CENTER FOR ASTROPHYSICS HARVARD & SMITHSONIAN

VERSION: 1.1
RELEASE DATE: December 9, 2024

TROPOSPHERIC EMISSIONS: MONITORING OF POLLUTION (TEMPO) PROJECT

Total Ozone Level 2 and 3 Data products: User Guide

December 9, 2024

Distributed by the Atmospheric Science Data Center
https://asdc.larc.nasa.gov

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REVISION HISTORY

Version	Item	Description	Release date
1.0	All	Initial version	May 20, 2024
1.1	- Known data product issues - Sections 2, 3.2.2 and 4.3	- Update known data product issues - Update validation status to provisional - Add a Section for data versioning and release history - Update quality flag explanation	December 9, 2024

PRODUCT to SCIENCE DATA PROCESSING CENTER PIPELINE VERSION

Version Designation	Science Data Processing Center Pipeline Version	Release
V03	4.4	May 20, 2024; first public release of TEMPO Level 2 and Level 3 products

KNOWN DATA PRODUCT ISSUES

Total Ozone (O3TOT)

(1) TEMPO Total column ozone (TCO) shows latitude-dependent biases compared to OMI and OMPS TCO, varying from ~5% at lower latitudes to ~-2% at high latitudes. This latitudinal dependence does not vary much with season. This latitudinal dependence is confirmed from validation using ground-based Pandora, Dobson and Brewer observations. Preliminary testings indicates that this latitudinal dependence results mainly from the spectral dependence of radiometric bias in the Sun-normalized radiances.

(2) TEMPO TCO also shows clear discontinuity when the algorithm switches from using the main pair of wavelengths (~317 and 331 nm) to a different wavelength pair (331 and 360 nm) at high solar zenith angle or viewing zenith angle, resulting in lower TCO values.

Contents

1. Before You Begin

1.1. Purpose of the Document

This document provides a quick guide for Tropospheric Emissions: Monitoring of Pollution (TEMPO) Total Ozone (O3TOT) 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 TEMPO O3TOT product

1.2. Acronyms, Abbreviations, and Definitions

AI	Aerosol Index
ASDC	Atmospheric Science Data Center
ATBD	Algorithm Theoretical Basis Document
BUV	Backscatter Ultraviolet
CCD	Charge-Coupled Device
CLDO4	TEMPO cloud algorithm
DU	Dobson Unit
FOV	Field of View
FWHM	Full Width at Half Maximum
HCHO	Formaldehyde
INR	Instrument Navigation and Registration
L1	Level 1
L2	Level 2
L3	Level 3
LUT	Look-Up Table
NASA	National Aeronautics and Space Administration
NM	Nadir-Mapper
NO2	Nitrogen Dioxide
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
TCO	Total Column Ozone
TEMPO	Tropospheric Emissions: Monitoring of Pollution
TOA	Top of the Atmosphere
TOMS	Total Ozone Mapping Spectrometer
QF	Quality Flag
SAO	Smithsonian Astrophysical Observatory
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 km × 4.75 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 V03 TEMPO L2 and L3 total ozone (O3TOT) products and a quick guide for the V03 TEMPO L2 and L3 O3TOT products, released on May 20, 2024. Note that the user guide for Level 2 and Level 3 ozone profile (O3PROF), and trace gas (NO_2 and HCHO) and cloud (CLD04) 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 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. As of December 9, 2024, these are declared at the Provisional maturity level. The TEMPO validation document defines the Provisional level as "the performance has been demonstrated through a large, but still (seasonally or otherwise) limited number of independent measurements. The analysis is sufficient for limited qualitative determinations of product fitness-for-purpose, and the product is potentially ready for testing by operational users and may be suitable for scientific publication." [TEMPO Validation Team, 2023]. The provisional maturity level was declared 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 O3TOT, and (4) L3 products. This is because L2 CLDO4 requires L1b as input, L2 trace gases require both L1b and L2 CLDO4 as inputs, and L3 products requires 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 that described in this document.

Product	**Level**	**Description**	**Spatial Resolution and Coverage**	**Validation maturity level**
O3TOT	L2	Total column ozone (TCO) and UV aerosol index (AI)	Native TEMPO ground pixel, one granule	Provisional
O3TOT	L3	TCO and UV AI on regular grid	All Level 2 granules merged for a single scan, on a 0.02° × 0.02° regular grid	Provisional

2.3. Level 2 products

2.3.1. O3TOT

The TEMPO O3TOT algorithm is composed of two parts: (1) The forward model calculation for simulating top of atmosphere (TOA) radiance and Jacobians of radiances and (2) the inverse model calculation for deriving the TCO from measured radiance. The TEMPO O3TOT algorithm is based on the OMTO3 V8.5 algorithm (called the Total Ozone Mapping Spectrometer (TOMS) V8.5). The detailed description of the algorithm is in the OMI ATBD for ozone products (https://eospso.gsfc.nasa.gov/sites/default/files/atbd/ATBD-OMI-02.pdf, chapter 2). For adapting to the TEMPO, two parts have been updated: (1) Expand viewing geometry to accommodate larger TEMPO's larger observing viewing zenith angle (VZA), (2) Update slit functions from BP (Bass and Paur, 1985) cross sections with a triangular slit of 0.45 nm Full Width at Half Maximum (FWHM) to BDM (Daumont et al., 1922; Brion et al., 1993; Malicet et al., 1995) cross sections with a triangular FWHM of 0.60 nm.

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 on to a 0.02° × 0.02°

regular grid over the domain of 155°W–24.5°W to 17.2°N–63.55°N. Gridding was performed using data filtered through different solar zenith angles, cloud fraction, data quality flag criteria as needed by each product.

3. Science algorithm overview

3.1. Ancillary data

TEMPO O3TOT L2 products require ancillary data. TEMPO O3TOT algorithm mainly used atmospheric trace gas and meteorological parameters from the TOMS climatology data. They are interpolated onto TEMPO pixels from their original resolutions.

For surface reflectance and effective cloud fraction, TEMPO O3TOT assumes 15% for surface albedo and 80% for cloud albedo to derive effective cloud fraction and directly retrieve surface/cloud albedo if the effective cloud fraction is ≤ 0 or ≥ 1. Snow and ice can dramatically change surface albedo and significantly influence cloud and trace gas results. Snow and ice fraction is specified through TOMS climatology data. The details of ancillary data are shown in Table 3.1.1.

Table 3.1.1. Ancillary data for TEMPO L2 O3TOT algorithm.

Input	**Source**
Cloud-top pressure	TEMPO CLDO4 product Defaults to cloud pressure climatology (OMI-derived) if cloud retrieval is unavailable.
Cloud fraction	Retrieved based on the MLER. If $f_c \leq 0$ or ≥ 1, it is set to 0 or 1, R_s or R_{cld} is retrieved instead.
Ozone profiles	TOMS V8 climatology (total ozone dependent, monthly / 10° zonally mean)
Temperature profiles	TOMS V8 climatology (monthly / 10° zonally mean)
Surface albedo	15% or directly retrieved as R_s if $f_c = 0$
Snow/ice fraction	Climatology at 1° × 1° from the TOMS V8
Terrain height pressure	Climatology at 1/3° × 1/3° from the TOMS V8
Aerosols	Not explicitly treated, but an aerosol correction is included

3.2. O3TOT

3.2.1. Algorithm overview

The TEMPO L2 O3TOT algorithm is based on the OMTO3 V8.5 algorithm (called TOMS V8.5) adapted for TEMPO. This algorithm has been described in detail in the OMI ATBD for ozone products (https://eospso.gsfc.nasa.gov/sites/default/files/atbd/ATBD-OMI-02.pdf, chapter 2).

There are several changes to adapt this algorithm for TEMPO L2 O3TOT. The first way to adapt to TEMPO is to update the radiance Look-Up Table (LUT). The viewing zenith angles in LUT were expanded to accommodate larger TEMPO's larger observing viewing zenith angle

(VZA). The Second way to adapt to TEMPO is to update the slit function, which is from Bass-Paur cross sections with a triangular slit function of 0.45 nm full width at half maximum (FWHM), to BDM cross sections with a triangular FWHM of 0.60 nm. The last update is to use the retrieved optical centroid cloud pressure from the new TEMPO CLDO4 product.

The basic algorithm uses 2 wavelengths (317.5 and 331.2 nm under most conditions, and 331.2 and 360 nm for high ozone and high solar zenith angle conditions). The longer of the two wavelengths is used to derive effective cloud fraction (f_c) based on the Mixed Lambert Equivalent Reflectivity (MLER) model that was developed to model the effect of clouds on Rayleigh scattering. This algorithm also calculates the absorbing aerosol index (AI) from the radiance residuals at 360 nm.

3.2.2. O3TOT usage recommendations

The quality_flag variable in the product group of the L2 file provides quality of the product. Retrieval of the highest quality have quality_flag equal to “0”. If a data user wants to perform an analysis with a lot of data, even if it is less accurate, the user can use quality_flag equal “5”, “8”, and “13”. Lastly, if a data user want to perform an analysis without considering the data quality, the user can use quality_flag is smaller than “4096”.

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 O3TOT filename have a format of

TEMPO_{GAS}_L2_V03_{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: O3TOT. (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_V03_{YYYY}{MM}{DD}T{HH}{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
O3TOT Level 2	TEMPO_O3TOT_L2_V03_{YYYY}{MM}{DD}T{HH}{NN}{SS}Z _S{XXX}G{YY}.nc
O3TOT Level 3	TEMPO_O3TOT_L3_V03_{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. 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	column_amount_o3	float (mirror_step, xtrack)	DU	Total ozone column
product	fc	float (mirror_step, xtrack)	none	Effective cloud fraction (mixed LER model)
product	uv_aerosol_index	float (mirror_step, xtrack)	none	UV aerosol index

The L2 O3TOT file also contains multiple useful variables to check the quality of the total ozone retrieval. The following variables are included in O3TOT L2 file:

- quality_flag in product group reports the detailed quality of the retrieval.
  - Bits 0 to 3 together contain several output error flags (Note in the case of multiple error flags, only the highest error flag is reported):
    - 0: Good sample
    - 1: Glint contamination (corrected)
    - 2: SZA > 84°
    - 3: 360 residual > threshold
    - 4: Residual at unused ozone wavelength > 4 sigma
    - 5: SOI > 4 sigma (SO_2 present)

        - 6: Non-convergence
        - 7: Abs (residual) > 16.0 (fatal)
        - 8: Row anomaly error (same as bit 6 in this field)
    - Bits 4 to 5 are reserved for future use (currently set to 0).
    - Bit 7 is set to 0 when TEMPO CLDO4 cloud pressure is used and set to 1 when climatological cloud pressure is used.
    - Bits 8 to 15 are flags that are set to 0 for FALSE (good value), or 1 for TRUE (bad value)
        - Bit 8: Geolocation error (anomalous FOV Earth location)
        - Bit 9: SZA > 88°
        - Bit 10: Missing input radiance
        - Bit 11: Error input radiance
        - Bit 12: Warning input Radiance
        - Bit 13: Missing input irradiance
        - Bit 14: Error input irradiance
        - Bit 15: Warning input irradiance

- algorithm_flags in support_data group reports the overall quality of the retrieval.
    - The algorithm flag associated with the ground pixel:
        - 0: Skipped
        - 1: Standard
        - 2: Adjusted for profile shape
        - 3: Based on C-pair (331 and 360 nm)
        - 10: Snow/Ice

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