Methodology for determination of the ozone vertical distribution elements from satellite spectral measurements of IR thermal radiation

Svetlana Akishina, Alexander Polyakov, Yana Virolainen

St. Petersburg State University, St. Petersburg, Russia

St Petersburg University

OZONE LAYER AND UPPER ATMOSPHERE RESEARCH LABORATORY

O3 Lab

Feel free to contact us:
s.akishina@spbu.ru
a.v.polyakov@spbu.ru
y.virolainen@spbu.ru

1. Introduction

Ozone (O_3) is crucial for the atmosphere's chemical and thermal balance.

On account of different lifetimes, different formation and degradation mechanisms, different variability trends and different roles in different atmospheric layers **it is important to obtain information on ozone spatial (vertical and horizontal) and temporal distribution**.

50 km

Stratospheric:
- Occurs during the Chapman cycle as a result of solar irradiation.
- Protecting the biosphere from the harmful effects of UV radiation.
- Lifetime can range from a few months to a few years.

10 km

Tropospheric:
- Occurs as a result of photochemical reactions with the pollutants CO, NOx, CH_4 and is transported from the stratosphere.
- Harmful to life due to its toxicity, contributing to the greenhouse effect.
- Lifetime ranges from 1-2 days in the near surface layer to several weeks in the free troposphere.

Meteor-M No.2

Satellite instruments **can provide** this information.

2. Methods

IKFS-2 details

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, mW/(m^2 sr cm^{-1})	0.35 , λ = 6 µm 0.15 , λ = 13 µm 0.45 , λ = 15 µm
spatial resolution at sub-satellite point	35 km
swath width	1000…2500 km
sampling period	0.6 s

- The IKFS-2 spaceborne infrared Fourier-transform spectrometer **measures outgoing infrared radiance** and can provide data on the atmosphere for various applications.
- IKFS-2 is located **aboard the Meteor-M No.2 series Russian meteorological satellite from 2015 to the present**.
- IKFS-2 instrument was **developed by the Keldysh Research Center** together with Krasnogorsky zavod and Bauman State Technical University (Moscow).

IKFS-2 ozone retrievals

Formulation of the forward/inverse problem using the optimal estimation method (OEM) *(Rodgers, 2000)*:

$$\tilde{\vec{y}} = \boldsymbol{B}(\vec{x}) + \vec{\varepsilon}\,,$$

a suitable estimation of the state vector $\tilde{\vec{x}}$ is obtained by minimizing the function $\Phi(\tilde{\vec{x}})$:

$$\Phi(\tilde{\vec{x}}) = \|\boldsymbol{B}(\tilde{\vec{x}}) - \tilde{\vec{y}}\|^2_{\boldsymbol{\Sigma}^{-1}} + \|\tilde{\vec{x}} - \bar{\vec{x}}\|^2_{\boldsymbol{D}^{-1}} \to min.$$

The algorithm for minimisation is iterative:

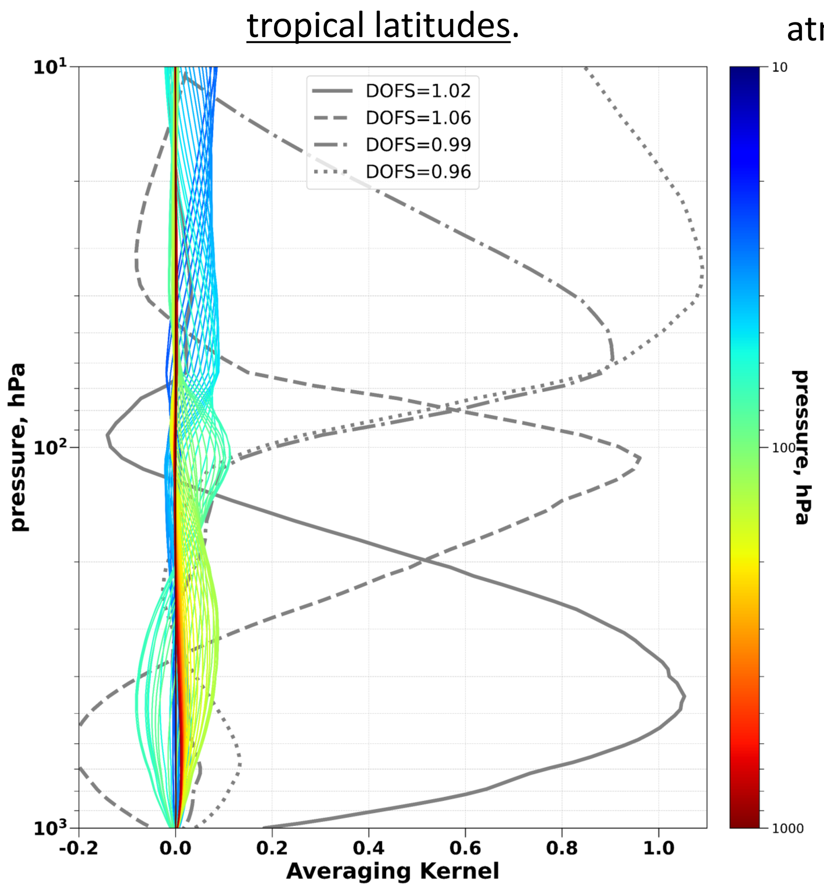
$$\tilde{\Phi}_k(\tilde{\vec{x}}_{k+1}) = \|\boldsymbol{A}_k\tilde{\vec{x}}_{k+1} - \tilde{\vec{y}}\|^2_{\boldsymbol{\Sigma}^{-1}} + \|\tilde{\vec{x}}_{k+1} - \bar{\vec{x}}\|^2_{\boldsymbol{D}^{-1}} + \|\tilde{\vec{x}}_{k+1} - \tilde{\vec{x}}_k\|_{\boldsymbol{L}^{-1}} \to min$$

$\boldsymbol{D}$ is the a priori covariance matrix of $\vec{x}$, $\boldsymbol{A}_k$ is the Jacobian matrix of $\boldsymbol{B}$ operator at a point $\tilde{\vec{x}}_k$, $\boldsymbol{\Sigma}$ is measurement error $\vec{\varepsilon}$ covariance matrix

- $\boldsymbol{L} = l\boldsymbol{L}_0$, $\boldsymbol{L}_0$ is diagonal of the a priori covariance matrix $\boldsymbol{D}$, l is positive number
- **ANN** method is used to obtain **an initial estimate**
- we use the **principal component method** in relation to the retrieved profiles to reduce the dimensionality of the problem

3. Results

IKFS-2 ozone averaging kernel functions, in partial column units, corresponding to tropical latitudes.



The DOFS number estimates of the IKFS-2 measurements relative to ozone for different atmospheric climate models (*Anderson et al., 1986*).

Climate model	DOFS
Tropics (15 N)	4.4
Mid-latitude, summer (45 N)	4.3
Mid-latitude, winter (45 N)	3.9
Subarctic, summer (60 N)	4.3
Subarctic, winter (60 N)	3.4

Peaks of sensitivity: ~ 450 hPa (6-7 km), 110 hPa (15-16 km), 55 hPa (20-21 km) and 30 hPa (24-25 km).

We divide the altitude range to **four vertical layers**:
1. surface–220 hPa (TROPO)
2. 220–80 hPa (UTLS)
3. 80–30 hPa (LMS)
4. 30–5 hPa (MS)

Summary of the retrieval settings

a priori information	Ozonesonde profiles (from 2015 to 2022) measured between 1000 and 6 hPa
forward problem-solving software	RTTOV v13.2
O3 initial approximation and number of principal components	by ANN method, 5 principal components
spectral window	1005-1054 cm^{-1}, excluding the channels with interfering effects of H2O absorption
surface pressure	NCEP GFS
H2O and T profiles, Ts	OEM, retrieved prior to ozone in the following order: **H2O(z), T(z), Ts**, then, for additional precision **H2O(z), Ts**
emissivity information	Database *(Borbas et al., 2017)*

We performed **closed-loop numerical experiments** to estimate the errors of the method with respect to the ozone vertical distribution elements retrieval. Uncertainties of the following parameters **were NOT included** in the experiments: the content of CO2, CO, N2O, CH4 (their absorption does not have a strong interfering effect on ozone), surface pressure, and the surface emissivity.

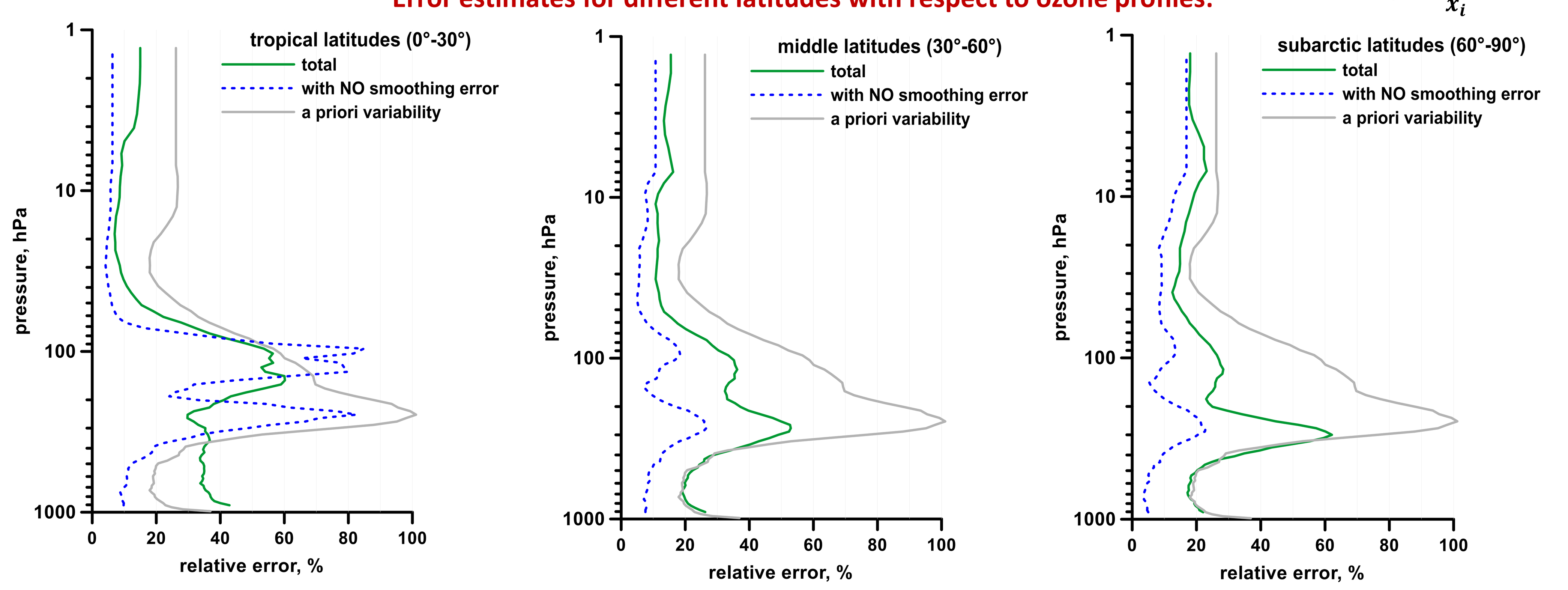
Error estimates for different latitudes with respect to the partial columns:

Layer	tropical latitudes (0°-30°) error, DU	tropical latitudes (0°-30°) error, %	middle latitudes (30°-60°) error, DU	middle latitudes (30°-60°) error, %	subarctic latitudes (60°-90°) error, DU	subarctic latitudes (60°-90°) error, %
above 30 hPa	7.3	4.6	8.0	6.4	10.8	10.8
80-30 hPa	4.3	8.1	9.0	9.7	12.8	12.2
220-80 hPa	3.2	34.6	6.6	15.1	9.8	14.0
p0-220 hPa	6.1	65.2	6.0	13.7	6.9	9.8
p0-300 hPa	5.7	26.5	4.9	16.6	4.0	14.4
Total column	**6.9**	**2.7**	**5.2**	**1.7**	**8.3**	**2.5**

p0 is surface pressure, **p0-300 hPa** is tropospheric ozone column

Error estimates for different latitudes with respect to ozone profiles:

$$var_i = \frac{\sqrt{D_{i,i}}}{\bar{x}_i} \cdot 100\%$$



4. Discussion

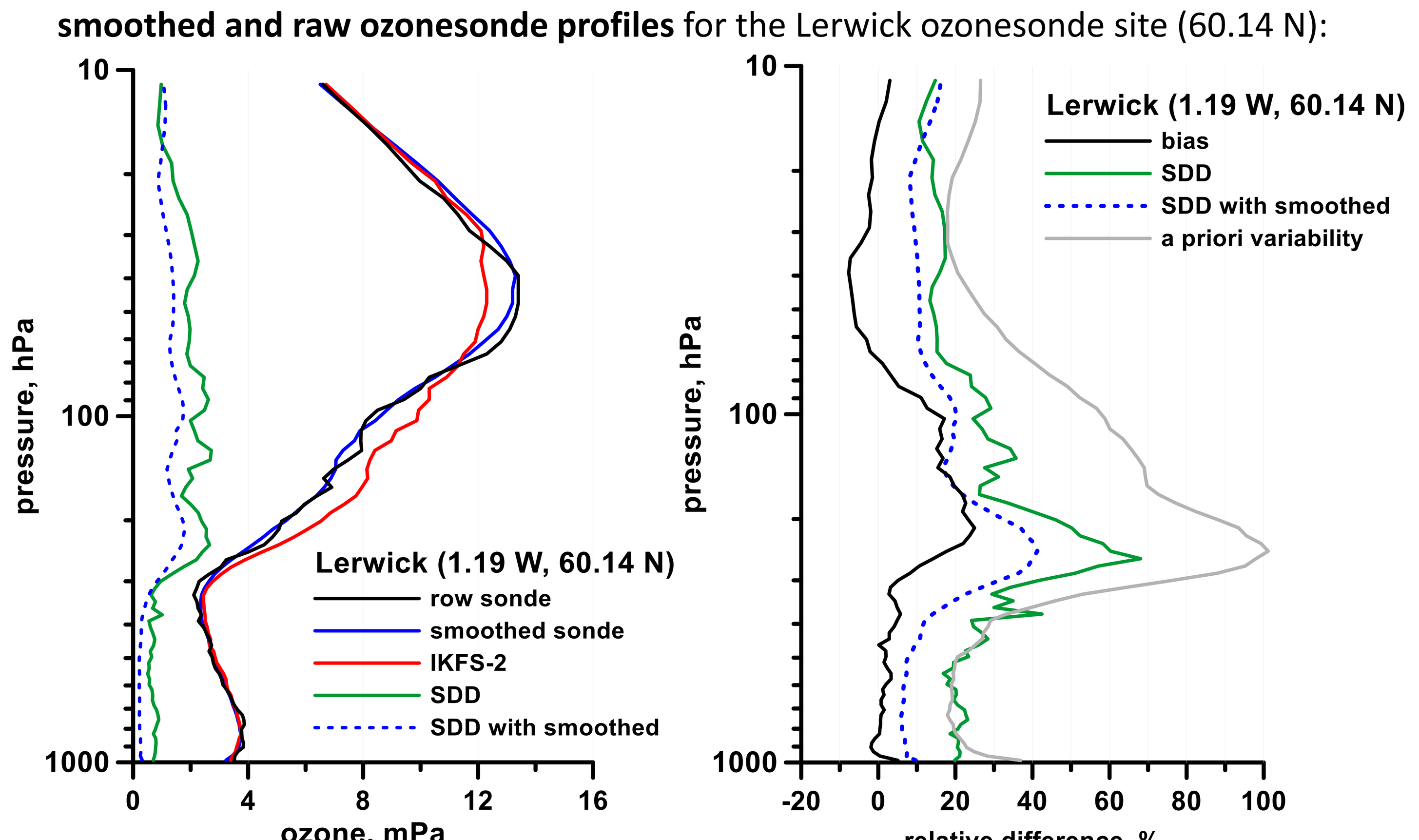
Validation vs ozonesondes

Comparison between the mean retrieved IKFS-2 partial columns with raw ozonesondes partial columns for all latitudes, taking into account IKFS-2-sonde coincidences for the **8-year (2015–2022)** period. Coincidence criteria: **70 km and ± 12h**.

Layer	all latitudes (0°-90°) Δ±SDD, DU	SDD, %	σ, %
30-10 hPa	3.0 ± 11.4	13.7	22.7
80-30 hPa	-4.3 ± 11.2	12.8	25.8
220-80 hPa	7.4 ± 11.7	26.9	63.4
p0-220 hPa	-0.2 ± 6.7	15.4	19.5
p0-300 hPa	-0.5 ± 4.9	17.9	18.6
Total column	**15.5 ± 31.5**	**10.4**	**18.7**

σ is natural ozone variability (SD) by ozonesondes

Example of comparison between the mean retrieved IKFS-2 profiles with the mean smoothed and raw ozonesonde profiles for the Lerwick ozonesonde site (60.14 N):



5. Conclusion

1. We obtained an optimal algorithm for solving the inverse problem by a physical and mathematical method based on the optimal estimation method with respect to the vertical ozone profile.
2. Total error estimate of the algorithm with respect to total ozone column is **2.3 %**. Ozone measurements at mid-latitudes have the highest accuracy (**1.7 %**). In the future, the uncertainty of the surface emissivity will have to be taken into account.
3. Numerical experiments show that in the troposphere the mean error in determining the ozone content from IKFS-2 measurements with no smoothing error is **5-10 %** depending on latitude (the smallest error occurs at high latitudes). The error in determining stratospheric ozone content is **5-15 %** (the smallest error occurs at low latitudes). The largest error with respect to the ozone profile is observed in the UTLS region, and is **20-30 %**, not taking into account low latitudes due to the very small ozone content in this area of tropical latitudes.
4. The comparison with ozonesonde vertical profiles shows that, on average, IKFS-2 algorithm overestimates O3 by **10-25 %** in the UTLS region, while it underestimates O3 by ~**5-10 %** in the stratosphere.

References

Anderson, G. & Clough, Shepard & Kneizys, F. & Chetwynd, J. & Shettle, Eric. (1986). AFGL Atmospheric Constituent Profiles (0.120km). 46.

Borbas, E.; Hulley, G.; Knuteson, R.; Feltz, M. MEaSUREs Unified and Coherent Land Surface Temperature and Emissivity (LST&E) Earth System Data Record (ESDR): CAMEL Users' Guide; 2017. https://lpdaac.usgs.gov/sites/default/files/public/product_documentation/cam5k30_v1_user_guide_atbd.pdf

Rodgers C.D. Inverse methods for atmospheric sounding. Theory and practice. Series on Atmospheric, Oceanic and Planetary Physics. V. 2. World Scientific. Singapore–New Jersey–London–Hong–Kong. 2000. 238 p.

Acknowledgements

The authors thank the SRC "Planeta" for providing access to the results of IKFS-2 spectral measurements. The authors thank the HEGIFTOM working group within the TOAR-II project for providing access to harmonized ozonesonde measurement data. This work was carried out with support from St. Petersburg State University, project code 116234986.