

Algorithm Description for the TEMPO Total Ozone Retrieval Algorithm

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Key Points:

- This article provides descriptions of the TEMPO total ozone retrieval algorithm from theoretical and practical perspectives.
- Evaluation of the TEMPO V3.0 (Beta) total ozone columns using the OMI and OMPS data.
- Known issues of the TEMPO V3.0 (Beta) total ozone retrieval algorithm.

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Abstract

For the Tropospheric Emissions: Monitoring of Pollution (TEMPO), the OMTO3 V8.5 (also called Total Ozone Mapping Spectrometer (TOMS) V8.5) based algorithm has been adapted to retrieve the total ozone columns. This algorithm uses two wavelength pairs, one (317.5 nm for Ozone and 331.2 nm for the reflectivity) is for most conditions and the other (331.2 and 360 nm) is for high ozone and high solar zenith angle conditions. For adapting to the TEMPO, three parts have been updated, first is expanding viewing geometry to accommodate larger TEMPO's larger observing viewing zenith angle (VZA), second is updated 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, and third is using optical centroid cloud pressure from the TEMPO cloud (CLDO4) product. The main product parameters are total column ozone (TCO) for the TEMPO each native spatial pixel. This algorithm also calculates the absorbing aerosol index (AI) from the radiance residuals at 360 nm.

Plain Language Summary

Ozone has a profound influence on the atmosphere and life on Earth. The ozone layer in the stratosphere acts as a protector of the Earth's life from harmful solar ultraviolet radiation and constitutes ~90% of total ozone. It is an important greenhouse gas in the upper troposphere and lower stratosphere and plays a very important role in tropospheric chemistry in the troposphere. It is a major pollutant and toxic to biota near the surface. So, it is essential to monitor both total ozone and its vertical distribution due to its key roles in different parts of the atmosphere. TEMPO (Tropospheric Emissions: Monitoring of Pollution) is a satellite mission in geostationary orbit used for measuring trace gases and aerosols of importance to air quality over North America. This document describes the retrieval algorithm and product details for the TEMPO total ozone product.

Keywords: TEMPO, Total Ozone, UV aerosol index

Version Description

This is Version 1.0 of the algorithm description for the TEMPO Level 2 total ozone retrieval algorithm.



1 Introduction

TEMPO is NASA's first Earth Venture Instrument (EVI-1) project, selected in 2012 (Zoogman et al., 2017). It is a PI-led instrument project at the Smithsonian Astrophysical Observatory (SAO) with project management at NASA Langley Research Center (LaRC) and instrument development at Ball Aerospace. TEMPO is NASA's first host payload. NASA LaRC was designated to manage the mission project to find the satellite provider and host and launch for TEMPO. After the TEMPO instrument delivery in November 2018, the TEMPO mission joined with the satellite provider Maxar in 2019 and the host IntelSat in 2020. The TEMPO instrument will launch on board the commercial geostationary communication satellite IntelSat-40e (IS-40e) via SpaceX Falcon 9 into a geostationary orbit at 91°W.

TEMPO uses the UV/visible spectroscopic technique to measure atmospheric pollution across North America, from Mexico City/Puerto Rico to the Canadian oil sands, and from the Atlantic to the Pacific, hourly and at high spatial resolution. TEMPO spectroscopic measurements in the ultraviolet and visible wavelengths provide a tropospheric measurement suite that includes the key gases of tropospheric air pollution chemistry. Measurements are made from geostationary orbit for nearly continuous daylight monitoring and to capture the inherent high variability in the diurnal cycle of emissions and chemistry. A small spatial footprint resolves pollution sources at a sub-urban scale. Together, high temporal and spatial resolution improves emission inventories, better monitors population exposure, and enables effective emission-control strategies.

The detailed descriptions of the TEMPO instrument and measurements are described in the previous study (Zoogman et al., 2017) and TEMPO L0-1 ATBD (Chong et al. 2024).



1.1 Scope of this ATBD

The purpose of this algorithm description document is to describe the TEMPO total ozone retrieval algorithm (O3TOT) briefly. This TEMPO O3TOT algorithm is based on TOMS V8.5 algorithm and the detailed descriptions are in the OMI algorithm theoretical basis document (ATBD) for ozone products (<https://eosps0.gsfc.nasa.gov/sites/default/files/atbd/ATBD-OMI-02.pdf>, chapter 2). The generated output contains the retrieved total ozone, SO₂ index, and UV aerosol index. It contains ozone columns below the cloud, effective cloud fraction, radiative cloud fraction, cloud pressure, surface reflectivity at 331 nm, surface refractivity at 360 nm, terrain height, and terrain pressure. The quality flag and algorithm are very useful parameters for evaluating a retrieved total ozone.



2 Algorithm Description

The TOMS algorithm is based on theoretical work developed by Dave and Mateer in 1967, making it a foundational concept in the field of atmospheric science for almost half a century. This algorithm uses two wavelengths (317.5 and 331.2 nm) to estimate the Total Column Ozone (TCO) based on BUV radiances from satellite observation. This TOMS algorithm was adapted to the TEMPO total ozone (O3TOT) algorithm.

The TEMPO algorithm uses two wavelength pairs, one is 317.5 and 331.2 nm under most conditions, the other is 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. In this MLER model, the scene consists of a clear-sky scene of surface reflectivity of 0.15 and a cloudy scene of cloud reflectivity of 0.8 based on the independent pixel approximation:

$$I = I_{clr} \times (1 - f_c) + I_{clد} \times f_c \quad (1)$$

where I , I_{clr} and $I_{clد}$ are the overall, clear, and cloudy scene radiances, respectively. When f_c becomes less than zero or when there is snow/ice, we assume that no cloud is present and use the Lambert Equivalent Reflectivity (LER) model to derive the clear scene reflectivity R . When f_c exceeds 1, we assume 100% cloud cover and derive cloud reflectivity using the LER model. Given the derivation of f_c and/or R from the longer wavelength, the shorter (stronger ozone-absorbing) wavelength is used to derive total ozone. The effective cloud-top pressure is taken from the retrieved Optical Cloud Centroid Pressure (OCCP) inferred from the newly implemented TEMPO O₂-O₂ cloud algorithm when available. Otherwise, it is taken from the climatological Optical Cloud Centroid Pressure (OCCP) from the OMCLDRR product. In either the MLER or LER model, the retrieved ozone column is the weighted ozone column above surface and OCCP by Cloud Radiative Fraction (CRF), defined as $f_c \times I_{clد} \div I$. To estimate the total column amount, the “un-measured” or ghost column below OCCP (also weighted by CRF) is estimated using an ozone climatology and added to retrieved ozone column.

The algorithm also calculates the absorbing Aerosol Index (AI) from the radiance residuals at 360 nm. The AI is useful for tracking global transport of smoke and dust, for it can



track these aerosols above and through clouds, as well as over snow/ice covered surfaces. Various studies have indicated that AI is very nearly proportional to the aerosol absorption optical depth at 360 nm. However, the proportionality constant varies with the altitude (of the center of mass) of the aerosol layer, the lower the altitude the smaller the constant. Most aerosols have stronger absorption in the UV than in the visible, including mineral dust from deserts and carbonaceous aerosols containing organic and black carbon. Since the AI is also affected by the spectral dependence of surface albedo caused by sea-glint and water-leaving radiance, and since there are residual errors in the MLER model in estimating Rayleigh scattering in presence of clouds, we recommend that only the AI values larger than +1 should be used for aerosol studies and areas contaminated by sea-glint should be avoided completely. Since absorbing aerosols causes the ozone derived from the basic ozone retrieval algorithm to be overestimated, a parametric relationship based on AI is used to correct the initial retrieved ozone column. This relationship also appears to remove a large portion of errors caused by sea-glint. Other than the three primary wavelengths mentioned above, the total ozone algorithm uses additional wavelengths for quality control and error correction in more restricted geophysical situations. These include correction for ozone profile shape errors at large solar zenith angles using 312.6 nm measurements, and the detection of strong sulfur-dioxide contamination using multiple wavelength pairs. For a more detailed description of the algorithm please refer to the Algorithm Theoretical Basis Document (ATBD) at <https://eosps0.gsfc.nasa.gov/sites/default/files/atbd/ATBD-OMI-02.pdf>, chapter 2.

The total ozone algorithm is one of the two algorithms that derive total ozone values from TEMPO. It performs retrieval at the native spatial resolution. The other is the ozone profile algorithm based on the optimal estimation approach. It takes advantage of TEMPO's hyperspectral measurements and can retrieve more vertical information from TEMPO radiance spectrum in the UV and visible. Therefore, it can potentially be more accurate. However, due to the involvement of on-line radiative transfer calculation, the ozone profile retrieval is very slow and is only performed on aggregated pixels (4 native spatial pixels coadded; currently 4 pixels across the track or in the N/S direction are).



2.1 Atmospheric Model and Trace Gas Profiles

The TEMPO O3TOT algorithm mainly uses atmospheric trace gas profiles and meteorological parameters from the TOMS V8 climatology data as shown in Table 1.

Table 1. Ancillary data used in the TEMPO O3TOT algorithm.

Input	Source
Cloud-top pressure	TEMPO O ₂ -O ₂ cloud 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 averaged)
Temperature profiles	TOMS V8 climatology (monthly / 10° zonally averaged)
Surface albedo	15% or directly retrieved as R_s if $f_c = 0$
Snow/ice fraction	Climatology at 1° × 1° from the TOMS V8.5
Terrain height pressure	Climatology at 1/3° × 1/3° from the TOMS V8.5
Aerosols	Not explicitly treated, but an aerosol correction is included

2.2 Quality Flags

TEMPO O3TOT product has two quality flags, one is `algorithm_flags` in `support_data` group reports the overall quality of the retrieval, the other is `quality_flag` in `product_group` reports the detailed quality of the retrieval.

Detailed descriptions for algorithm flag and quality flag are shown in Table 2 and Table 3, respectively.

Table 2. Algorithm flags in the TEMPO O3TOT product.

Value	Descriptions
0	Skipped
1	Standard



2	Adjusted for profile shape
3	Based on C-pair (331 and 360 nm)
10	Snow/Ice

Table 3. *Quality flags in the TEMPO O3TOT product.*

Value	Descriptions
Bits 0 to 3 together contain several output error flags	
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

2.3 Algorithm Output Variables

Table 4 presents key variables in the TEMPO L2 O3TOT product file.

Table 4. Key variables in the TEMPO L2 O3PROF product file.

Name	Long name	Unit
/product/column_amount_o3	Column amount o3	DU
/product/fc	fc	-
product/ o3_below_cloud	o3 below cloud	DU
/product/quality_flag	quality flag	-
/product/radiative_cloud_frac	radiative cloud frac	-
/product/so2_index	so2 index	-
/product/uv_aerosol_index	uv aerosol index	-
/support_data/a_priori_layer_o3	a priori layer o3	DU
/support_data/algorithm_flags	algorithm flags	-
/support_data/cloud_pressure	cloud pressure	hPa
/support_data/lut_wavelength	lut wavelength	nm
/support_data/step1_o3	step1 o3	DU
/support_data/step2_o3	step2 o3	DU
/support_data/surface_reflectivity_at_331nm	surface reflectivity at 331nm	percent
/support_data/surface_reflectivity_at_360nm	surface reflectivity at 360nm	percent
/support_data/terrain_height	terrain height	m
/support_data/terrain_pressure	terrain pressure	hPa



3. Algorithm Usage Constraints

This article aims to describe the TEMPO O3TOT algorithm briefly. Therefore, detailed descriptions and the underlying theory are provided in the OMI ATBD (<https://eosps0.gsfc.nasa.gov/sites/default/files/atbd/ATBD-OMI-02.pdf>, chapter 2). It is recommended to read the User Guide document before utilizing the TEMPO Level 2 total ozone product.



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