



TROPOSPHERIC EMISSIONS: MONITORING OF POLLUTION (TEMPO) PROJECT

Ozone Profile Level 2 and 3 Data products: User Guide

September 17, 2025

DOI: 10.5067/doc/tempo/O3PROF_L2-3UserGuide_V2.0

AUTHORS

Junsung Park (Center for Astrophysics | Harvard & Smithsonian)

Xiong Liu (Center for Astrophysics | Harvard & Smithsonian)

John Houck (Center for Astrophysics | Harvard & Smithsonian)

Kelly Chance (Center for Astrophysics | Harvard & Smithsonian)

CONTRIBUTIONS:

TEMPO Science Team, Center for Astrophysics | Harvard & Smithsonian

TEMPO Ground System Team, Center for Astrophysics | Harvard & Smithsonian

NASA Langley Research Center

NASA Goddard Space Flight Center

NASA Ames Research Center

University of Maryland

Pusan National University

REVISION HISTORY

Version	Item	Description	Release date
2.0	All	First public release: Version 04 (V04)	September 17, 2025
		TEMPO O3PROF	

PRODUCT to SCIENCE DATA PROCESSING CENTER PIPELINE VERSION

Version Designation	Science Data Processing Center Pipeline Version	Release
V03	4.4	First limited release of TEMPO O3PROF Level 2 and Level 3 products to TEMPO validation team
V04	4.7	September 17, 2025; First public release of TEMPO O3PROF Level 2 and Level 3 products

KNOWN DATA PRODUCT ISSUES

Ozone Profile (O3PROF)

Preliminary evaluations and validations of V04* (before final V04) O3PROF data products were conducted using very limited correlative data sets. Most of the V04* O3PROF retrievals are based on Version 1 (V1) Goddard Earth Observing System – Composition Forecast (GEOS-CF) a priori profiles rather than V2 GEOS-CF a priori profiles. Here are preliminary evaluation summaries of:

(1) Tropospheric column ozone (TrCO)

- a. An inter-comparison was conducted with satellite observations from the Ozone Monitoring Instrument (OMI; provided by Juseon Bak from Pusan National University), the Earth Polychromatic Imaging Camera (EPIC; the high-resolution EPIC product provided by Jerry Ziemke from NASA GSFC), and the TROPOSpheric Monitoring Instrument (TROPOMI; provided by Juseon Bak based on the Smithsonian Astrophysical Observatory (SAO) O3PROF algorithm (Bak et al., 2025)). The TrCO retrievals exhibit strong spatial consistency across these satellite datasets, with a correlation coefficient of ~0.6, a root mean square error (RMSE) of ~8 DU, and a mean bias (MB) of 1–2 DU.
- b. Comparisons with Tropospheric Ozone Lidar Network (TOLNet) ground-based lidar observations show generally good agreement, although with approximately 10% systematic TEMPO low bias.

(2) 0–2 km column ozone

- a. The 0–2 km subcolumn ozone was evaluated against TOLNet ground observations and a near-surface subcolumn product derived from airborne-lidar High Spectral Resolution Lidar (HSRL-2) ozone profiles during the August 2023 NASA Synergtic TEMPO Air Quality Science (STAQS) campaign. TEMPO and HSRL-2 measurements coincide over Chicago, IL (8, 12, and 15 August 2023) and New York City, NY (5 and 9 August 2023). Overall (1289 coincidences), TEMPO 0–2 km subcolumns had a small bias (2.34 ppb, 4.8%) against HSRL-2. Results varied between cities with a low bias (-6.02 ppb, -11.5%, n = 455) in Chicago, IL and a high bias (6.91 ppb, -14.5%, n = 834) in New York City, NY.
- b. Evaluation against TOLNet shows similar behavior, with an approximate 10% systematic TEMPO low bias. HSRL-2 and TOLNet 0–2 km subcolumn coincidences (n =17) during STAQS were well correlated (R = 0.85).

Contents

AUT	THORS	2
REV	ISION HISTORY	3
PRO	DUCT to SCIENCE DATA PROCESSING CENTE	ER .
	OWN DATA PRODUCT ISSUES	
	one Profile (O3PROF)	
	tents	
1.	Before You Begin	
1.1.		
1.2.	Acronyms, Abbreviations, and Definitions	7
2.	Introduction	9
2.1.		
2.2.		
2.3.	Level 2 products	10
2	.3.1. O3PROF	11
2.4.	Level 3 product	11
3.	Science algorithm overview	12
3.1.	Ancillary data	12
3.2.	O3PROF	13
3	.2.1. Algorithm overview	13
3	.2.2. O3PROF usage recommendations	13
4.	Data Organization and Format	15
4.1.	Filename	15
4.2.	Format	15
4.3.	Key variables	16
4	.3.1. TEMPO Level 2 O3TOT files	16

References	17
Version: V2.0	
Ozone Profile Level 2 and 3 Data products: User Guide	6

1. Before You Begin

1.1. Purpose of the Document

This document provides a quick guide for Tropospheric Emissions: Monitoring of Pollution (TEMPO) Ozone Profile (O3PROF) Level 2 (L2) and Level 3 (L3) products.

This user guide provides the following:

- 1) Algorithm overview
- 2) File descriptions
- 3) Key variables
- 4) Updates from the previous version
- 5) Known issues for the TEMPO O3PROF product

1.2. Acronyms, Abbreviations, and Definitions

ASDC Atmospheric Science Data Center

ATBD Algorithm Theoretical Basis Document

BUV Backscatter Ultraviolet
CCD Charge-Coupled Device
CLDO4 TEMPO cloud algorithm

DU Dobson Unit

EPIC Earth Polychromatic Imaging Camera

FOV Field of View

FWHM Full Width at Half Maximum
GEOS Goddard Earth Observing System

GEOS-CF Goddard Earth Observing System – Composition Forecast

GLER a geometry-dependent surface Lambertian Equivalent Reflectivity

GOME Global Ozone Monitoring Experiment

HCHO Formaldehyde

HSRL-2 High Spectral Resolution Lidar

IMS Interactive Multisensor Snow & Ice Mapping System

INR Instrument Navigation and Registration

L1 Level 1
L2 Level 2
L3 Level 3

LUT Look-Up Table

MB Mean bias

NASA National Aeronautics and Space Administration

NM Nadir-Mapper NO2 Nitrogen Dioxide

OCP Optical Centroid Pressure

OE Optimal Estimation

OMI Ozone Monitoring Instrument
OMPS Ozone Mapping and Profiler Suite

OMTO3 OMI Level-2 Total Column Ozone Data Product

O3TOT TEMPO total ozone algorithm
O3PROF TEMPO ozone profile algorithm
PCA Principal component analysis

RMSE Root mean square error TCO Total Column Ozone

TrCO Tropospheric Column Ozone

TEMPO Tropospheric Emissions: Monitoring of Pollution

TOA Top of the Atmosphere

TOLNet Tropospheric Ozone Lidar Network
TOMS Total Ozone Mapping Spectrometer

QF Quality Flag

SAO Smithsonian Astrophysical Observatory
STAQS Synergistic TEMPO Air Quality Science

SZA Solar Zenith Angle

SDPC Science Data Processing Center

TEMPO Tropospheric Emissions: Monitoring of Pollution

TOMS Total Ozone Mapping Spectrometer

UV Ultraviolet
V01 Version 1
V02 Version 2
V03 Version 3
VIS Visible

VZA Viewing Zenith Angle

2. Introduction

The Tropospheric Emissions: Monitoring of Pollution (TEMPO) is a geostationary satellite mission to monitor air quality over North America, from Mexico City to the Canadian oil sands and from the Atlantic to the Pacific. It has hourly temporal resolution during sunlight times of the day and high spatial resolution ($2 \text{ km} \times 4.75 \text{ km}$ at the center of the field of regard) (Zoogman et al., 2017).

The TEMPO products are generated by the Science Data Processing Center (SDPC) at the Smithsonian Astrophysical Observatory (SAO). After being generated at SAO, all products are sent to the NASA Atmospheric Science Data Center (ASDC) for public distribution. In rare cases, Level 2 (L2) and Level 3 (L3) product files may be missing even if corresponding Level 1b (L1b) files exist due to failed Instrument Navigation and Registration (INR) processing, which results in a lack of geolocation information.

This User Guide document includes a brief description of the V04 TEMPO L2 and L3 ozone profile (O3PROF) products and a quick guide for the V04 TEMPO L2 and L3 O3PROF products, released on September 17, 2025. Note that the user guides for Level 2 and Level 3 total ozone (O3TOT), trace gas (NO₂ and HCHO), and cloud (CLDO4) products are provided separately.

The SAO team welcomes and relies on feedback from data users to make improvements to TEMPO products.

2.1. Data versioning and release history

Updates to the SDPC operational pipeline result in periodic new data releases. When this occurs, a new collection is created that includes all data products. The collection version number can be found in the data filename and has the format VXX, where XX denotes the collection version. Since first light on August 2, 2023, the SAO science team has been working to improve the processing pipeline and science products with assistance from the TEMPO validation team. On February 5, 2024, a limited set of preliminary unvalidated TEMPO Version 1 (V01) products were released for users to become familiar with the file format and content. On February 26, 2024, the SDPC pipeline was updated to produce Version 2 (V02) products for the public release of the V02 L1b (irradiance and radiance) products. On May 20, 2024, the SDPC was updated to produce Version 3 (V03) L1, L2, and L3 products. V03 products constitute the first public release of TEMPO L2 and L3 products, excluding the TEMPO O3PROF product. In June 2025, the V03 TEMPO O3PROF L2 and L3 products were released to a limited group of users, including the validation team. On September 17, 2025, the SDPC software was updated to produce Version 4 (V04) L2, L2, and L3 products, including the TEMPO O3PROF products. As of September 17, 2025, the V04 TEMPO O3PROF is declared at Beta maturity level. The TEMPO validation document defines the Beta level as "the product is minimally validated but

may still contain significant errors; based on product quick looks using the initial calibration parameters. Publication of research based on Beta maturity products is not recommended and highly discouraged." (TEMPO Validation Team, 2023). The maturity is anticipated to be declared provisional after validation team approval. Users should consult the relevant data landing pages for current product maturity.

2.2. Science data processing overview

The SDPC generates TEMPO products in the following order: (1) L1b, (2) L2 CLDO4, (3) L2 O3PROF, and (4) L3 products. This is because L2 CLDO4 requires L1b as input, other L2 products require both L1b and L2 CLDO4 as inputs, and L3 products require L2 products as inputs. Table 2.1.1 lists the L2 and L3 products described in this document. More details for each product can be found in the corresponding ATBD and algorithm description document.

Table 2.1.1.	TEMPO	L2 and L3	products t	that are	described in this document.	
					Spatial Resolution and	

Product	Level	Description	Spatial Resolution and Coverage	Validation maturity level
O3PROF	L2	Ozone profile, Total column ozone (TCO), Tropospheric column ozone (TrCO), and Stratospheric column ozone (SCO)	4-pixel in N/S direction are coadded from the native TEMPO ground pixel, one granule	Beta
O3PROF	L3	Ozone profile, Total column ozone (TCO), Tropospheric column ozone (TrCO), and Stratospheric column ozone (SCO)	All Level 2 granules merged for a single scan, on a $0.04^{\circ} \times 0.04^{\circ}$ regular grid	Beta

2.3. Level 2 products

TEMPO O3PROF Level 2 data products are organized in terms of the scan number (e.g., S004) and granule number (e.g., G01) for each day. Note that files use UTC format. Each scan is a sweep from the East to the West, and nominally takes one hour to complete. The data collected during each scan is divided into different granules to keep the data volume for each file manageable. Each granule contains data collected during a short time range (~6.7 minutes in nominal operations). Each granule file contains all spatial pixels in the North-South direction, but only a portion of the East-West coverage of a full scan.

The granule number (e.g., G01, G02, etc.) does not always correspond to the same geographic location, but rather to the order in which the granule was collected for the scan. In

some cases, Level 2 O3PROF scans may be missing early granules (e.g., G01) when twilight (city light) measurements were made.

2.3.1. O3PROF

For V04 TEMPO O3PROF, the optimal estimation (OE) based algorithm has been optimized to retrieve ozone profiles from backscattered radiances in the spectral range ~308-340 nm in the ultraviolet (UV) band. This TEMPO O3PROF algorithm is adapted from our UV-only Global Ozone Monitoring Experiment (GOME) and OMI ozone profile retrieval algorithm as described in detail in Liu et al. (2005, 2010) and Bak et al. (2024). We plan to update the algorithm to utilize both UV and visible wavelengths in the future version (spectral fitting windows are subject to change in future updates). This algorithm implements time-consuming online radiative transfer calculation, and thereby retrievals are done at spatially co-added pixels (currently 4 pixels in the N/S direction are coadded) required by TEMPO science requirements. The main product parameters are partial ozone columns with units of Dobson Unit (DU) at 24 layers from the surface to ~ 60 km with the first layer from surface to surface + 2 km (i.e., 0-2 km ozone above surface), and their random-noise and smoothing error profiles with total, stratospheric, and tropospheric ozone columns. A detailed description of the algorithm can be found in the TEMPO O3PROF ATBD (Park et al., 2025).

2.4. Level 3 product

TEMPO L3 products are generated using an area-weighted gridding program. For each variable of interest, the program maps the corresponding L2 variable onto a $0.04^{\circ} \times 0.04^{\circ}$ regular grid over the domain of $155^{\circ}W-24.5^{\circ}W$ to $17.2^{\circ}N-63.55^{\circ}N$. Gridding was performed using data filtered through different solar zenith angles, cloud fraction, and data quality flag criteria as needed by each product.

3. Science algorithm overview

3.1. Ancillary data

TEMPO O3PROF L2 products require ancillary data. The TEMPO O3PROF algorithm mainly uses atmospheric trace gas profiles and meteorological parameters from the Goddard Earth Observing System (GEOS) Composition Forecasting (GEOS-CF) model system (Keller et al., 2021; Knowland et al., 2022a) as shown in Table 3.1.1. The GEOS-CF is a chemical forecasting system produced by NASA's Global Modeling and Assimilation Office (GMAO). The details on the GEOS-CF system and performance tropospheric simulation can be found in Keller et al. (2021), and the stratospheric component of the GEOS-CF is described and evaluated in Knowland et al. (2022a). Its implementation, emission inventories, and outputs are described in Knowland et al. (2022b). If, for some reason, the GEOS-CF forecast becomes unavailable, the TEMPO processing pipeline defaults to using trace gas from GEOS-CF climatology (monthly averaged) and meteorological parameters provided in the GEOS-CF TEMPO daily forecasts. The detailed description of the GEOS-CF processing step and usage of the ancillary data are in the TEMPO O3PROF ATBD (Park et al., 2025). Surface albedo is based on a geometry-dependent surface Lambertian Equivalent Reflectivity (GLER) (Qin et al., 2019; Fasnacht et al., 2019) climatology. It is calculated for a given location, specific viewing geometry (varying with month and time) at 340 nm. The GLER is based on MODIS BRDF and USGS surface albedo spectra for land/snow surface and the Cox-Munk BRDF model for water surface. Cloud information is taken from the cloud Optical Centroid Pressure (OCP) of the TEMPO O₂-O₂ cloud product. If the TEMPO CLDO4 product is not available, the OCP is based on an OMCLDRR climatology.

Table 3.1.2 shows the list of reference spectra for trace gases used in the TEMPO O3PROF algorithm. These reference spectra can be updated or changed in future algorithm updates.

Table 3.1.1. Ancillar	y data for TEMPO	L2 O3PROF algorithm.
------------------------------	------------------	----------------------

Input	Source		
Cloud-top pressure	TEMPO CLDO4 product (O ₂ -O ₂ spectral fitting)		
Cloud fraction	Initial derived from ~347 nm, futher fitted		
Ozone profiles	GEOS-CF v2 + Tropopause-based Climatology (Bak et al., 2013)		
Other trace gases	Chemical model based climatolgies		
Temperature profiles	GEOS-CF v2		
Surface albedo	GLER v2		
Snow/ice fraction	L1b, Interactive Multisensor Snow & Ice Mapping System (IMS)		
Terrain height	L1b, GEMTED2010 (Danielson and Gesch, 2010) with 30 arcs		
Surface pressure	GEOS-CF v2 with correction		
Tropopause pressure	GEOS-CF v2		
Aerosols	None, implicitly included in the cloud/albedo treatment		

Species/Component	Details
O_3	Birk and Wagner (2021)
O_2 - O_2	Finkenzeller and Volkamer (2022)
NO_2	Vandaele et al. (1998), 220 K
BrO	Wilmouth et al. (1999), 228 K
НСНО	Chance and Orphal (2011), 300 K
SO ₂	SCIAMACHY FM (Bogumil et al., 2003)

Table 3.1.2. Reference spectra used in the TEMPO O3PROF algorithm.

3.2. **O3PROF**

3.2.1. Algorithm overview

The TEMPO L2 O3PROF algorithm is proposed to use both TEMPO UV and visible radiances based on the optimal estimation technique. However, we first optimized the UV-only algorithm. The publicly released V04 TEMPO L2 O3PROF algorithm is adapted from the SAO UV-only GOME and OMI ozone profile retrieval algorithms, as described in detail in Liu et al. (2005, 2010a) and Bak et al. (2024). The spectral fitting window of 308-340 nm has been used based on the normalized difference between TEMPO observation and VLIDORT simulation (during the evaluation of the soft calibration performance).

TEMPO radiance and solar irradiance and corresponding random measurement errors from L1b data are used in the retrievals. As the retrievals are time-consuming due to online radiative transfer calculations, and we do not have enough computational resources, the spatial coadding (4-pixel in N/S direction are coadded) strategy has been employed to perform retrievals over the entire FOR.

The TEMPO slit function is derived for the spectral fitting window using a super-Gaussian function for each coadded cross-track pixel. In addition, to improve the radiometric calibration, soft calibration has been employed for BUV retrievals due to inadequate radiometric calibration or forward model simulations (Liu et al. 2010a; Bak et al., 2017, 2024). This soft calibration has been calculated using 15 scans of TEMPO observation in July and August 2024. Additionally, to improve the radiative transfer calculation for both accuracy and speed, the forward model is based on a combination of principal component analysis (PCA) applied to a hyperspectral optical property dataset and look-up tables of radiance corrections (Bak et al., 2021). The details of this algorithm have been described in detail in the TEMPO PROF ATBD (Park et al., 2025).

3.2.2. O3PROF usage recommendations

The quality_flag variable is not provided in the TEMPO L2 O3PROF product. Therefore, to use the highest quality of data, the user should filter out the low-quality data using the variable of (1) "eff cloud fraction" in the support data group,

- (2) "solar zenith angle" and "viewing zenith angle" in the geolocation group,
- (3) "fit_RMS", "avg_residual", and "retrieval_exit_status" in the qa_statistics group. The most recommended filtering criteria is as follows:
 - (1) "eff cloud fraction" is greater than 0.5.
 - (2) "solar_zenith_angle" and "viewing_zenith_angle" are greater than 80 degrees.
 - (3) "fit_RMS" is greater than 3, "avg_residual" is greater than 0.3, and "retrieval_exit_status" is less than 1 or greater than 99.

To ensure the data quality strictly, users should filter out the thick cloud scenes, snow/ice covered scenes, and abnormally large values from "fit_RMS" and "avg_residual" in the qa_statistics group.

In the case of the TEMPO L3 O3PROF product. Because the meaning of the qa_statistics variables could change after averaging pixels, we can't provide the qa_statistics group in the TEMPO L3 O3PROF product. Therefore, the TEMPO L3 O3PROF product applied data filtering with "fit_RMS", "avg_residual", and "retrieval_exit_status" as described above before producing the TEMPO L3 O3PROF product. Additional filtering with "eff_cloud_fraction", "solar zenith angle", and "viewing zenith angle" could be applied for better quality.

4. Data Organization and Format

TEMPO data products are organized in terms of the scan number (e.g., S004) and granule number (e.g., G01) for each day. Each scan is a sweep from the East to the West, and nominally takes one hour to complete. The data collected during each scan is divided into different granules to keep the data volume for each file manageable. Each granule contains data collected within a few minutes.

4.1. Filename

Table 4.1.1 shows the TEMPO Level 2 and 3 file naming convention. The Level 2 O3PROF filename have a format of

$$TEMPO_{GAS}_{L2}V04_{YYYY}\{MM\}\{DD\}T\{HH\}\{NN\}\{SS\}Z_{S}\{XXX\}G\{YY\}.nc,$$

with YYYY (year), MM (month), DD (day), HH (hour), NN (minute), and SS (second) denoting the GMT time stamp at the beginning of the time period covered by the file, and XXX and YY denoting the scan and granule numbers, respectively. The segment GAS represents the product type: O3PROF. (Note that the curly brackets are added here for display purposes; they don't exist in actual filenames.)

The TEMPO Level 3 filenames have a format of

$$TEMPO_{GAS}_L3_V04_{YYYY}_{MM}_{DD}_{THH}_{NN}_{SS}Z_S_{XXX}.nc,$$

Again, with YYYY (year), MM (month), DD (day), HH (hour), NN (minute), and SS (second) denoting the GMT time stamp at the beginning of the time period covered by the file and _S{XXX} the scan number.

Table 4.1.1 TEMPO Level 2 and 3 file naming convention.

Product	Filename format
O3PROF Level 2	TEMPO_O3PROF_L2_V04_{YYYY}{MM}{DD}T{HH}{NN}{SS}Z _S{XXX}G{YY}.nc
O3PROF Level 3	TEMPO_O3PROF_L3_V04_{YYYY}{MM}{DD}T{HH}{NN}{SS}Z_S{XXX}.nc

4.2. Format

TEMPO products are in the self-explanatory NetCDF4 format. The content of a NetCDF file can be reviewed by a command "ncdump -h {FILENAME}" on Linux systems or explored on a graphical interface using the software "Panoply," distributed by NASA Goddard Institute for

Space Studies (https://www.giss.nasa.gov/tools/panoply/). NetCDF files can be read using FORTRAN, C, Python, Matlib, IDL, etc.

Each file contains several groups (named "diagnostic", "geolocation", "product", "qa_statistics", and "support_data") and global attributes. Each group contains a number of variables. Each variable is described by its attributes.

Dimensions used for the variables are defined in each netcdf file. Typically, the xtrack = 2048 dimension is fixed along the North-South direction. However, the TEMPO O3PROF product has xtrack = 512 due to the 4-pixel coadding in N/S direction. The first and last few pixels in the North-South direction contain fill values as they are not suitable for retrieval. The granule builds in the East-West scanning direction and contains data collected within a few minutes. The corner = 4 dimension is used for the 4 corners of each ground pixel.

4.3. Key variables

Key variables for TEMPO L2 and L3 files in this release are provided below. For the full list of variables, please use NetCDF manipulation software.

4.3.1. TEMPO Level 2 O3TOT files

Table 4.3.1. TEMPO Level 2 O3TOT key variables

Group	Name	Format (dimension)	Unit	Description
product	ozone_profile	float (mirror_step, xtrack, layer)	DU	vertical ozone profile with 24 layers
product	Total_ozone_column	float (mirror_step, xtrack)	DU	Total column ozone
product	Tropospheric_ozone_ column	float (mirror_step, xtrack)	DU	Tropospheric column ozone
product	Stratospheric_ozone_ column	float (mirror_step, xtrack)	DU	Stratospheric column ozone

References

- Bak, J., Liu, X., Wei, J. C., Pan, L. L., Chance, K., & Kim, J.H. (2013). Improvement of OMI ozone profile retrievals in the upper troposphere and lower stratosphere by the use of a tropopause-based ozone profile climatology. *Atmospheric Measurement Techniques*, 6(9), pp.2239-2254. https://doi.org/10.5194/amt-6-2239-2013.
- Bak, J., Liu, X., Kim, J. H., Haffner, D. P., Chance, K., Yang, K., & Sun, K. (2017).
 Characterization and correction of OMPS nadir mapper measurements for ozone profile retrievals. *Atmospheric Measurement Techniques*, 10(11), pp.4373-4388.
 https://doi.org/10.5194/amt-10-4373-2017.
- Bak, J., Liu, X., Spurr, R., Yang, K., Nowlan, C. R., Miller, C. C., Abad, G. G., & Chance, K. (2021). Radiative transfer acceleration based on the principal component analysis and lookup table of corrections: optimization and application to UV ozone profile retrievals. *Atmospheric Measurement Techniques*, *14*, pp.2659–2672. https://doi.org/10.5194/amt-14-2659-2021.
- Bak, J., Liu, X., Yang, K., Gonzalez Abad, G., O'Sullivan, E., Chance, K., & Kim, C.H. (2024). An improved OMI ozone profile research product version 2.0 with collection 4 L1b data and algorithm updates. *Atmospheric Measurement Techniques*, *17*(7), pp.1891-1911. https://doi.org/10.5194/amt-17-1891-2024.
- Bak, J., Liu, X., Abad, G. G., & Yang, K. (2025). An extension of ozone profile retrievals from TROPOMI based on the SAO2024 algorithm. *Remote Sensing*, *17*(5), 779. https://doi.org/10.3390/rs1750779.
- Birk, M., & G. Wagner (2021). ESA SEOM-IAS Measurement and ACS database O3 UV region (II) [Data set],, Zenodo, https://doi.org/10.5281/zenodo.4423918.
- Bogumil, K., Orphal, J., Homann, T., Voigt, S., Spietz, P., Fleischmann, O. C., Vogel, A., Hartmann, M., Kromminga, H., Bovensmann, H., & Frerick, J. (2003). Measurements of molecular absorption spectra with the SCIAMACHY pre-flight model: instrument characterization and reference data for atmospheric remote-sensing in the 230–2380 nm

- region. *Journal of Photochemistry and Photobiology A: Chemistry*, *157*(2-3), pp.167-184. https://doi.org/10.106/S1010-6030(03)00062-5.
- Chance, K., & Orphal, J., (2011). Revised ultraviolet absorption cross sections of H2CO for the HITRAN database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 112(9), pp.1509-1510. https://doi.org/j.jqsrt.2011.02.002.
- Danielson, J.J., & Gesch, D.B. (2011). *Global multi-resolution terrain elevation data* 2010 (*GMTED2010*) (No. 2011-1073). US Geological Survey.
- Fasnacht, Z., Vasilkov, A., Haffner, D., Qin, W., Joiner, J., Krotkov, N., Sayer, A. M. and Spurr, R. (2019). A geometry-dependent surface Lambertian-equivalent reflectivity product for UV–Vis retrievals–Part 2: Evaluation over open ocean. *Atmospheric Measurement Techniques*, *12*(12), pp.6749-6769. https://doi.org/10.5194/amt-12-6749-2019.
- Finkenzeller, H., & Volkamer, R. (2022). O2–O2 CIA in the gas phase: Cross-section of weak bands, and continuum absorption between 297–500 nm. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 279, p.108063. https://doi.org/10.1016/j.jqsrt.2021.108063.
- Gordon, I. E., Rothman, L. S., Hargreaves, E. R., Hashemi, R., Karlovets, E. V., Skinner, F. M., Conway, E. K., Hill, C., Kochanov, R. V., Tan, Y., & Wcisło, P. (2022). The HITRAN2020 molecular spectroscopic database. *Journal of quantitative spectroscopy and radiative transfer*, 277, p.107949. https://doi.org/10.1016/j.jqsrt.2021.107949.
- Keller, C. A., Knowland, K. E., Duncan, B. N., Liu, J., Anderson, D. C., Das, S., Lucchesi, R. A., Lundgren, E. W., Nicely, J. M., Nielsen, E., & Ott, L.E. (2021). Description of the NASA GEOS composition forecast modeling system GEOS-CF v1. 0. *Journal of Advances in Modeling Earth Systems*, 13(4), p.e2020MS002413. https://doi.org/10.1029/2020MS002413.
- Knowland, K. E., Keller, C. A., Wales, P. A., Wargan, K., Coy, L., Johnson, M. S., Liu, J., Lucchesi, R. A., Eastham, S. D., Fleming, E., & Liang, Q. (2022). NASA GEOS composition forecast modeling system GEOS-CF v1. 0: Stratospheric

- composition. *Journal of advances in modeling earth systems*, *14*(6), p.e2021MS002852. https://doi.org/10.1029/2021MS002852.
- Knowland, K. E., Keller, C. A., & Lucchesi, R. A. (2022). File specification for GEOS-CF products. *GMAO Office Note*.
- Liu, X., Bhartia, P.K., Chance, K., Spurr, R.J.D., & Kurosu, T.P. (2010a). Ozone profile retrievals from the Ozone Monitoring Instrument. *Atmospheric Chemistry and Physics*, *10*(5), pp.2521-2537. https://doi.org/10.5194/acp-10-2521-2010.
- Liu, X., Chance, K., Sioris, C. E., Spurr, R. J. D., Kurosu, T. P., Martin, R. V., & Newchurch, M. J. (2005). Ozone profile and tropospheric ozone retrievals from the Global Ozone Monitoring Experiment: Algorithm description and validation. *Journal of Geophysical Research: Atmospheres*, 110(D20). https://doi.org/10.1029/2005JD006240.
- Qin, W., Fasnacht, Z., Haffner, D., Vasilkov, A., Joiner, J., Krotkov, N., Fisher, B., & Spurr, R. (2019). A geometry-dependent surface Lambertian-equivalent reflectivity product for UV–Vis retrievals–Part 1: Evaluation over land surfaces using measurements from OMI at 466 nm. *Atmospheric Measurement Techniques*, *12*(7), pp.3997-4017. https://doi.org/10.5194/amt-12-3997-2019.
- TEMPO Validation Team (2023). Tropospheric Emissions: Monitoring of Pollution (TEMPO) Level 2 Science Data Product Validation Plan, SAO-DRD-11.
- Vandaele, A. C., Hermans, C., Simon, P. C., Carleer, M., Colin, R., Fally, S., Merienne, M. F., Jenouvrier, A., & Coquart, B. (1998). Measurements of the NO2 absorption cross-section from 42 000 cm—1 to 10 000 cm—1 (238–1000 nm) at 220 K and 294 K. *Journal of Quantitative Spectroscopy and Radiative Transfer*, *59*(3-5), pp.171-184. https://doi.org/10.1016/S0022-4073(97)00168-4.
- Wilmouth, D. M., Hanisco, T. F., Donahue, N. M., & Anderson, J.G. (1999). Fourier transform ultraviolet spectroscopy of the A 2Π3/2← X 2Π3/2 transition of BrO. *The journal of physical chemistry a*, 103(45), pp.8935-8945. https://doi.org/10.1021/jp991651o.
- Zoogman, P., Liu, X., Suleiman, R. M., Pennington, W. F., Flittner, D. E., Al-Saadi, J. A., Hilton, B. B., Nicks, D. K., Newchurch, M. J., Carr, J. L. Janz, S. J., Andraschko, M. R., Arola,

- A., Baker, B. D., Canova, B. P., Chan Miller, C., Cohen, R. C., Davis, J. E., Dussault, M. E., Edwards, D. P., Fishman, J., Ghulam, A., González Abad, G., Grutter, M., Herman, J. R., Houck, J., Jacob, D. J., Joiner, J., Kerridge, B. J., Kim, J., Krotkov, N. A., Lamsal, L., Li, C., Lindfors, A., Martin, R. V., McElroy, C. T., McLinden, C., Natraj, V., Neil, D. O., Nowlan, C. R., O'Sullivan, E. J., Palmer, P. I., Pierce, R. B., Pippin, M. R., Saiz-Lopez, A., Spurr, R. J. D., Szykman, J. J., Torres, O., Veefkind, J. P., Veihelmann, B., Wang, H., Wang, J., & Chance, K. (2017). Tropospheric emissions: Monitoring of pollution (TEMPO). *Journal of Quantitative Spectroscopy and Radiative Transfer*, *186*, 17-39. https://doi.org/10.1016/j.jqsrt.2016.05.008.
- Park, J., Liu, X., Bak, J., Houck, J., Chance, K., Suleiman, R. M., Davis, J, E., Chong, H., Hou, W., Flittner, D. E., Carr, J., O'Sullivan, E., González Abad, G., Knowland, K. E., Chan Miller, C., Nowlan, C. R., Wang, H., Fitzmaurice, J., Carpenter, L., Spurr, R., & Newchurch, M. J. (2025). Algorithm theoretical basis document for the TEMPO Ozone Profile Retrieval Algorithm.
- Park, J., Liu, X., Houch, J., Haffner, D., & Chnace, K. (2024). Algorithm Description for the TEMPO Total Ozone Retrieval Algorithm.