy being 4%. The discrepancies for the CTM are a little larger, 2 and 8%, respectively. The CC is maximal for the comparison between the EMAS and the experimental data. It can be noted that the EMAS model generally agrees better with satellite measurements in this layer.

The distribution functions for the TOC and ozone column in the 15–60 km layer are compared in Fig. 1 for example. A good agreement is seen for all three ensembles and layers. It can only be noted that the EMAS model provides for a slightly larger number of realizations with a low TOC and ozone column in the 0–25 km layer in comparison with satellite data and the CTM. This feature of the model (some underestimation of ozone) was also noted earlier.

The seasonal variations in simulated and measured TOCs and ozone columns in the 25–60-km layer are exemplified in Figs. 2 and 3, where the monthly mean ozone columns, calculated from three data ensembles, and the difference between the experimental and model data are shown. Both models describe the seasonal variations in the TOC with high accuracy. The EMAC model underestimates the TOC in comparison with satellite measurements (by 20–40 DU on the average). When simulating in the CTM, the differ-

**Fig. 1.** Distribution histograms of TOC and ozone column in the 25–60 km layer.

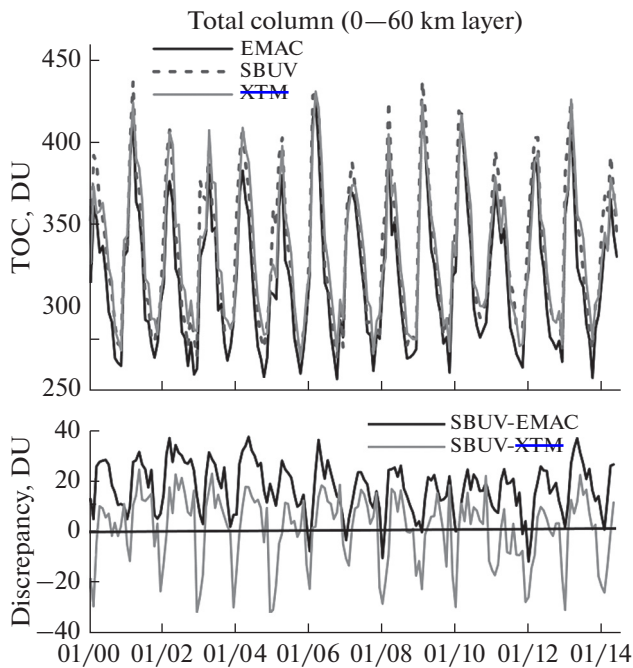


Fig. 2. Seasonal variations in the monthly mean TOC values for different ensembles and their discrepancy in the 0–60 km layer.

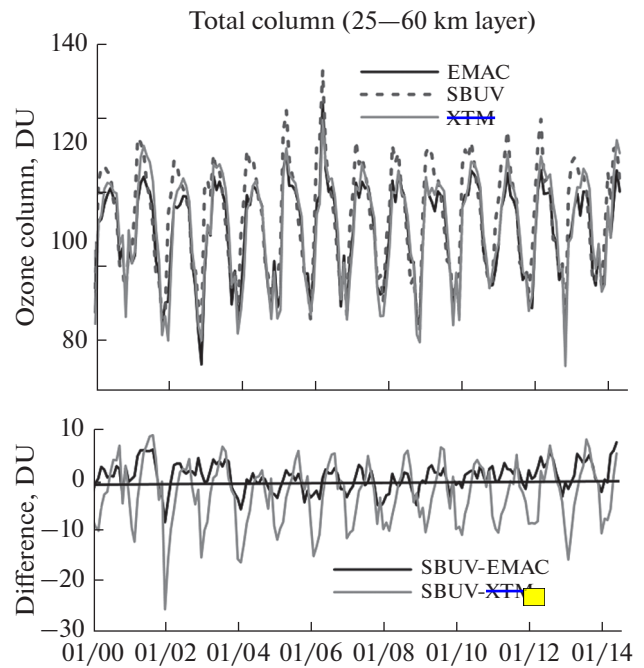


Fig. 3. Seasonal variations in the monthly mean ozone partial column in the 25–60 km layer for different ensembles and their discrepancy.

ences in TOC are usually no higher than 20–30 DU. Let us note that a similar pattern is observed for the 0–25 km layer, where the atmospheric ozone is mainly accumulated.

The CTM overestimates the ozone column in the 25–60-km layer on average (by up to 10–15 DU at maxima) in comparison with the measurements (Fig. 3). The EMAC model properly reflects the seasonal variations in SBUV data on ozone; the difference between the two ensembles does not exceed 5 DU.

Short-Term Ozone Layer Depletion

The reproducibility of rapid and significant decreases in ozone by the models is important for forecasts of the increase in UV illumination of the surface. The analysis of the SBUV data allows one to identify 131 cases of rapid and short-term 10% (or more) decreases in TOC during the day in the vicinity of St. Petersburg over 15 years.

Figure 4 exemplifies such changes in TOC in February–May of 2011. Sharp decreases in TOC were observed in early March and in late March–early April. According to the satellite measurements, those changes were ~100–120 DU. Let us note that such ozone depletion can result in a ~30% increase in UV fluxes on the Earth’s surface under certain conditions. In late February–early March, the EMAS model reproduces the drop in ozone the most accurately; in late March–early April, both models reproduce the

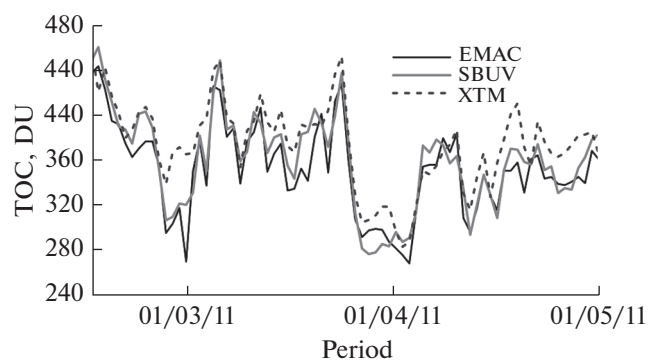


Fig. 4. Variations in TOC in spring 2011 according to data of different ensembles.

changes in TOC approximately equally accurately, but the EMAS is more accurate.

Table 3 presents the statistical characteristics of the discrepancy between the experimental (SBUV) and

Table 3. Statistical characteristics of the comparison between different ensembles for 131 days of observation of a rapid 10% increase in TOC

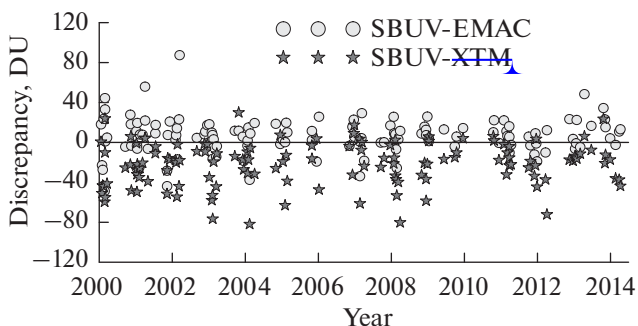
Ensemble	Discrepancy		CC
	DU	%	
SBUV-EMAC	6 ± 18	2 ± 6	0.93 ± 0.01
SBUV- XTM	-22 ± 22	-7 ± 7	0.92 ± 0.01

Table 4. Quantitative characteristics of trends (linear regression) in the daily mean ozone column in the layers per year (in DU) and decade (in %) and the trend uncertainties in a 96% confidence interval

Layer, km	0–25		25–60		0–60	
	DU/year	%/decade	DU/year	%/decade	DU/year	%/decade
ensemble						
SBUV	-0.28 ± 0.27	-1.24 ± 1.17	+0.13 ± 0.08	+1.3 ± 0.8	-0.15 ± 0.31	-0.4 ± 0.9
EMAC	+0.19 ± 0.29	+0.9 ± 1.3	+0.075 ± 0.002	+0.74 ± 0.02	+0.27 ± 0.32	+0.9 ± 1.0
XTM	+0.12 ± 0.27	+0.5 ± 1.2	+0.10 ± 0.09	+0.9 ± 0.8	+0.22 ± 0.32	+0.7 ± 1.0

model data for the days of a 10% decrease in TOC with respect to the previous days. The EMAC model slightly underestimates the TOC minima (by 2%), while CTM overestimates them (by 7%). The random components of the discrepancy between the experimental and model data are 6 and 7% for the EMAC and CTM, respectively. The CC for both models exceeds 0.9. When comparing these data for all measurement days with the data from Table. 2, it can be seen that the accuracy of the description of measurements in the EMAC model depends little on the intensity of variations in TOC; i.e., the EMAC model qualitatively reacts to a sharp decrease in ozone, but it quantitatively underestimates its depth. At the same time, when comparing the SBUV data and CTM results (Table 3), a significant increase in systematic errors is observed; i.e., the CTM usually significantly overestimates the ozone column in days of its decrease. Thus, the CTM does not show a rapid or sharp decreases in TOC.

Figure 5 shows the discrepancies between the SBUV measurement data and the TOC values simulated in the two models. This figure visualizes the data presented from Table 3. Thus, the discrepancy between the measurements and the CTM results is negative in most cases; i.e., CTM overestimates the ozone values at its minima. The EMAC model slightly underestimates the ozone-column minima on the average, which is typical for the results of a comparison between the EMAC and SBUV data.

**Fig. 5.** Discrepancy between the measured and simulated TOC values in days of its 10% decrease.

Long-Term Ozone Trends

A relatively long period of analysis (about 15 years) allows estimating the long-term trends in the ozone column. We made such estimates using a simple linear trend model for TOC and the ozone column in the 0–25 and 25–60 km layers for all three time series (Table 4).

First and foremost, we note that the resulting trends are close to zero for all the cases under study and often lower than the calculation errors. Boldface numbers are statistically significant values of the given trends. According to SBUV data, there is a minor negative trend in the 0–25 km layer (a little more than 1% per decade). For the 25–60 km layer, all three time series give a small positive trend, no larger than 1.3% per decade (according to satellite data). Taking into account the trend calculation errors, we can say that both measurements and simulation generally point out to minor trends in the ozone column in the region of St. Petersburg in 2000–2014.

MAIN RESULTS AND CONCLUSIONS

SBUV measurements of TOC and ozone partial columns in two atmospheric layers—0–25 and 25–60 km—were compared with numerical simulation data for St. Petersburg within the CTM and EMAC models: the daily and monthly means, short-term decrease in TOC (mini-holes), and long-term trends for 2000–2014. This study allows us to draw the following main conclusions.

1. The results of calculations in the two models are in a good agreement with SBUV measurements for the conditions of St. Petersburg. Statistical characteristics of the three time series (the means, SD, medians, asymmetry factors, etc.) are well matched. The statistical parameters of the temporal distribution of TOC and the ozone partial column in the 0–25 km layer according to the CTM agree better on the average with the satellite data when compared to the EMAC model. This is due to the use of the MERRA data on wind, temperature, humidity, and pressure fields in the CTM. The opposite is true for the 25–60 km layer: EMAC parameters agree on average better with the satellite data.

2. The EMAS model can underestimate TOC by 16 DU (5%) on average in comparison with the satellite data; the random component of the discrepancies reaches 16 DU (5%). For CTM, there are practically no systematic discrepancies, SD is 23 DU (7%). The EMAS model also underestimates the ozone values in the 0–25 km layer on average when compared to satellite measurements (by 15 DU, 7%), and the random component of the discrepancies between them is relatively small (15 DU, 7%). The same comparisons with CTM data show very small systematic discrepancies (2 DU, 1%), but a large random component (20 DU, 9%). For the 25–60 km layer, the discrepancies between the models and the experimental data are also small. The EMAS model differs from the satellite data by 1%, with random discrepancies of 4%. Slightly larger discrepancies are observed for CTM: –2 and 8%, respectively. The CC are maximal for the comparison between the SBUV and EMAS data, but are quite high when compared with the CTM.

3. Examples of comparisons of the ozone distribution functions (histograms) between satellite and model data show their similarity. It can only be noted that the EMAS model gives a slightly larger number of realizations with low values of TOC and ozone column in the 0–25 km layer in comparison with satellite data and CTM.

4. A comparison of the seasonal variations between different ozone data shows the high quality of the model description of the interannual variations, which manifest themselves in variations in the monthly mean minima and maxima. However, the EMAS model gives on the average lower values of the monthly mean TOC than the satellite measurements (up to 20–40 DU). When modeling in the CTM, the differences with the experiment usually do not exceed 20–30 DU.

5. Both models describe the sharp decreases in ozone well, but the EMAS model does this with a much higher accuracy than the CTM; the CTM often overestimates the observed minima in the ozone column.

6. The simplest estimates of long-term linear trends in ozone show that they are close to zero both in the experimental and model data for the period 2000–2014.

Note that numerous comparisons with the EMAS simulation results are contained in works (Righi et al., 2015; Jöckel et al., 2016). The validation of the ozone-content simulation results shows that the model is in a good agreement with the measurements.

The qualitative reproduction of zonal mean ozone columns is remarkable, in particular, high ozone levels in spring in the Northern hemisphere. However, the tropospheric ozone values are overestimated by this model by about 20%. The differences are smaller in the stratosphere; the model underestimates the measurements by 5% on average. Only in summer (June–September) do the discrepancies reach 20%. Our comparisons between the EMAS data and SBUV

measurements near St. Petersburg show significantly smaller discrepancies on average.

Finally, our estimates of long-term trends are in a good agreement with the estimates from the work (Harris et al., 2015). For a close time period (1998–2012), the estimates of trends from various experimental data (ground-based and satellite) are close to zero for the 35°–60°N latitude belt.

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