OZONE LAYER AND UPPER ATMOSPHERE RESEARCH LABORATORY

St Petersburg University

Neural network approach to determination of total and tropospheric ozone columns from spectral measurements of outgoing thermal radiation

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Introduction

The role of atmospheric ozone and our measurements approach

- 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.
- **We present the techniques based on the artificial neural network (ANN) approach and the principal component (PC) analysis for deriving the 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.**

Methods for measuring the atmospheric ozone content

- **In situ:** near surface, aircraft, balloon (ozonesondes)
- **Remote:**

Ground – based (local)

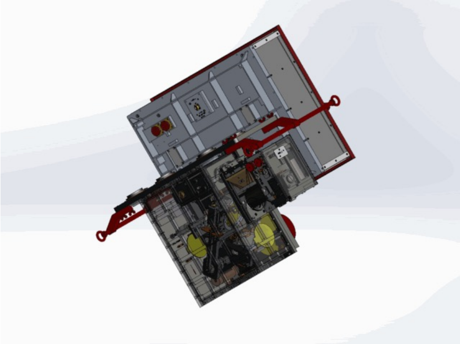
- Direct Solar Radiation: IR, UV, VIS (FTIR; Dobson and Brewer instruments – «reference standard»)
- Scattered solar radiation UV, VIS, NIR (SOAZ, DOAS)
- Scattered solar radiation at low Sun (Umkehr)
- Microwave thermal radiation
- Lidars

Satellite (global)

- Scattered-reflected solar radiation (OMI, TROPOMI)
- Transmittance - solar occultation (ACE-FTS), stars occultation
- <u>Outgoing thermal IR radiation (IASI, CrIS, AIRS, IKFS-2)</u>
- Microwave radiation (limb - MLS)
- Measurements of emissions in UV, VIS and NIR regions of the spectrum

IKFS-2 instrument

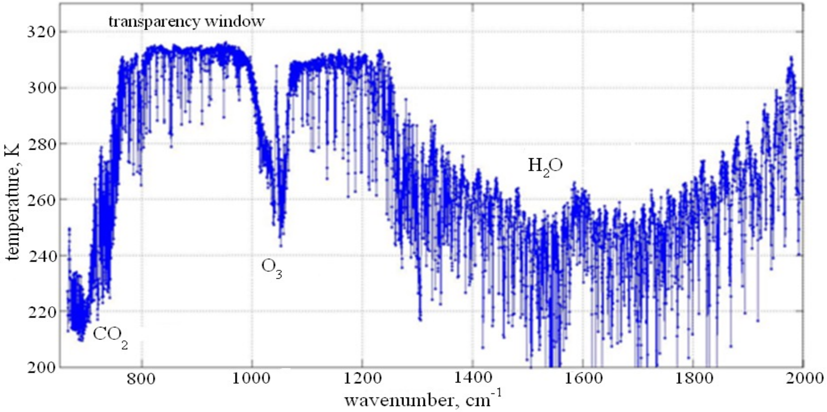
- **The IKFS-2 spaceborne infrared Fourier-transform spectrometer measures outgoing infrared radiance** and can provide data on the atmosphere for numerical weather prediction and various applications in the field of atmospheric and climate sciences.
- **IKFS-2 is located aboard the Meteor-M No.2 Russian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



Main modules:

- the interferometer module
- the pointing system
- the radiation refrigerator
- the electronics module

An example of measured spectrum:



2701 spectral channels with an apodized spectral resolution of 0.7 cm^{-1} in the 660–1210 cm^{-1} spectral region, and of 1.4 cm^{-1} in the 1210–2000 cm^{-1} region

parameter	requirement
spectral range	5-15 µm (660-2000 cm^{-1})
spectral resolution	0.4 cm^{-1}
calibration error, no more than	0.5 K
NESR, [$W/(m^2\ sr\ cm^{-1})$]	$3.5 \cdot 10^{-4}$, 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

Description of the retrieval technique

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 March 2015 to December 2022).
2. Calculation of the average spectrum, covariance matrices, Empirical Orthogonal functions (EOF).
3. Preparation of ozone data, OMI (level 2) data for TOC and ozonesonde (the HEGIFTOM collection) data for TrOC.

2. Building a training sample

1. Measurement pairs matching.
2. Calculation of the PCs and assembly of the training data sets.
3. ANN (three-layer perceptron) training.

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

4. Validation

Description of the retrieval technique

Results of the ANN training

	Data source	Mismatch parameters	Pairs number	Input values set	Approximation error
TOC	OMI AURA, level2 data	70 km, 5 hours	2×10^7	Satellite zenith angel, Day of Year, latitude, 50 PCs of ozone band, 25 PCs whole spectrum, 40 NHLN	8.8 DU
TrOC	HEGIFTOM ozonesonde data collection	200km, 24 hours	5.6×10^5	Satellite Zenith Angle, Day of year, latitude, 0 PCs of ozone band, 35 PCs of whole spectrum, 55 NHLN	2.7 DU (400 hPa) 3.7 DU (300 hPa)

Comparison the IKFS-2 TOC vs ground-based and satellite measurements

Satellite data level 2		Ground-based hourly data	
TROPOMI, QF>0.9, TOCs >100 and TOCs < 650 DU		Dobson and Brewer, Direct Sun, 21 stations	
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 TOC retrieval: Differences for single stations (WOUDC)

N	Station	Latitude, Degrees	Longitude, Degrees	Altitude, m	Pairs Number	Bias, %	SDD, %
Brewer instrument							
1	Eureka	80.050	−86.420	9	82,767	−0.2	2.6
2	Resolute	74.700	−94.970	68	11,979	−0.6	2.1
3	Churchill	58.750	−94.070	26	8360	−1.6	3.0
4	Obninsk	55.100	36.610	100	1044	−0.2	2.7
5	Edmonton	53.550	−114.110	752	8496	1.0	3.1
6	Goose Bay	53.310	−60.360	26	11,752	0.0	2.2
7	Lindenberg	52.209	14.121	127	9472	−1.3	2.9
8	De Bilt	52.100	5.180	24	12,558	−2.6	2.1
9	Saturna Island	48.770	−123.130	202	7686	0.4	2.6
10	Aosta	45.740	7.360	570	1022	0.3	2.0
11	Egbert	44.230	−79.780	264	7493	−1.6	2.1
12	Toronto	43.780	−79.470	202	50,937	−1.0	2.2
13	Kislovodsk	43.730	42.660	2070	3783	1.6	2.4
14	Thessaloniki	40.634	22.956	60	6959	−1.0	2.2
15	Mauna Loa (HI)	19.540	−155.580	3397	24,581	3.2	3.5
16	Paramaribo	5.806	−55.210	16	10,880	−0.5	2.1
Dobson instrument							
17	Kyiv-Goloseyev	50.364	30.497	206	3763	−0.1	1.9
18	Lannemezan	44.129	0.370	590	131	2.4	2.0
19	University of Tehran	35.730	51.380	1419	674	1.1	2.0
20	Natal	−5.835	−35.207	49	32	0.5	1.2
21	Cachoeira-Paulista	−22.69	−46.200	574	26	−3.5	1.6

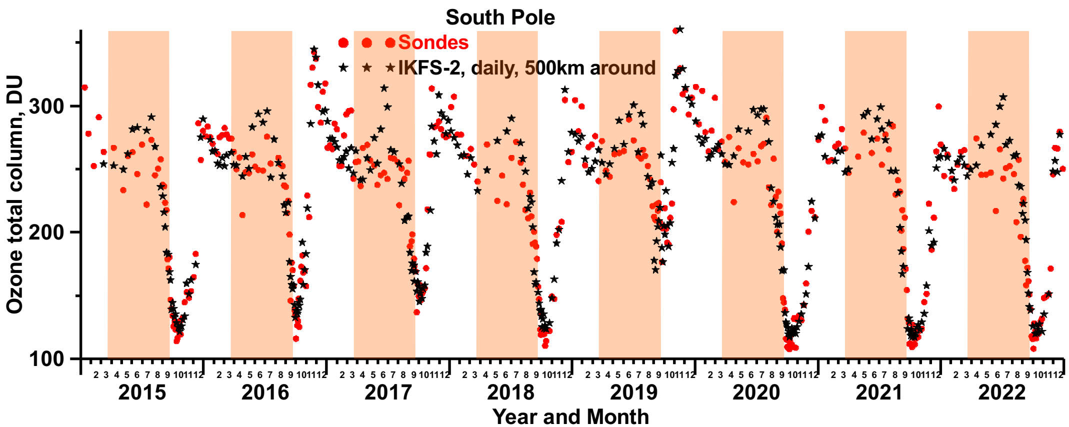
Dobson and Brewer, Direct Sun	
1 hour, 70 km	
March 2015 – Dec 2022	
Bias, %	**SDD, %**
-0.41	**2.67**

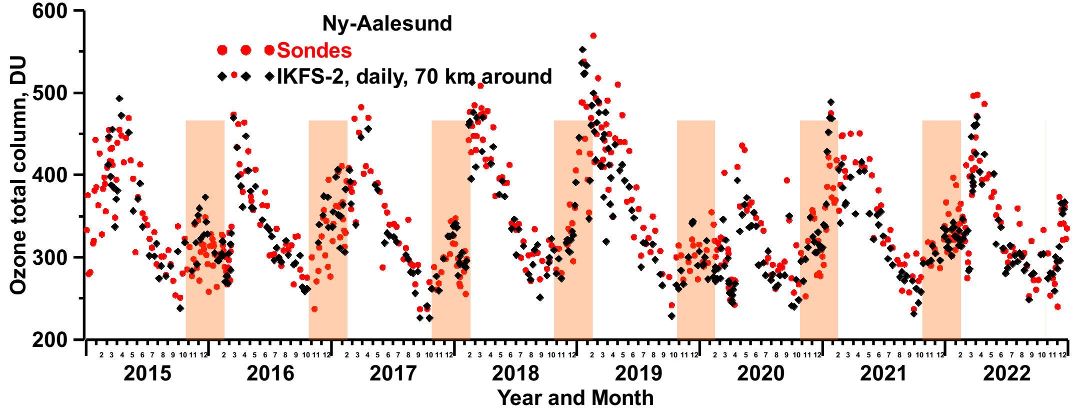
Validation of the IKFS-2 TOC retrieval

Differences between IKFS-2 and ozonesonde TOCs

Ozonesonde 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**

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





Daily averaged TOCs in a distance of 500 km (and 70 km) at the South Pole (and Ny-Ålesund) station. The polar night periods are showed.

Comparison against FTIR data

Ground-based (GB) data
FTIR measurements, NDACC network
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 all sites considered:

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

Biases vary significantly for different sites

That can be explained by:

- the peculiarities of the station location (stability of air masses, altitude, surroundings, etc.)
- different retrieval methods of IR spectroscopic data

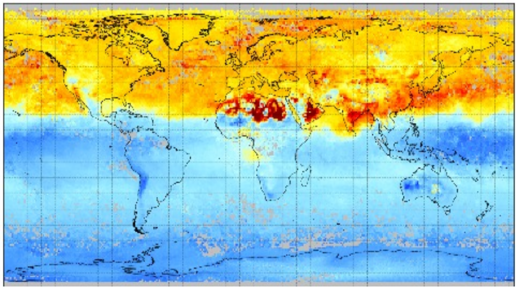
Differences for each site considered (in DU):

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
Total	**7069**		**2.99**

Validation of the IKFS-2 TrOC retrieval

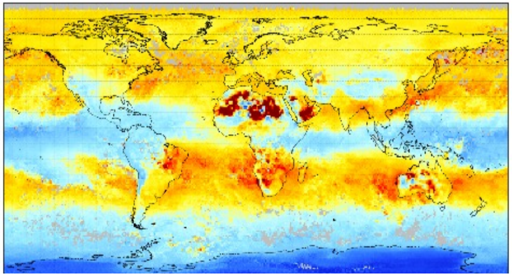
Comparison of monthly TrOC (up to 300 mbar) distribution derived by IKFS-2 and IASI

Monthly average Tropospheric Ozone by IKFS-2 (Day and Night) in May 2019

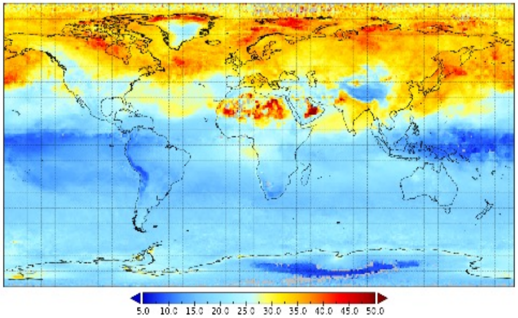


IKFS-2

Monthly average Tropospheric Ozone by IKFS-2 (Day and Night) in Nov 2019

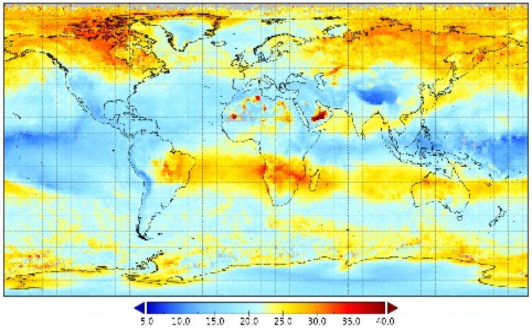


Monthly average Tropospheric Ozone by IASI (Day and Night) in May 2019

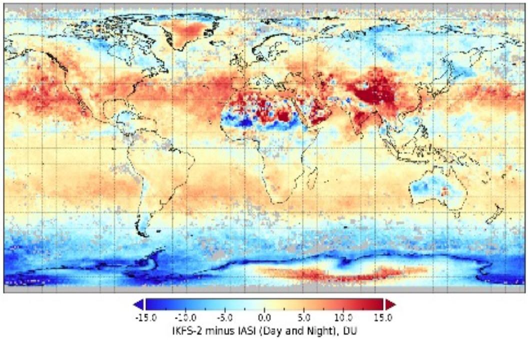


IASI

Monthly average Tropospheric Ozone by IASI (Day and Night) in Nov 2019

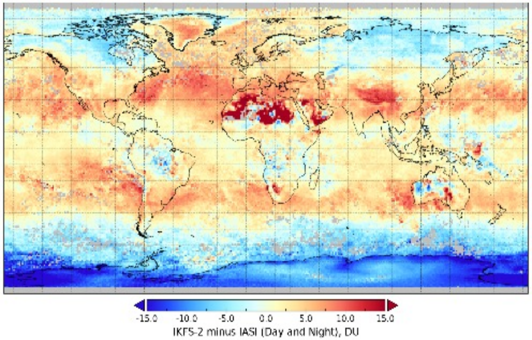


Differences in monthly averaged tropospheric ozone, May 2019



Differences

Differences in monthly averaged tropospheric ozone, Nov 2019



Conclusions

- A technique for estimating the TOCs and TrOCs from the IKFS-2 spectral measurements based on the PC and ANN methods has been developed.
- The ANNs were trained on OMI TOC data and ozonesonde TrOC data. The mean errors in the approximation of the OMI TOC data are **8.3 DU**, in the approximation of the ozonesonde TrOC data are **2.7 DU and 3.7 DU** for tropospheric layers below 400 and 300 hPa.
- The average differences between IKFS-2 and ground-based TOC data range from -0.6 to -0.8%; the standard deviations of these differences are usually less than 3%.
- The average differences between IKFS-2 and TROPOMI TOC measurements range from -2 to 0%; the standard deviations of the differences are from 2 to 4%.
- The developed technique (IR method) can be used during polar nights when measurements with the OMI and TROPOMI equipment (method of scattered and reflected solar radiation) are impossible.
- The average TrOC differences between IKFS-2 and FTIR measurements depend on altitude and location of a site, the SD of the differences are both layers are within 3 DU.
- In general, IKFS-2 and IASI satellite measurements demonstrate nearly similar spatial and temporal variability in observed TrOCs with various biases in different latitudes.
- The use of a sufficiently broad and statistically complete dataset for the ANN training, an optimally simple ANN, and continuous training on the entire dataset allow us to construct an accurate efficient technique for solving the inverse problems of atmospheric optics.

Thank you for attention!

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

SRC "Planeta" for providing access to the results of IKFS-2 spectral measurements,

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

the IRWG-NDACC PIs for providing the access to FTIR ozone data.

The authors acknowledge Saint-Petersburg State University for a research grant No. 116234986.

Useful information and links

- **Polyakov, A.; Virolainen, Y.; Nerobelov, G.; Kozlov, D.; Timofeyev, Y. Six Years of IKFS-2 Global Ozone Total Column Measurements // Remote Sens. 2023, 15, 2481.** https://doi.org/10.3390/rs15092481
- Polyakov, A., Virolainen, Y., Nerobelov, G., Timofeyev, Y. & Solomatnikova, A. Total ozone measurements using IKFS-2 spectrometer aboard MeteorM N2 satellite in 2019–2020 // International Journal of Remote Sensing. 42, 22, pp. 8709–8733, 2021.
- Yu. M. Timofeev, G. M. Nerobelov, A. V. Polyakov, and Ya.A. Virolainen, Satellite Monitoring of the Ozonosphere // Russian Meteorology and Hydrology, 2021, Vol. 46, No. 12, pp. 849–855. DOI: 10.3103/S1068373921120062
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- A. S. Garkusha, A. V. Polyakov, Yu. M. Timofeev, Ya. A. Virolainen, and A. V. Kukharsky Determination of the Total Ozone Content in Cloudy Conditions based on Data from the IKFS-2 Spectrometer Onboard the Meteor-M no. 2 Satellite // Izvestiya, Atmospheric and Oceanic Physics, 54, No. 9(2018) 1244–1248.
- Garkusha, A. S., Polyakov, Timofeev, Y. M., A. V. & Virolainen, Y. A. Determination of the total ozone content from data of satellite IR Fourier-spectrometer // Izvestiya, Atmospheric and Oceanic Physics. 2017, 53, 4, pp. 433–440.

The website of the ozone layer and upper atmosphere laboratory

O_3 Lab

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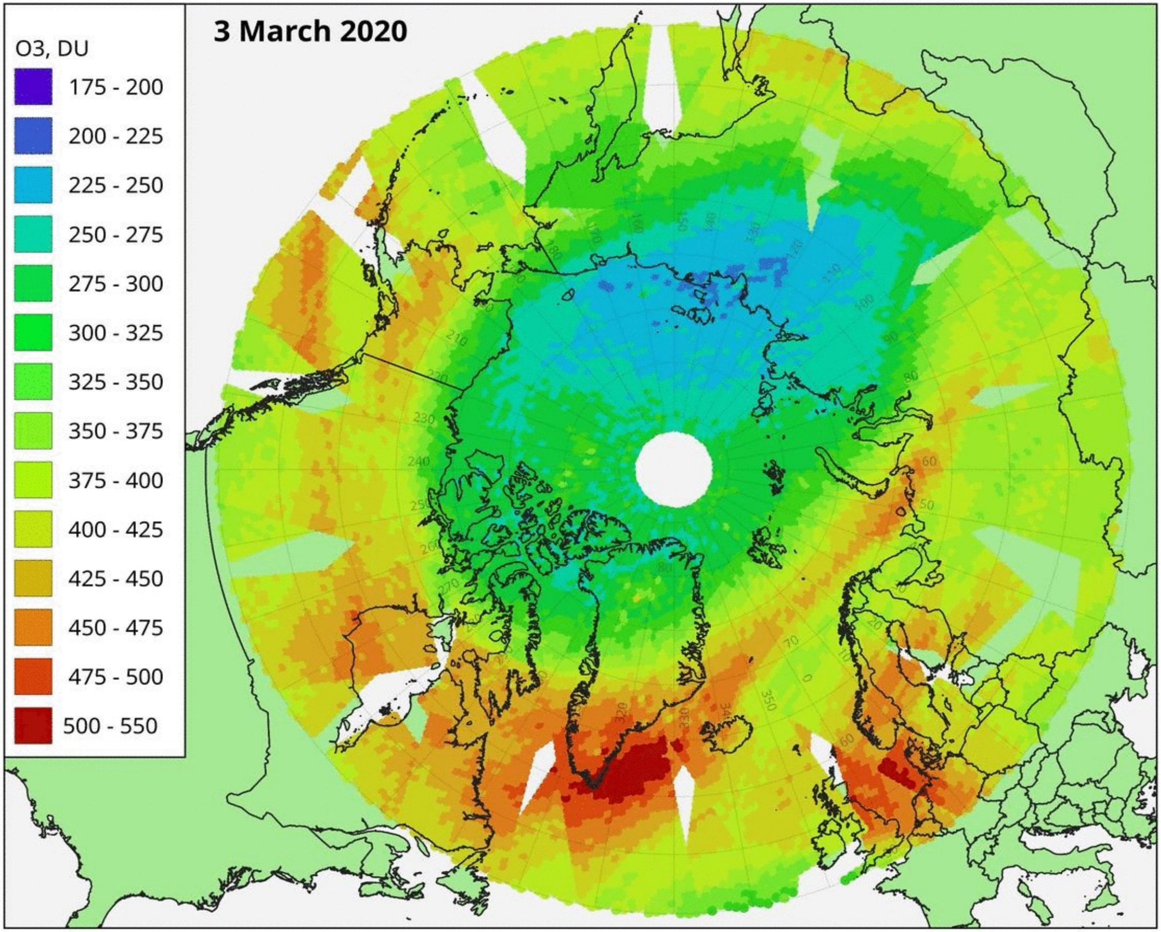
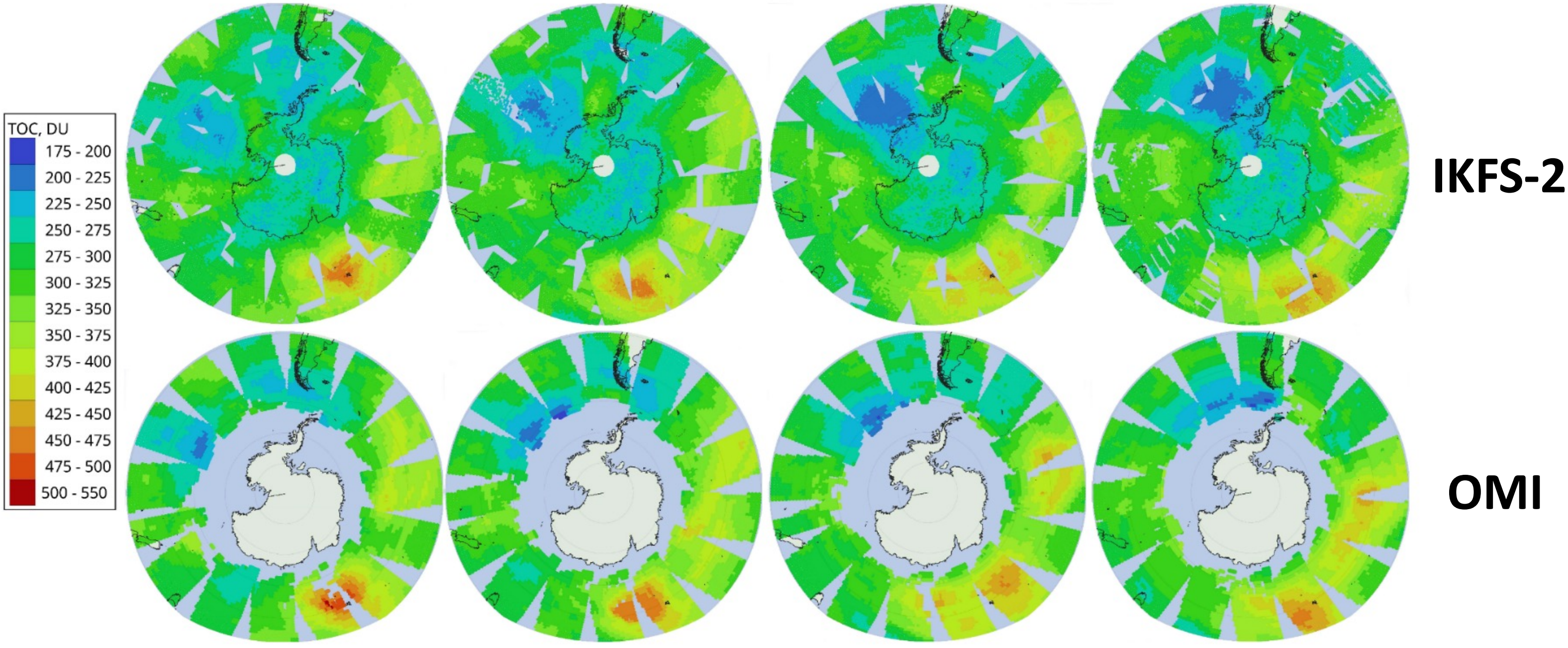
IKFS-2 TOCs in March 2020



IKFS-2 and OMI TOC retrievals - measurements are taken even in regions under polar nights.

22–25 July 2020



Figures from: Polyakov, A.; Virolainen, Y.; Nerobelov, G.; Kozlov, D.; Timofeyev, Y. Six Years of IKFS-2 Global Ozone Total Column Measurements. Remote Sens. 2023, 15, 2481. https://doi.org/10.3390/rs15092481

Comparison of IKFS-2 TOC with ozone sounding data (100km, 24 hours)

site	Latitude, degrees	ozonesonde		IKFS-2		Absolute differences		Relative differences	
		средне е	STD	средне е	STD	Δ, DU	б, DU	Δ, %	б, %
Alert	82.5	336.3	58.1	342.1	63.3	5.8	31.7	2.0	10.8
Eureka	79.99	365.7	81.4	372.8	91.4	7.1	32.9	1.7	8.8
Ny-Alesund	78.93	342.6	65.6	336.7	66.36	-5.9	26.1	-1.6	7.2
Resolute	74.71	not enough data							
Scoresbysund	70.48	331.5	55.9	339.8	52.7	8.3	27.3	3.0	8.0
Sodankyla	67.36	340.0	61.9	335.8	58.2	-4.2	26.2	-0.7	9.0
Lerwick	60.13	326.9	49.5	327.8	46.8	0.8	25.0	0.6	7.6
UCCLE	50.48	321.2	44.3	318.9	40.3	-2.3	23.7	-0.3	7.3
Madrid	40.47	313.4	34.2	309.5	33.1	-3.9	17.2	-1.1	5.3
Hohenpeisen	47.8	299.0	33.7	318.8	33.4	19.8	19.4	6.9	6.8
Costa Rica	9.980	inadequate data (about 200 DU, tropics)							
Ascension Is.	-7.970	inadequate data (many less than 200 DU, tropics)							

South Pole site not captured by IKFS-2 scan, minimum distance 150km