# Global Modeling and Assimilation Office

*GMAO Office Note No. 22 (Version 1.0)*

# Supplemental Documentation for GEOS Aerosol Products

Release Date: 03/02/2023

**Global Modeling and Assimilation Office**
**Earth Sciences Division**
**NASA Goddard Space Flight Center**
**Greenbelt, Maryland 20771**

This page intentionally left blank.

# Supplemental Documentation for GEOS Aerosol Products

Document maintained by Allison Collow (GMAO, UMBC)

This document should be cited as
Collow, A., V. Buchard, M. Chin, P. Colarco, A. Darmenov, and A. da Silva, 2023: Supplemental Documentation for GEOS Aerosol Products. GMAO Office Note No. 22 (Version 1.0), 8 pp, available from http://gmao.gsfc.nasa.gov/pubs/office_notes.

Approved by:

_________________________________

Steven Pawson Date

Head, Global Modeling and Assimilation Office
Code 610.1, NASA GSFC

**REVISION HISTORY**

| Version Number | Revision Date | Extent of Changes |
|---|---|---|
| 1.0 | 03/02/2023 | Baseline |

# Table of Contents

# 1. Introduction

This document provides information pertinent for the interpretation and analysis of aerosol products in the Goddard Earth Observing System (GEOS) produced using the Goddard Chemistry Aerosol Radiation and Transport (GOCART) module. GOCART was initially developed as an offline model, driven by assimilated meteorological fields, to represent the lifecycle of aerosols (Chin et al., 2000, 2002; Ginoux et al., 2001). It has since been incorporated as an online module within GEOS (Colarco et al. 2010) and has been used to analyze and forecast the aerosol lifecyle and their interaction with radiation (Randles et al., 2017; Buchard et al., 2017). GOCART is used in near-real time (NRT), reanalysis, and subseasonal to seasonal (S2S) GEOS products as summarized in Figure 1. NRT products include GEOS FP (Lucchesi, 2018), GMAO's weather and forecast system, GEOS-CF (Knowland et al., 2022), focused on chemical constituents, and a semi-stationary system used to provide data to instrument teams, termed FP-IT and slated to be replaced by GEOS-IT. Additionally, GOCART aerosols are included in GMAO's flagship reanalysis, MERRA-2 (Bosilovich et al., 2016), and S2S systems (Nakada et al., 2018). Users are referred to the respective documentation for each individual product for more information. In version 1 of GEOS-CF, two aerosol modules are run in parallel, with GOCART coupled to the meteorology (Keller et al., 2021). Aerosol output from GOCART within GEOS-CF is currently limited and used as a measure of uncertainty (Knowland et al., 2022). Caution is recommended if using details in this document alongside output from GEOS-CF as it may not be applicable.

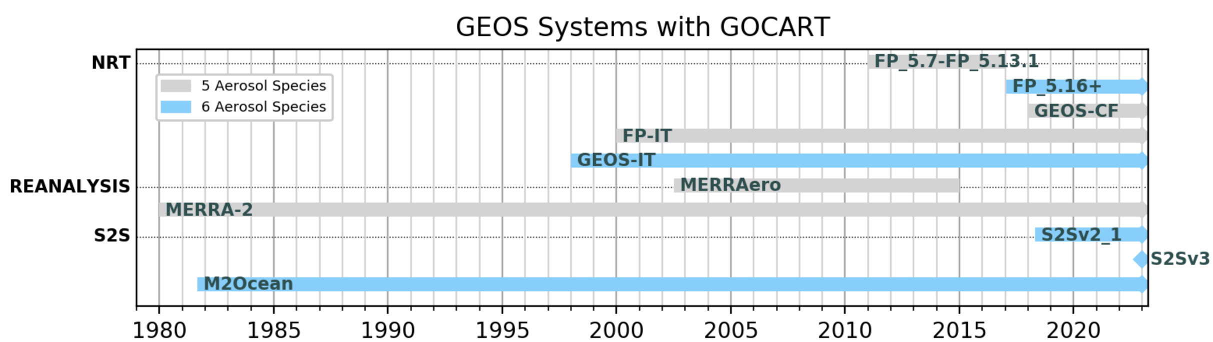



Figure 1: Timeline of GEOS products that include GOCART colored based on the number of aerosol species as discussed in Section 2.

# 2. Aerosol Speciation

Depending on the configuration, GOCART provides five to seven species of aerosol: dust, sea salt, sulfate, black carbon, organic carbon, nitrate (GEOS 5.16 and later), ammonium (GEOS 5.16 and later), and brown carbon (GOCART2G and later). In the real world, each of these species would be present in the atmosphere with a size distribution. For computational efficiency, dust and sea salt are binned into five size groupings and nitrate is proportioned into three bins. This binning allows for particle size to be incorporated into the production, deposition, and optical properties of the aerosol. For other aerosol components, lognomal distributions of particle sizes are imposed, with modal and effective radius varying with ambient relative humidity. Furthermore, carbonaceous aerosols (black carbon, organic aerosol) are grouped into hydrophobic and hydrophilic components to represent aerosol particles that do and do not swell, respectively, in the presence of elevated relative humidity. The bulk properties of each aerosol species are described in more detail in the following subsections.

## 2.1 Dust

### 2.1.1 GEOS FP 5.29.4, MERRA-2, GEOS-IT, GEOS S2S

Dust aerosol is considered hydrophobic and is represented with five mass bins that correspond to dry size ranges (in μ) and densities (kg $m^{-3}$) as follows:

| | DU001 | DU002 | DU003 | DU004 | DU005 |
|---|---|---|---|---|---|
| Radius (μm) | 0.73 | 1.4 | 2.4 | 4.5 | 8 |
| Radius Lower Bound (μm) | 0.1 | 1 | 1.8 | 3 | 6 |
| Radius Upper Bound (μm) | 1 | 1.8 | 3 | 6 | 10 |
| Density (kg $m^{-3}$) | 2500 | 2650 | 2650 | 2650 | 2650 |

In the optical property calculations, the first bin DU001 is split into four sub-bins with differing optical properties following the sub-bin particle size distribution in Table 1 of Tegen and Lacis (1996).

## 2.2 Sea Salt

### 2.2.1 GEOS FP 5.29.4, MERRA-2, GEOS-IT, GEOS S2S

Sea salt aerosol is represented with five bins that correspond to dry size ranges (in μ) and densities (kg $m^{-3}$) as follows:

| | SS001 | SS002 | SS003 | SS004 | SS005 |
|---|---|---|---|---|---|
| Radius (μm) | 0.079 | 0.316 | 1.119 | 2.818 | 7.772 |
| Radius Lower Bound (μm) | 0.03 | 0.1 | 0.5 | 1.5 | 5 |
| Radius Upper Bound (μm) | 0.1 | 0.5 | 1.5 | 5 | 10 |
| Density (kg $m^{-3}$) | 2200 | 2200 | 2200 | 2200 | 2200 |

Salt is considered hydrophilic such that the size of each sea salt bin will change as the particle grows due to humidity.

## 2.3 Nitrate

### 2.3.1 GEOS FP 5.29.4, GEOS-IT, GEOS S2S

Nitrate aerosol, represented with three size bins, and the associated chemistry tracers, ammonia ($NH_3$) and ammonium ion ($NH_4^+$), are included in GEOS products beginning with GEOS-5.16 in 2017. Fine mode nitrate is placed in bin 001, while bins 002 and 003 represent the heterogenous production of nitrate on sea salt and dust aerosols, respectively. The dry size ranges (in μm) and densities used for calculating settling velocities (kg $m^{-3}$) for aerosol involved in the lifecycle of nitrate are as follows:

| | $NH_4^+$ | NI001 | NI002 | NI0033 |
|---|---|---|---|---|
| Radius (µm) | 0.2695 | 0.2695 | 2.1 | 7.57 |
| Density (kg $m^{-3}$) | 1769 | 1725 | 2200 | 2650 |

### 2.4 Sulfate

#### 2.4.1 GEOS FP 5.29.4, MERRA-2, GEOS-IT, GEOS S2S
Sulfate has a dry particle radius of 0.35 µm and a density of 1700 kg $m^{-3}$, which are used for settling.

### 2.5 Carbonaceous Aerosol

#### 2.5.1 GEOS FP 5.29.4, MERRA-2, GEOS-IT, GEOS S2S
Carbonaceous aerosol is divided into black and organic carbon. Upon emission, each carbon species is partially hydrophobic and becomes hydrophilic with time. From an optics perspective, the size distribution for the hydrophilic portion of carbon changes with relative humidity according to a growth factor. Despite being termed organic carbon, a factor of 1.8 is already applied to convert source masses of organic carbon into particulate organic matter (POM). The settling radii and densities for all carbon species are 0.35 µm and 1800 kg $m^{-3}$, respectively.

#### 2.5.2 GOCART-2G
Beginning with the implementation of GOCART-2G, brown carbon is included as the organic aerosol emitted from biomass burning that is distinct from organic aerosols with anthropogenic and biogenic sources. Brown carbon is assumed to be hydrophobic, and its physical and optical properties are similar to organic aerosols but with stronger absorption at ultraviolet wavelengths.

## 3. Computation of Surface $PM_{2.5}$

GEOS outputs the surface mass concentration of aerosol particles with diameters smaller than 2.5 µm individually for each aerosol species using the geometric size of an aerosol particle at 0% relative humidity. These fields can then be used to compute the total $PM_{2.5}$, however the formulation is dependent on humidity and the number of species included in the version of GEOS. In the presence of water vapor, hydrophilic carbon, sulfate, sea salt, and nitrate will swell and effectively increase the aerosol mass concentration. Below are the suggested formulas for the computation of total $PM_{2.5}$ based on the variety of aerosol speciations in GEOS products. This formulation neglects the possibility that an aerosol particle may swell to be larger that 2.5 microns with elevated humidity.

### 3.1 MERRA-2

MERRA-2 contains five aerosol species, black carbon, dust, organic carbon, sea salt, and sulfate. The geometric $PM_{2.5}$ can be computed as follows utilizing output from the tavg1_2d_aer_Nx file collection:

$$PM2.5 = DUSMASS25 + f_{rh,oc} * OCSMASS + f_{rh,bc}*BCSMASS + f_{rh,ss}*SSSMASS25 + f_{rh,so4}*SO4SMASS*1.3756$$

where $f_{rh,x}$ is the particle growth factor at ambient RH for specie x and the multiplication of sulfate by 1.3756 is to convert sulfate, $SO_4$, to ammonium sulfate, $(NH_4)_2SO_4$, as the most likely form of sulfate in the atmosphere. Details on determining $f_{rh,x}$ can be found in Section 3.4.

## 3.2 GEOS 5.16+ and GEOS-IT

Beginning with GEOS-5.16, which includes the currently operational GEOS FP and upcoming GEOS-IT, GOCART includes six aerosol species: black carbon, dust, organic carbon, sea salt, sulfate, and nitrate. The geometric $PM_{2.5}$ can be computed as follows utilizing output from the tavg1_2d_aer_Nx file collection:

$$PM2.5 = DUSMASS25 + f_{rh,oc} * OCSMASS + f_{rh,bc}*BCSMASS + f_{rh,ss}*SSSMASS25 + f_{rh,so4}*SO4SMASS + f_{rh,ni}*NISMASS25 + NH4SMASS$$

where $f_{rh,x}$ is the particle growth factor at ambient RH for specie x. The multiplication factor of 1.3756 used in the MERRA-2 formulation is not required due to the inclusion of an ammonia tracer. Details on determining $f_{rh,x}$ can be found in Section 3.4.

## 3.3 GOCART2G

Beginning with the implementation of GOCART-2G, there are seven aerosol species: black carbon, brown carbon, dust, organic carbon, sea salt, sulfate, and nitrate. The geometric $PM_{2.5}$ can be computed as follows utilizing output from the tavg1_2d_aer_Nx file collection:

$$PM2.5 = DUSMASS25 + f_{rh,oc} * OCSMASS + f_{rh,br} * BRSMASS + f_{rh,bc}*BCSMASS + f_{rh,ss}*SSSMASS25 + f_{rh,so4}*SO4SMASS + f_{rh,ni}*NISMASS25 + NH4SMASS$$

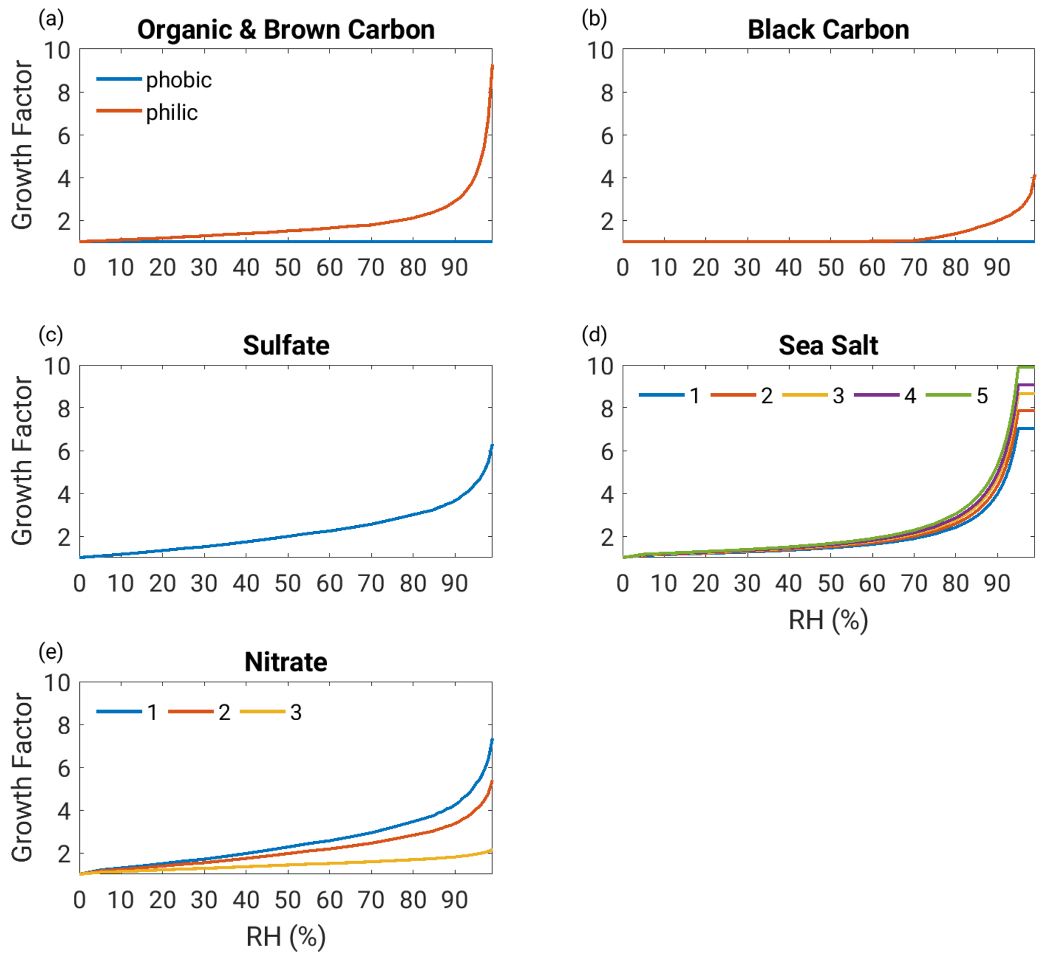
where $f_{rh,x}$ is the particle growth factor at ambient RH for specie x. The multiplication factor of 1.3756 used in the MERRA-2 formulation is not required due to the inclusion of an ammonia tracer. Details on determining $f_{rh,x}$ can be found in Section 3.4.

## 3.4 Growth Factors Due to Relative Humidity

A self-consistent growth factor to account for the mass of water for a given species and relative humidity can be computed using the formula:

$$Growth\ Factor\ =\ 1 + \left(\left(\left(\frac{Radius\ at\ Wet\ RH}{Radius\ at\ Dry\ RH}\right)^3 - 1\right) x\ \frac{\rho_{Water}}{\rho_{Dry\ Species}}\right)$$

The dry densities for each species can be found in Section 2, while the effective radius at varying relative humidity for each species can be found in the optics tables described in Section 4. This results in the growth curves as shown in the figure below.




## 3.5 Aerodynamic $PM_{2.5}$

Observations of $PM_{2.5}$, such as those from the Environmental Protection Agency (EPA) and Interagency Monitoring of Protected Visual Environments (IMPROVE), are often representative of an aerodynamic particle size as opposed to geometric (Hand et al., 2011). When comparing GEOS $PM_{2.5}$ data to observations it is necessary to account for the fact that the aerodynamic diameter of a particle is generally larger than the geometric diameter for non-spherical particles and/or for particle density higher than 1 g $cm^{-3}$ (e.g., Reid et al., 2003). The geometric and aerodynamic diameters are related according to

$$d_a = d_g \sqrt{\frac{\rho}{\chi}}$$

where $d_a$ is the aerodynamic diameter, $d_g$ is the geometric diameter, $\rho$ is the particle density in g $cm^{-3}$, and $\chi$ is a shape factor.

This yields an aerodynamic particle size of 2.5 µm equivalent to a geometric size of 1.83 µm for dust and 1.69 µm for sea salt.

Unlike the computation of total $PM_{2.5}$ with a geometric particle size, the mass concentration of each species must come from the diagnostics based on size bin in the aerosol collection that provides the entire vertical profile, inst3_3d_aer_Nv. The fractional contribution, fPM, of a given bin, n, can be determined by

$$fPM(n) = \log(rPM/r\_low(n)) \,/\, \log(r\_up(n)/r\_low(n)),$$

where rPM is the threshold radius and r_low and r_up are the upper and lower bounds for the sea salt and dust bins given in the tables above.

An example formula using the seven aerosol species in GOCART2G is given below, where multiplicative factors are added for bin 1 of dust and bin 3 of sea salt to account for the fractional contribution of those bins.

$$PM_{2.5} = (0.9614*DU001 + f_{rh,ss1} * SS001 + f_{rh,ss2} * SS002 + f_{rh,ss3} * 0.3871 *SS003 + BCPHILIC + BCPHOBIC + f_{rh,oc} * OCPHILIC + OCPHOBIC + f_{rh,br} * BRPHILIC + BRPHOBIC + NH4A + f_{rh,ni1} * NO3AN1 + f_{rh,su} * SO4)*AIRDENS$$

# 4. Optics Calculations

Here we briefly describe the optics calculations that are used to compute the scattering and absorption extinction in GEOS due to aerosol. Aerosols are considered externally mixed. Each aerosol species has its own optics look up table that defines the aerosol intensive properties based on the Optical Properties of Aerosols and Clouds refractive indices (OPAC; Hess et al. 1998) and assuming Mie scattering. The resulting optics files for each aerosol species contains the scattering, extinction, mass scattering and mass extinction efficiencies, asymmetry parameter, and real and imaginary refractive indices as a function of wavelength, relative humidity, and particle radius. These fields are used to compute the scattering and absorption for each species and gridbox, which are then added linearly to arrive at the total aerosol optical depth. Single scattering albedo is defined in the same manner as the ratio of the scattering extinction to the total extinction. Additional details regarding the generation of the optics look up tables can be found in Kemppinen et al. (2022). A record of the optics files used in GEOS products can be found in Appendix B. Netcdf files containing the optics parameters are available for download at https://portal.nccs.nasa.gov/datashare/iesa/aerosol/AerosolOptics/.

# References

Bosilovich, M. G., R. Lucchesi, and M. Suarez (2016). MERRA-2: File Specification. GMAO Office Note No. 9 (Version 1.1), 73 pp, available from http://gmao.gsfc.nasa.gov/pubs/office_notes.

Buchard, V., C. A. Randles, A. da Silva,A. S. Darmenov, P. R. Colarco,R. C. Govindaraju, R. A. Ferrare, J. W. Hair, A. Beyersdorf, L. D. Ziemba, and H. Yu (2017). The MERRA-2 Aerosol Reanalysis, 1980-onward, Part II: Evaluation and Case Studies. J. Clim , 30, 6851-6872. doi: 10.1175/JCLI-D-16-0613.1, Chin, M., Rood, R. B., Lin, S.-J., Müller, J.-F., and Thompson, A. M. (2000), Atmospheric sulfur cycle simulated in the global model GOCART: Model description and global properties, J. Geophys. Res., 105( D20), 24671– 24687, doi:10.1029/2000JD900384.

Chin, M., Ginoux, P., Kinne, S., Torres, O., Holben, B. N., Duncan, B. N., Martin, R. V., Logan, J. A., Higurashi, A., and Nakajima, T. (2002), Tropospheric Aerosol Optical Thickness from the GOCART Model and Comparisons with Satellite and Sun Photometer Measurements, J. Atmos. Res., 59(3), 461-483. doi:10.1175/1520-0469(2002)059<0461:taotft>2.0.co;2.

Colarco, P., da Silva, A., Chin, M., and Diehl, T. (2010), Online simulations of global aerosol distributions in the NASA GEOS-4 model and comparisons to satellite and ground-based aerosol optical depth, J. Geophys. Res., 115, D14207, doi:10.1029/2009JD012820.

Ginoux, P., M. Chin, I. Tegen, J. Prospero, B. Holben, O. Dubovik, and S.-J. Lin (2001), Sources and global distributions of dust aerosols simulated with the GOCART model, J. Geophys. Res. 106, 20,255-20,273. doi: 10.1029/2000JD000053.

Keller, C. A., K.E. Knowland, B. N. Duncan, J. Liu, D. C. Anderson, S. Das, R. A. Lucchesi, E. W. Lundgren, J. M. Nicely, E. Nielsen, L. E. Ott, E. Saunders, S. A. Strode, P. A. Wales, D. J. Jacob, and S. Pawson (2021). Description of the NASA GEOS Composition Forecast Modeling System GEOS-CF v1.0. Journal of Advances in Modeling Earth Systems, 13 (4), e2020MS002413. doi: 10.1029/2020MS002413.

Kemppinen, O. and Coauthors (2022). GEOS aerosol optical table calculation package pygeosmie. NASA Technical Report, in preparation.

Knowland, K.E., C.A. Keller, and R. Lucchesi (2022). File Specification for GEOS-CF Products. GMAO Office Note No. 17 (Version 1.2), 53 pp, available from https://gmao.gsfc.nasa.gov/pubs/office_notes.php.

Hand, J., and Coauthors (2011). Spatial and seasonal patterns and temporal variability of haze and its constituents in the United States: Report V June 2011. Cooperative Institute for Research in the Atmosphere, Colorado State University, 507 pp. [Available online at http://vista.cira.colostate.edu/Improve/spatial-and-seasonal-patterns-and-temporal-variability-of-haze-and-its-constituents-in-the-united-states-report-v-june-2011/.]

Hess, M., P. Koepke, and I. Schult (1998). Optical Properties of Aerosols and Clouds: The Software Package OPAC, Bulletin of the American Meteorological Society, 79(5), 831-844, doi: 10.1175/1520-0477(1998)079<0831:OPOAAC>2.0.CO;2.

Nakada, K., R. Kovach, J. Marshak, and A. Molod (2018). S2S-2_1: File Specification. GMAO Office Note No. 16 (Version 1.0), 78 pp, available from http://gmao.gsfc.nasa.gov/pubs/office_notes.

Randles, C. A., A. da Silva, V. Buchard, P. R. Colarco, A. S. Darmenov, R. C. Govindaraju, A. Smirnov, R. A. Ferrare, J. W. Hair, Y.Shinozuka, and C. Flynn (2017). The MERRA-2 Aerosol Reanalysis, 1980-onward, Part I: System Description and Data Assimilation Evaluation. J. Clim , 30, 6823-6850. doi:10.1175/JCLI-D-16-0609.1.

Reid, J. S., et al. (2003), Comparison of size and morphological measurements of coarse mode dust particles from Africa, J. Geophys. Res., 108, 8593, doi:10.1029/2002JD002485, D19.

Tegen, I., and Lacis, A. A. (1996), Modeling of particle size distribution and its influence on the radiative properties of mineral dust aerosol, J. Geophys. Res., 101( D14), 19237– 19244, doi:10.1029/95JD03610.

# Appendix

## A. GOCART Version History on GitHub

| GEOS GCM Git Release | GOCART Git Release |
|---|---|
| 10.21.1 and earlier | 1.0.1 |
| 10.22.0 | 2.0.5 |

## B. Optics File History Beginning with MERRA-2

| | MERRA-2 | GEOS 5.29.4 |
|---|---|---|
| Black Carbon | v1_3 | v1_3 |
| Brown Carbon | n/a | n/a |
| Dust | v14_2 | v15_3 |
| Nitrate | n/a | v2_5 |
| Organic Carbon | v1_3 | v1_3 |
| Sea Salt | v3_3 | v3_3 |
| Sulfate | v1_3 | v1_3 |
| Number of Bands | 18 | 30 |