Нейронно-сетевой подход к определению общего и тропосферного содержания озона из спектральных измерений ИКФС-2

Neural network approach to determination of total and tropospheric ozone columns from spectral measurements of IKFS-2

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The role of atmospheric ozone

Ozone plays a crucial role in climate formation, and it shields life on Earth from harmful UV radiation. Ozone in the troposphere is a pollutant and greenhouse gas. Therefore, it is essential to monitor both total and tropospheric ozone columns.

The global ozone monitoring system includes remote, ground-based, and local methods. Only satellite methods can be used to monitor the global distribution of ozone.

Satellite methods that use the measurements of outgoing thermal radiation provides information on ozone not depending on solar illumination.

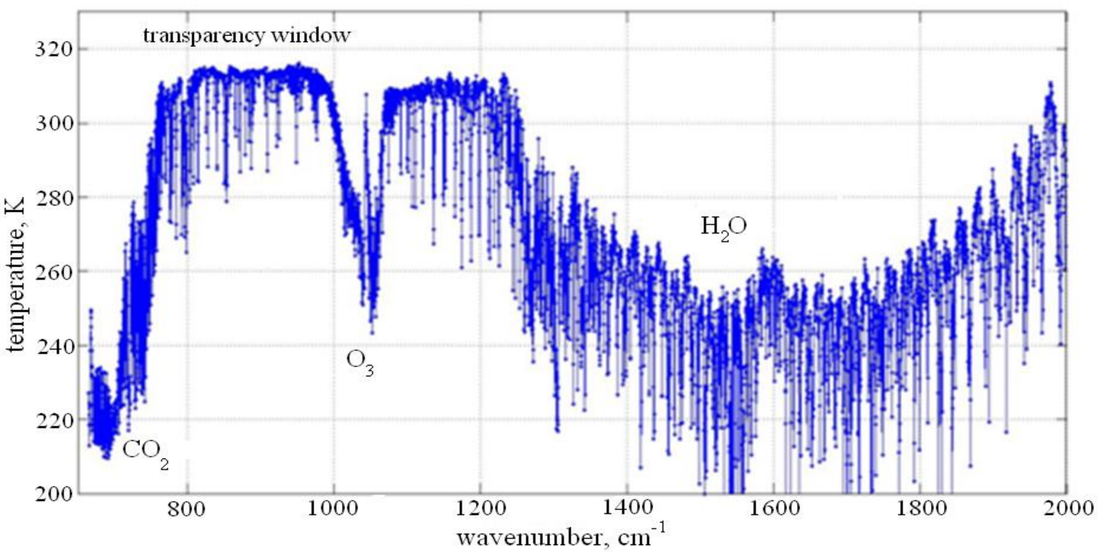
We present the techniques for deriving information on total ozone columns (TOCs) and tropospheric ozone columns (TrOCs) from spectra of outgoing thermal radiation measured by the IKFS-2 instrument aboard the “Meteor-M” No. 2 satellite, which are based on the artificial neural network (ANN) approach and the principal component (PC) analysis.

Methods for measuring the atmospheric ozone content

1. In situ: near surface, aircraft, balloon (ozonesondes)
2. Remote
   1. Ground – based (local)
      1. Direct Solar Radiation: IR,UV, VID
         FTIR; Dobson and Brewer instruments – «reference standard»
      2. Scattered solar radiation UV, VID, NIR
      3. Scattered solar radiation at low Sun (Umkehr)
      4. Microwave thermal radiation
      5. Lidars
   2. Satellite (global)
      1. Scattered-reflected solar radiation (OMI, TROPOMI)
      2. Transmittance - Solar occultation (ACE-FTS), stars occultation
      3. **Outgoing thermal IR radiation (IASI, CrIS, IKFS-2 etc)**
      4. Microwave radiation (limb - MLS)
      5. Measurements of emissions in UV, VIS and NIR regions of the spectrum

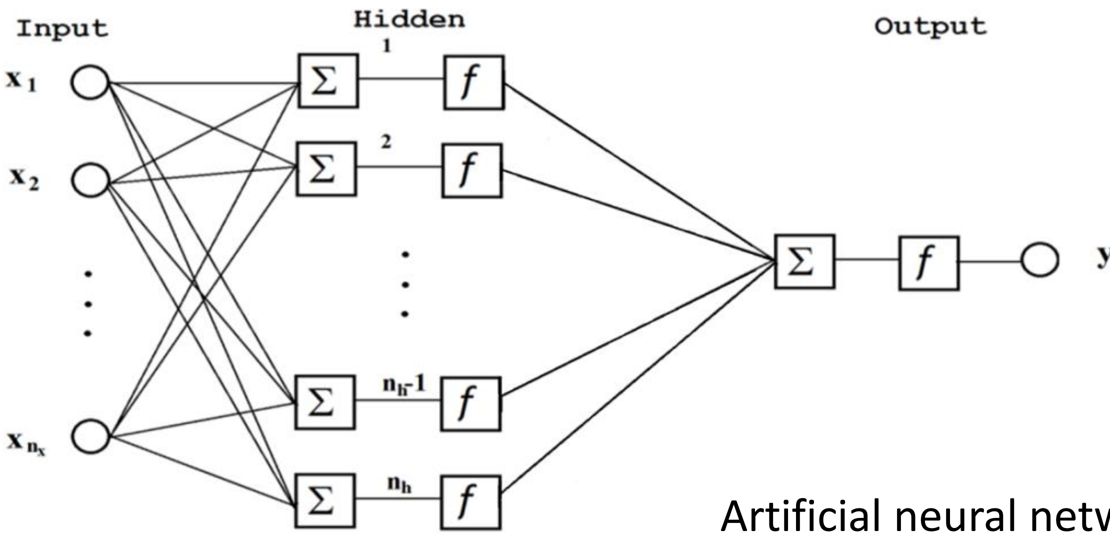
IKFS-2 instrument

The IKFS-2 spaceborne infrared Fourier-transform spectrometer measures outgoing infrared radiance and provides data on the atmosphere for numerical weather prediction and various applications in the field of atmospheric and climate sciences.
IKFS-2 is one of the key instruments of the Meteor-M №2 satellite. The instrument was developed by the Keldysh Research Center together with Krasnogorsky zavod and Bauman State Technical University (Moscow).



parameter	requirement
spectral range	5-15 µm
spectral resolution	0.4 cm^{-1}
calibration error, no more than	0.5 K
NESR, $[W \cdot m^{-2} sr^{-1} cm]$	$3.5 \cdot 10^{-4}$, λ = 6 µm $1.5 \cdot 10^{-4}$, λ = 13 µm $4.5 \cdot 10^{-4}$, λ = 15 µm
spatial resolution at sub-satellite point	35 km
swath width	1000…2500 km
sampling period	0.6 s

Ozone retrieval technique



f – activation function

x_j – one of input parameters

$b_i^1, \omega_{i,j}^1, \omega_i^2, b^2$ - coefficients

Artificial neural network (ANN) is a three-layer perceptron. Activation function is logistic.

$$Ozone = y = f(b^2 + \sum_{i=1}^{N_h} \omega_i^2 f(b_i^1 + \sum_{j=1}^{N} \omega_{i,j}^1 x_j)) \qquad (1)$$

Description of the retrieval technique and procedure

Algorithm for constructing the solution operator

1. Preparation of data for the training sample
    1. Preparation of IKFS-2 spectral measurements (***233,673,330*** spectra from 2015 to December 2022 - all data with a swath width 1000 and 1500 km***)***
    2. Calculation of the average spectrum, covariance matrices, EOF.
    3. Preparation of ozone data, OMI data for TOC and ozonesonde data for TrOC

2. Building a training sample

    1. Measurement pair matching,

        TOC: 70 km, 5 hours with OMI –> 20,262,148 pairs

        TrOC: 200km, 24 hours with ozonosondes –> 561,625 pairs

    2. Calculation of the PC and assembly of the training data sets

    3. ANN training (expression (1) minimization)

4. Testing of various ANNs (different number of PCs, number of hidden layer neurons (NHLN), inclusion of latitudinal-seasonal parameters in predictors)

5. Validation

Results of the ANN training

Training for TOCs:

Training set was based on the OMI level 2 data.
Selection conditions: time mismatch less than 5 hours, distance less than 70 km.
20,262,148 pairs of the IKFS-2 spectra and OMI TOCs were selected.
Optimal predictors set: Satellite Zenith Angle, Day of the year, 50 PCs of ozone absorption band, 25 PCs of the whole measured spectrum, 40 NHLN.
Training results: approximation error calculated with the whole (100%) data set equals **8.8 DU**

Training for TrOCs:

Training set was based on the HEGIFTOM ozonosonde data collection.
Selection conditions: time mismatch less than 24 hours, distance less than 200 km.
561,625 pairs of IKFS-2 spectra and ozonosonde data were selected.
Optimal predictors set: Satellite Zenith Angle, Day of year, 35 PC of whole measured spectrum, and 55 NHLN.
Training results: approximation error calculated with the whole (100%) data set equals **2.7 DU and 3.7 DU for layers lower 400 and 300 hPa**

Validation of the IKFS-2 TOC retrieval by comparison with ground-based and satellite measurements

Satellite data		Ground-based data	
TROPOMI, QF>0.9, TOCs >100 and TOCs < 650 DU		**Dobson and Brewer**, Direct Sun	
6 hours, 35 km		1 hour, 70 km	
May 2018-Dec 2022		March 2015 – Dec 2022	
Bias, %	**SDD, %**	**Bias, %**	**SDD, %**
-2.22	**2.73**	**-0.41**	**2.67**

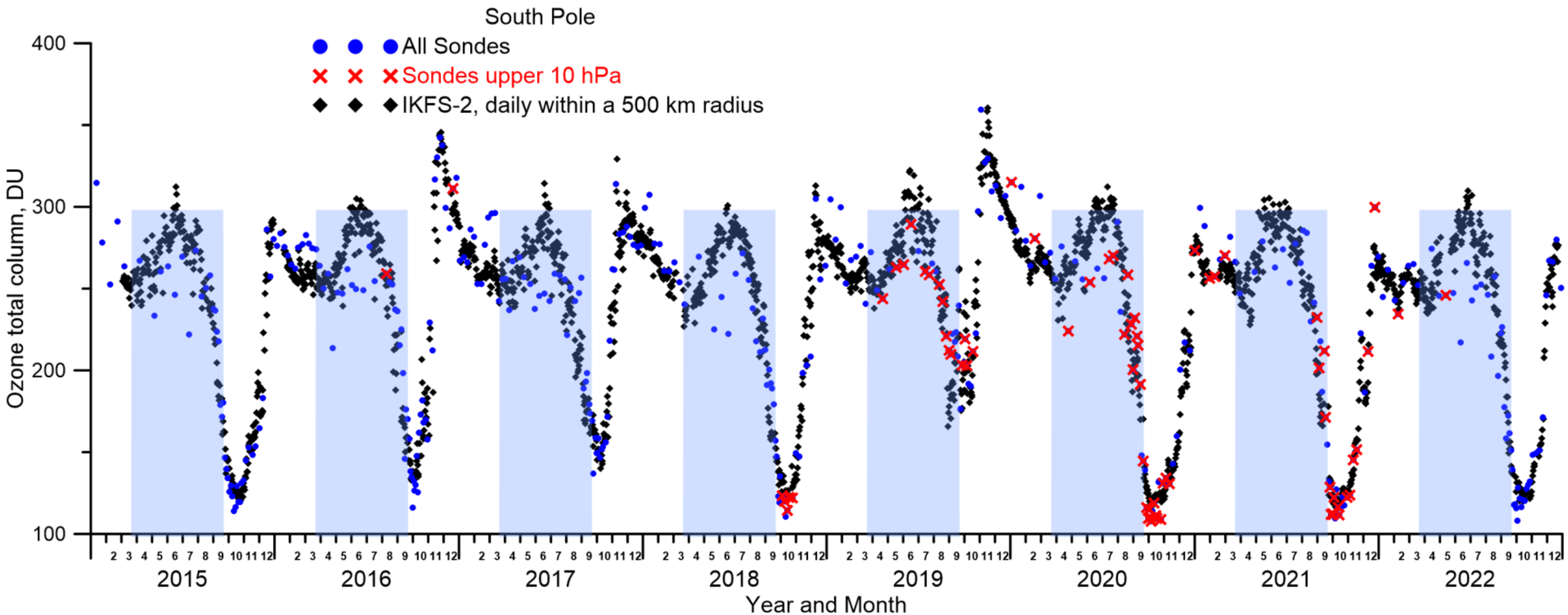
Validation of the IKFS-2 TOCs by comparison with ozonosonde data

Ozonosonde data	
HEGIFTOM homogenized data	
1 hour and 70 km distance (for South Pole 200 km distance)	
March 2015 - Dec 2022 (for South Pole 2021-2022)	
Single stations	
Bias, %	SDD, %
-1.6 – 6.9	**5.3 – 11**
Mean	
Bias, %	SDD, %
1.2	**7.9**

The differences are consistent with the uncertainty of the TOC retrievals obtained from the ozone sounding data.

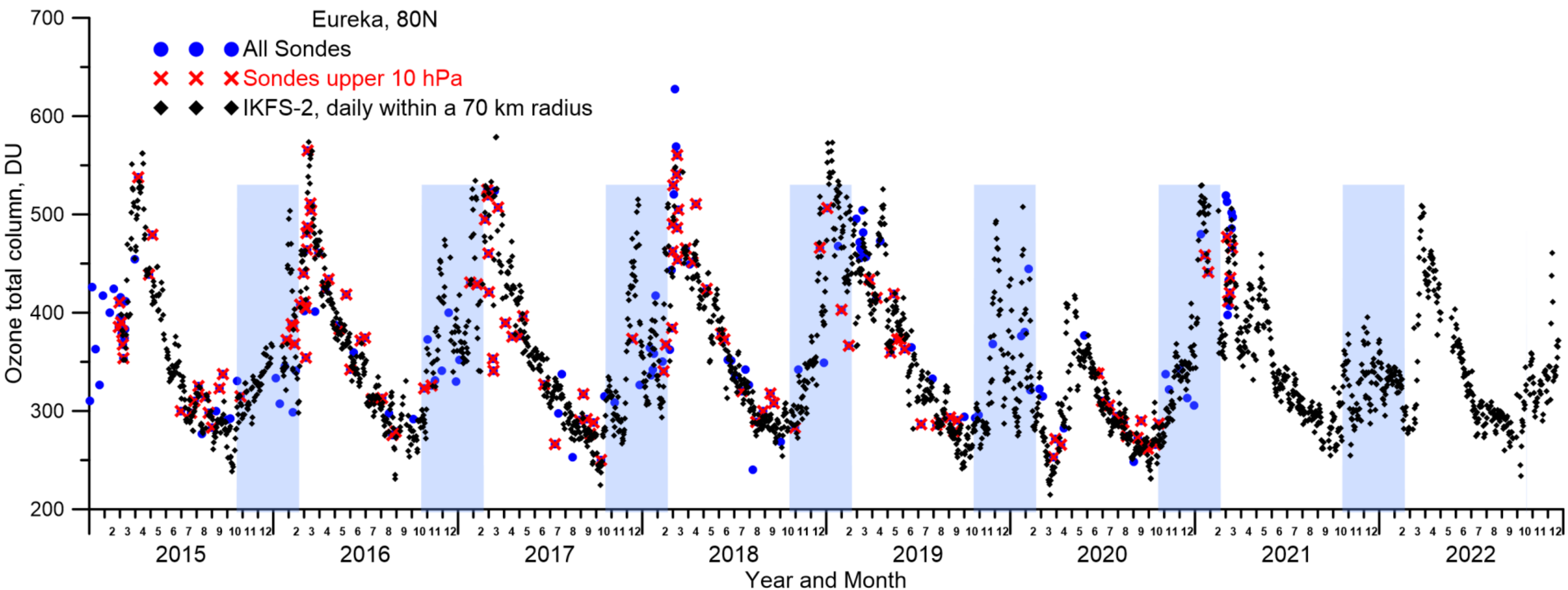
Specific conditions of comparison for the South Pole stations are caused by the Meteor-M N2 satellite orbit and the swath width of IKFS-2

Validation of the IKFS-2 TOCs by comparison with ozonosonde data



TOCs obtained from ozonesounding data and IKFS-2 daily averaged TOCs in a circle with a radius of 500 km and a center **at the South Pole station**. The periods of **the polar night are highlighted** in color.

Validation of the IKFS-2 TOCs by comparison with ozonosonde data



TOCs obtained from ozonesounding data and the IKFS-2 daily averaged TOCs in a circle with a radius of 70 km and a center **at the Eureka station (80°N)**. The periods of **the polar night are highlighted** in color.

Validation of the IKFS-2 TrOCs comparison with the FTIR data

Ground-based data
FTIR measurements, NDACC network, daily averaged TrOCs
IKFS-2 daily averaged TrOCs in a circle with a radius of 100 or 200 km to GB stations
March 2015-Dec 2022

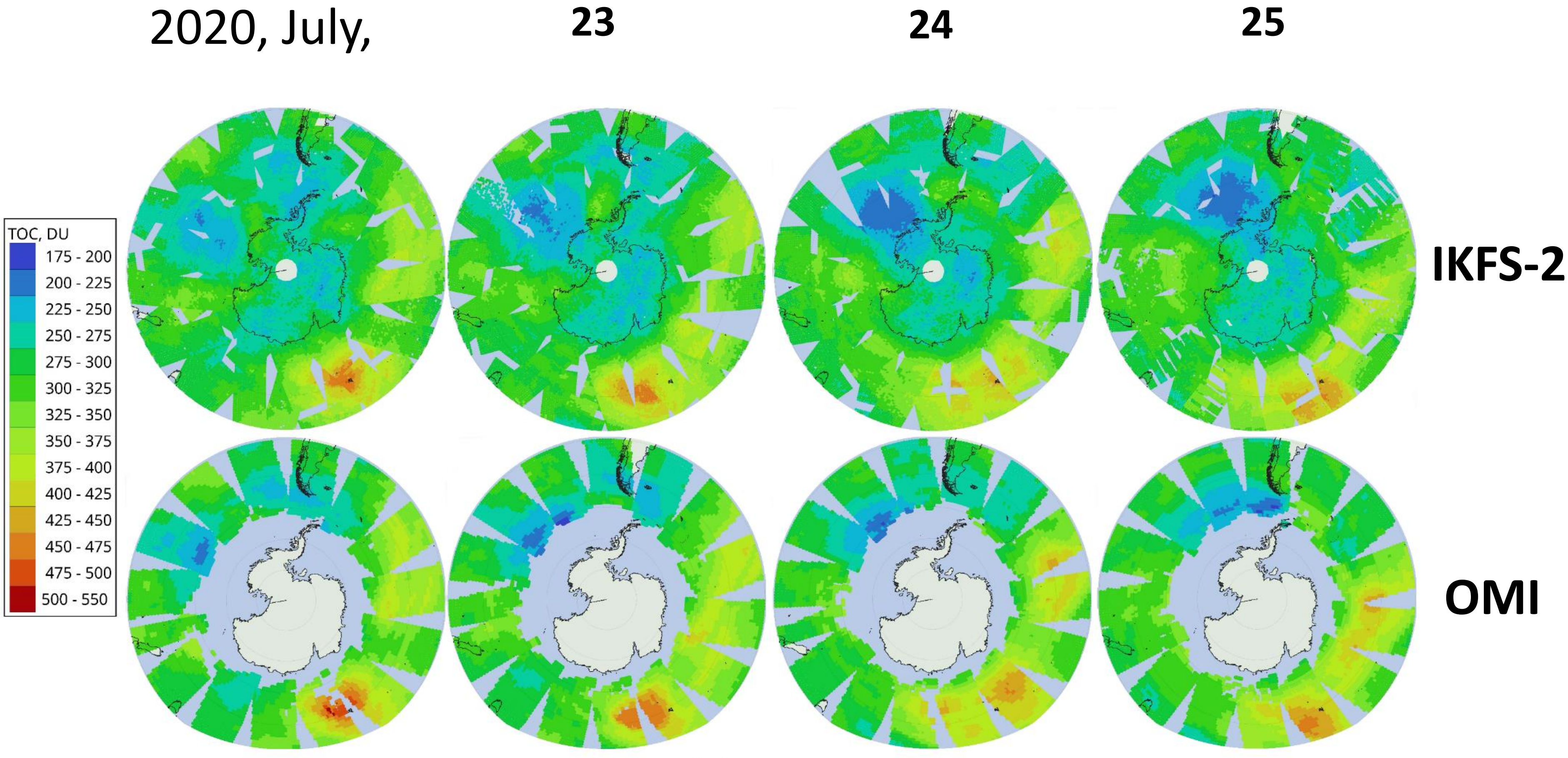
Mean SDDs for sites, DU

Lower	Averaging radius, km	
	100	200
300 hPa	2.91	2.95
400 hPa	3.00	2.99

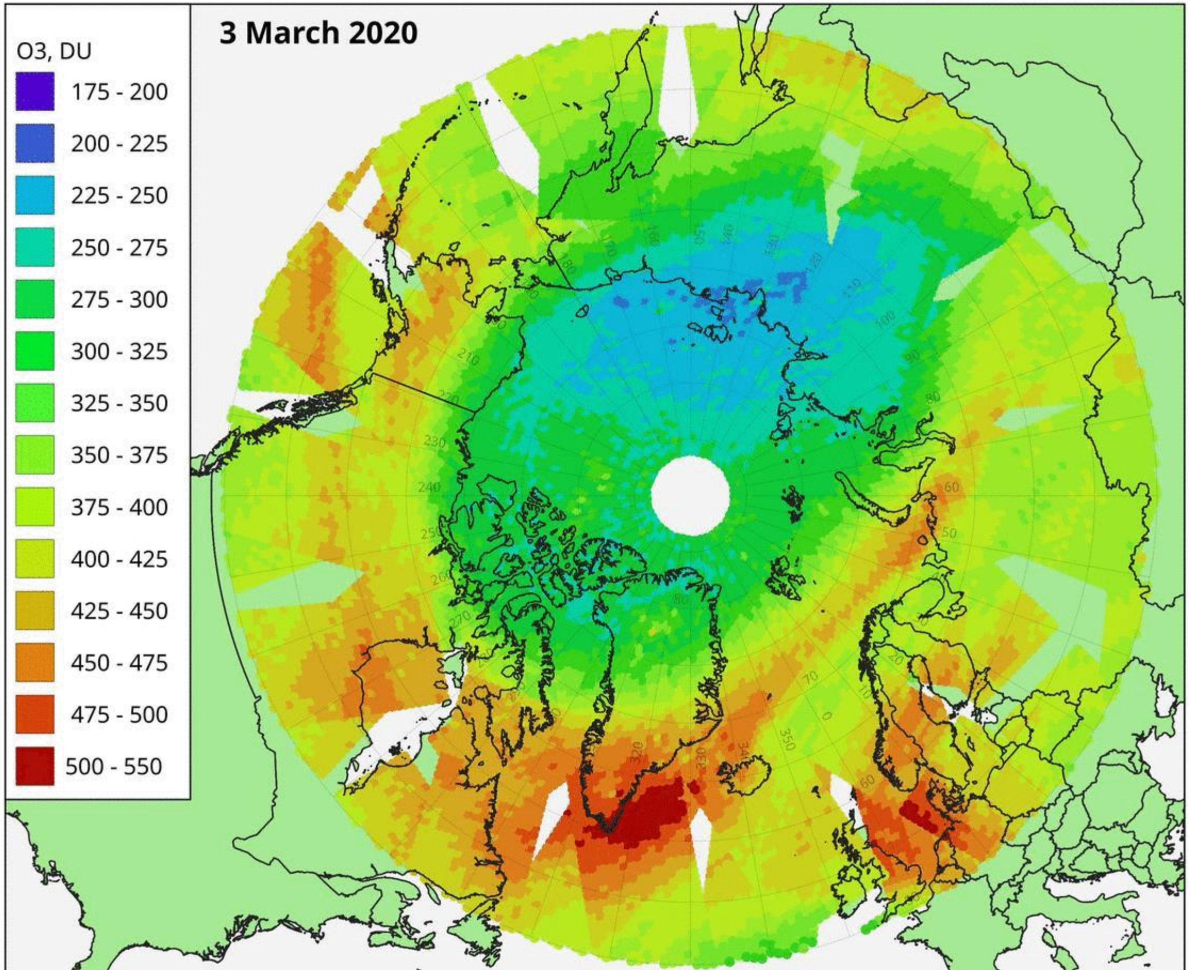
Bias and SDD, DU

Site	N (200 km)	Lower 400 hPa	
		Δ	σ
Eureka	282	+3.6	4.2
Ny Ålesund	120	-0.13	4.4
Thule	553	+2.0	3.4
Kiruna	491	+1.3	3.8
Harestua	153	-0.41	2.5
St. Petersburg	247	+0.84	3.6
Bremen	129	+0.64	2.7
Zugspitze	559	-10.4	3.1
Jungfraujoch	441	-12.5	2.0
Toronto – TAO	679	+1.9	4.1
Rikubetsu	100	-1.2	3.5
Boulder	367	-1.9	2.2
Tsukuba	184	+2.6	4.1
Izaña	395	-8.2	2.0
Mauna Loa	659	-8.5	2.1
Altzomoni	216	-11.1	2.2
Maido	342	-5.8	2.1
Wollongong	212	+2.7	2.8
Lauder	940	+1.2	2.1
all	**7069**		**2.99**

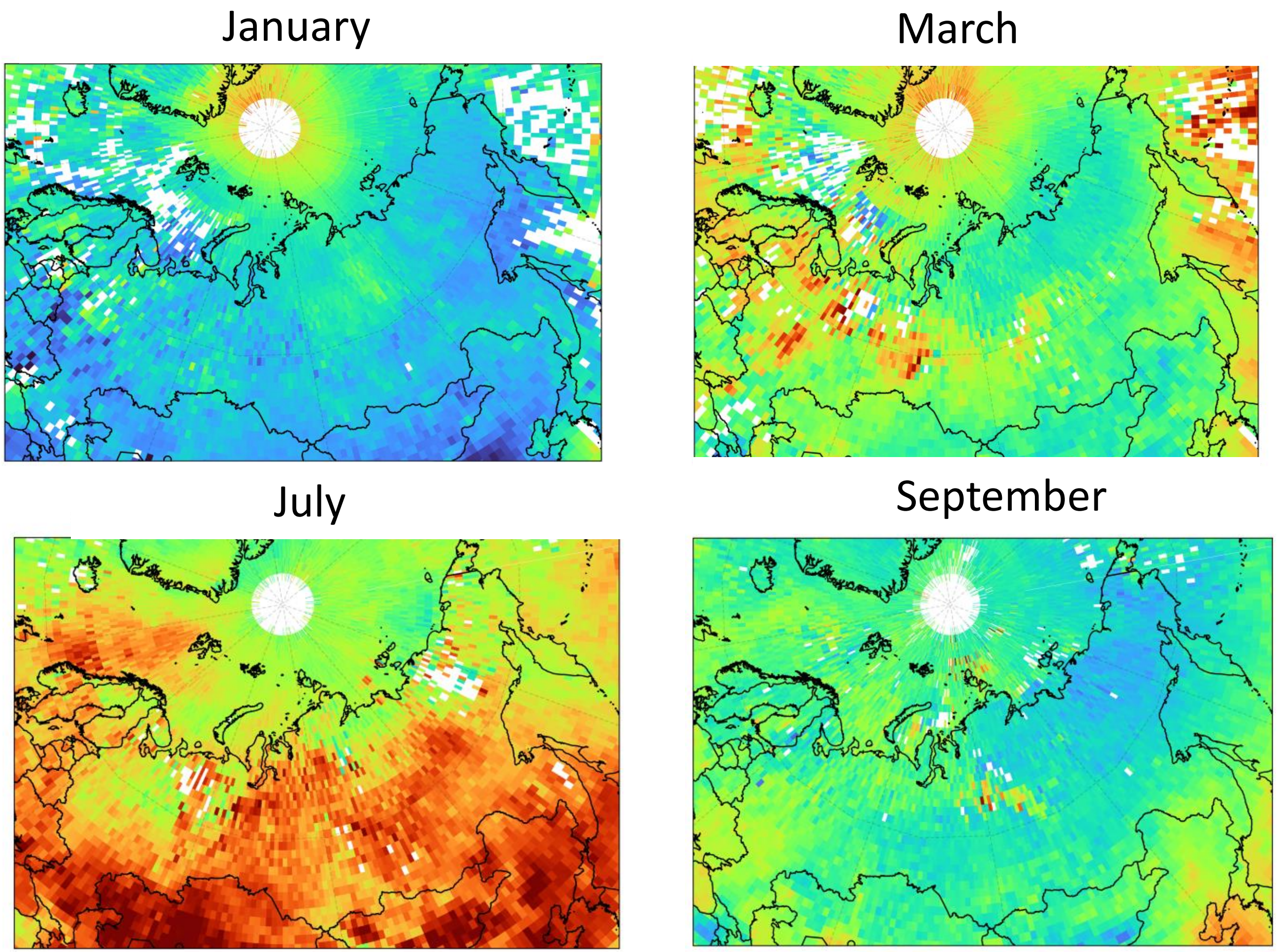
IKFS-2 TOC retrievals



IKFS-2 TOCs in March 2020



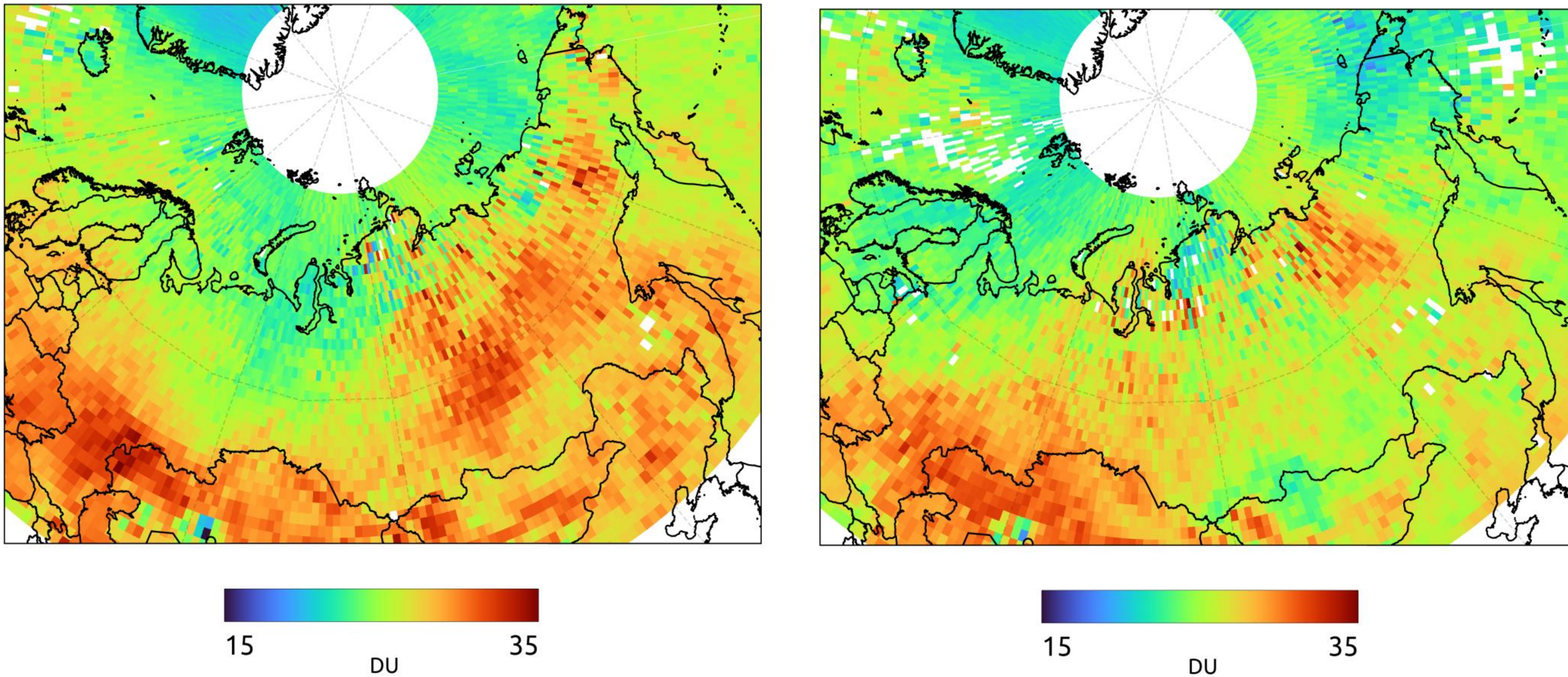
IKFS-2 monthly TrOC (up to 300 mbar) distribution in 2019



IKFS-2 monthly mean TrOC values for January, March, July and September 2019 (left to right, top to bottom)

Satellite measurements of TrOCs allow tracking the temporal variations of TrOCs on global and regional scales.

IKFS-2 monthly TrOC (up to 400 mbar) distribution in July an August 2021



The summer of 2021 was one of the hottest in the last 10 years of observations, especially in July there were many fires in Siberia, also leading to an increase in TrOC in these areas.

Выводы

- Разработана методика оценки ОСО и ТрСО по спектральным измерениям ИКФС-2.
- Средние погрешности аппроксимации данных ОСО OMI по разработанной методике составляют 8.3 е.Д.
- Средние ошибки аппроксимации данных озонозондирования ТрСО по разработанной методике составляют 2.7 е.Д. и 3.7 е.Д. для тропосферных слоев ниже 400 и 300 гПа.
- Сравнение методики для ИКФС-2 и данных наземных измерений показало: средние разности ОСО составляют от -0,6 до -0,8%, а стандартные отклонения этих разностей не превышают 3%.
- Сравнение методики для ИКФС-2 и данных TROPOMI показало средние разности от -2 до 0%, стандартные отклонения разностей составляют от 2 до 4%.
- Показано преимущество ИК-метода перед измерениями методом рассеянного и отраженного солнечного излучения (OMI и TROPOMI), возможность проведения измерений в период полярной ночи.
- Показано, что использование достаточно широкого и статистически полного набора данных для обучения ИНС, оптимально простой ИНС и продолжительного обучения на всем наборе данных позволяют построить точную эффективную методику решения обратных задач атмосферной оптики.

Thank you for attention

We thank the GES DISC Data and Information Service Centre for providing access to TROPOMI and OMI data,

НИЦ «Планета» за предоставление доступа к результатам спектральных измерений ИКФС-2, and

the HEGIFTOM working group within the TOAR-II project for providing access to the harmonized data of ozonesonde measurements.

Работа выполнена при поддержке проекта СПбГУ № 116234986.