README Document for NASA Ocean Biogeochemical Model

Last Revised July 2017

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July 2017

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Revision History

Revision Date	***Changes***	***Author***
2008	Original version	Gregg W.W.
March 2012	R2012.3	Gregg W.W. and Rousseaux C.S.
February 2015	See “1.4. What’s New?”	Gregg W.W. and Rousseaux C.S.
July 2017	R2017, See “1.4. What’s New?”	Gregg W.W. and Rousseaux C.S.

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1.0 Introduction

This document provides basic information for using NASA Ocean Biogeochemical Model products.

The NASA Ocean Biogeochemical Model (NOBM) is a comprehensive, interactive ocean biogeochemical model coupled with a circulation and radiative model in the global oceans (Gregg and Casey 2007). It spans the domain from -84° to 72° latitude in increments of 1.25° longitude by 2/3° latitude, including only open ocean areas where bottom depth >200m. NOBM contains 4 phytoplankton groups, 4 nutrient groups, a single herbivore group, and 3 detrital pools, and the major ocean carbon components, dissolved organic and inorganic carbon (DOC and DIC).

1.1 Dataset Description

The NASA Ocean Biogeochemical Model has been extensively validated (Gregg and Casey 2007; Gregg et al. 2003), involving a comparison of 9 of the 14 model state variables against in situ and/or satellite data sets (only herbivores, the 3 detrital components, and dissolved organic carbon have not been validated). The model contains 4 explicit phytoplankton taxonomic groups: diatoms, cyanobacteria, chlorophytes, and coccolithophores. As with nutrients and total chlorophyll, the phytoplankton groups in the model have been validated against in situ data (Gregg and Casey 2007, publicly available at http://gmao.gsfc.nasa.gov/research/oceanbiology/).

In the model, all biological processes are assumed to cease in the presence of sea ice. We provide a variable called 'ice' that represents the distribution of sea ice cover. The variables chlorophytes, diatoms, coccolithophores, cyanobacteria and total chlorophyll have been normalized to the fraction of ice (data=data(100-ice/100)).

The model is constrained by satellite data assimilation of total chlorophyll from SeaWiFS and MODIS-Aqua (Gregg 2008). The satellite data sets are adjusted for consistency using the Empirical Satellite Radiance-In situ Data (ESRID) methodology (Gregg and Casey 2010; Gregg et al. 2009).

The model is spun up from prescribed initial conditions (Gregg and Casey 2007) in free-run mode (not assimilated) for 35 years using climatological forcing from Modern-Era Retrospective analysis for Research and Applications (MERRA; Rienecker et al. 2011). It is then run with climatological forcing and data assimilation using climatological ESRID-MODIS chlorophyll for an additional 65 years for a 100-year total simulation. Very minor drift in nutrient concentrations (not chlorophyll) continue to be present, and we find a 15-year segment with the smallest change for all three nutrients (nitrate, silicate, and dissolved iron), which is 0.19% y^{-1} (mean) beginning in simulation year 77. We begin our transient run using these conditions for September 1997, the first year and month of SeaWiFS data collection. We run forward from this time until 2012 using transient forcing from MERRA, switching from ESRID-SeaWiFS to ESRID-MODIS in January 2003.

Phytoplankton relative abundances are not directly affected by the data assimilation, but they can be affected indirectly via changes in concentration gradients, light availability, and nutrient availability that are derived from changes in total chlorophyll.

The NOBM uses a multi-variate assimilation methodology where the imbalances derived from the assimilation of satellite chlorophyll are corrected using a mechanistic approach involving the nutrient-to chlorophyll ratios embedded in the model (Rousseaux and Gregg 2012). The difference between the chlorophyll assimilation results and the prior chlorophyll produced by the model (the analysis increments) are used to adjust the nutrient concentrations. The multi-variate assimilation is applied to silica and dissolved iron, as well as nitrate.

The multi-variate assimilation of nutrients begins with the assimilation of satellite chlorophyll

$$\Delta C_T = C_T(\mathrm{ana}) - C_T(\mathrm{model}) \tag{1}$$

$$C_T(\mathrm{model}) = \sum_i C_i \tag{2}$$

$$\Delta N = b_n \Delta C_T \tag{3}$$

where ΔC_T (Eq. 1) is the difference between the analyzed total chlorophyll, $C_T(\mathrm{ana})$, and the model, $C_T(\mathrm{model})$. $C_T(\mathrm{model})$ is the total chlorophyll (sum of all 4 phytoplankton components, Eq. 2), C_i is the i^{th} phytoplankton chlorophyll component, and f_i is the fraction of the i^{th} phytoplankton component of the total chlorophyll. The change in nitrate ΔN is simply a function of the analysis increment of total chlorophyll ΔC_T modified by the nitrate-to-chlorophyll ratio b_n (Eq. 3). We only allow the assimilation to change nitrate by a maximum of one-half in each assimilation event to reduce model instability resulting from outliers in the satellite chlorophyll data

$$N(\mathrm{assim}) = N(\mathrm{model}) + \min[\Delta N, 0.5N(\mathrm{model})] \tag{4}$$

where N(assim) is the new assimilated nitrate.

We extend this multi-variate approach to silica, except that silica is related strictly to the analysis increment of diatoms

$$\Delta Si = b_s f_i \Delta C_T \qquad (5)$$

$$f_i = C_i(\text{model})/C_T(\text{model}) \qquad (6)$$

where b_s is the silica-to-chlorophyll ratio, and f_i is the fraction of the i^{th} phytoplankton group to the total (in this case it is the diatom component). Like nitrate, Si(assim) is not allowed to change model prior Si by more than half.

$$Si(\text{assim}) = Si(\text{model}) + \min[\Delta Si, 0.5Si(\text{model})] \qquad (7)$$

For dissolved iron, the approach is the same as for to nitrate and silica, as expressed in Eqs. 1-7. However, under conditions of persistent negative ΔC_T and low atmospheric deposition, which occurs in the South Pacific, the assimilated dissolved iron concentrations can approach zero. To rectify this problem, we apply a special case for iron assimilation that only applies for $\Delta Fe<0$ (and therefore $\Delta C_T<0$):

$$Fe(\text{assim}) = Fe(\text{model}) + \min[w\Delta Fe, 0.5Fe(\text{model})] \qquad (8)$$

where Eq. 8 is the same as Eqs. 4 and 7 for nitrate and silica, respectively, except for a weighting factor w. This weighting factor is a function of the prior concentration of Fe.

$$w = 33.3Fe - 5.0 \qquad (9)$$

The weighting is applied globally and provides a smooth transition of the analysis increment to prevent iron concentrations from becoming so low as to prohibit all phytoplankton growth.

1.3 Contact information

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1.4 What's New?

The R2017 (released in July 2017) uses the most recent ocean color data product (R2014) from SeaWiFS, MODIS and Suomi-NPP. We use the Empirical Satellite Radiance-In situ Data (ESRID) methodology (Gregg et al., 2009) to increase the length of the data while keeping the global coverage of our approach. This approach uses relationships between satellite water-leaving radiances and in situ data after full processing, i.e., at Level-3, to improve estimates of surface variables while relaxing requirements on post-launch radiometric re-calibration (Gregg et al. 2009). It improves the quality, reliability, and consistency of ocean color data, while promoting a unified description of ocean biology from satellite and in situ platforms.

ESRID applies the standard processing bio-optical algorithm after processing completion, using satellite water-leaving radiances, and in situ chlorophyll (chl):

$$\log chl = a_0 + a_1R + a_2R^2 + a_3R^3 + a_4R^4 \qquad (10)$$

$$R(\lambda) = \rho(\lambda_1)/\rho(\lambda_2) \qquad (11)$$

where R is the reflectance ratio, ρ is the water-leaving reflectance at a specific wavelength λ, and a_0-a_4 are empirical coefficients. The empirical coefficients absorb biases in the radiances, most notably radiometric calibration but many others, including band location, and most out-of-band and electronic crosstalk errors. This reduces bias in the derived chlorophyll values.

We developed and evaluated ESRID using the latest versions of data produced by NASA and global in situ fluorometric chlorophyll data collected from the National Oceanographic Data Center (NODC; Conkright et al. 2002), NASA in situ (Werdell and Bailey 2005), and Atlantic Meridional Transect (Aiken et al. 2000) archives, that were quality controlled (Gregg et al. 2009). ESRID is substituted for the OCx component of the standard algorithm for chlorophyll concentrations greater than 0.2 mg m^{-3}.

There is insufficient in situ data in the major in situ archives to apply ESRID to VIIRS. Instead we utilize a modification where ESRID-MODIS retrieved chlorophyll is used instead of in situ data to derive empirical relationships with VIIRS satellite radiances. Called ESRIDS, with the second S for satellite, we find that a sixth-order polynomial provides the necessary consistency of VIIRS with MODIS needed here. We only use 2012 for the empirical characterization. ESRID and ESRIDS empirical coefficients are provided in the Appendix of Gregg and Rousseaux (2017). More information on the methodology used can be found in Gregg and Rousseaux (2017).

Additional details on the methodology can be found in:

- Gregg W.W. and C.S. Rousseaux, 2017. Global Trends in Ocean Phytoplankton: A New Assessment Using revised Ocean Color data. Remote Sensing Letters. DOI: 10.1080/2150704X.2017.1354263

2.0 Data Organization

In the model, all biological processes are assumed to cease in the presence of sea ice. We provide a variable called 'ice' that represents the distribution of sea ice cover. The variables chlorophytes, diatoms, coccolithophores, cyanobacteria and total chlorophyll have been normalized to the fraction of ice (data=data(100-ice/100)).

2.1 File Naming Convention

Depending on the data set downloaded the file names will either start by 'mon' for monthly dataset or 'day' for daily data set:

monyyyymm**.R2017.nc4** **(for monthly data set)**

dayyyyymmdd**.R2017.nc4** **(for daily data set)**

where:

- yyyy = 4 digit year number [1998 - 2015].
- mm = 2 digit month number [01-12]
- dd = day of month [01-31]

Example of filename for monthly data: mon199802.R2017.nc4

2.2 File Format and Structure

NOBM Data set files are in NetCDF-4-Classic. The NOBM spans the domain from -84° to 72° latitude in increments of 1.25° longitude by 2/3° latitude. Each monthly file contains the variables included in Table 2.

3.0 Data Contents

3.1 Global Attributes

In addition to arrays containing variables and dimension scales, global metadata is also stored in the files. Some metadata are required by standard conventions, some are present to meet data provenance requirements and others as a convenience to users of NOBM products. A summary of global attributes present in all files is shown in Table 1.

Global Attribute	Description
Map_Projection	Equidistant Cylindrical
Latitude_Units	degrees North
Longitude_Units	degrees East
Northernmost_Latitude	72.0
Southernmost_Latitude	-84.0
Westernmost_Latitude	-180.0
Eaternmost_Latitude	180.0
Latitude_Step	0.66666698
Longitude_Step	1.25
First_Point_Latitude	-84.0
First_Point_Longitude	-180.0

Table 1: Global metadata attributes associated with each NetCDF-4 file.
A floating point value of -9999 is used to identify missing data.

3.2 Products/Parameters

The following NOBM products are available:

Variables	Description	Units
tot	Total chlorophyll *a* concentration	mg chl a/m^3
chl	Chlorophyte concentration	mg chl a/m^3
dia	Diatom concentration	mg chl a/m^3
coc	Coccolithophores concentration	mg chl a/m^3
cya	Cyanobacteria concentration	mg chl a/m^3
irn	Iron concentration	Nano mole/L
rno	Nitrate concentration	Micro mole/L
h	Mixed layer depth	m
ice	Percentage of sea ice cover	%

Table 2: Name of the variables as used in the netcdf-4 files, their full description and units.

4.0 More Information

The NOBM is provided by the Global Modeling and Assimilation Office at NASA Goddard Space Flight Center http://gmao.gsfc.nasa.gov/research/oceanbiology/

6.0 Acknowledgements

This project is funded by the NASA EOS, MODIS Science of Terra and Aqua and MAP Programs.

References

Aiken, J., Rees, N., Hooker, S., Holligan, P., Bale, A., Robins, D., Moore, G., Harris, R., & Pilgrim, D. (2000). The Atlantic Meridional Transect: overview and synthesis of data. *Progress in Oceanography, 45*, 257-312

Conkright, M., Antonov, J., Baranova, O., Boyer, T., Garcia, H., Gelfeld, R., Johnson, D., Locarnini, R., Murphy, P., & O'Brien, T. (2002). World Ocean Database, 2001. Volume 1, Introduction

Gregg, W.W. (2008). Assimilation of SeaWiFS ocean chlorophyll data into a three-dimensional global ocean model. *Journal of Marine Systems, 69*, 205-225

Gregg, W.W., & Casey, N.W. (2007). Modeling coccolithophores in the global oceans. *Deep-Sea Research Part II, 54*, 447-477

Gregg, W.W., & Casey, N.W. (2010). Improving the consistency of ocean color data: A step toward climate data records. *Geophysical research letters, 37*, L04605

Gregg, W.W., Casey, N.W., O'Reilly, J.E., & Esaias, W.E. (2009). An empirical approach to ocean color data: Reducing bias and the need for post-launch radiometric re-calibration. *Remote Sensing of Environment, 113*, 1598-1612

Gregg, W.W., Ginoux, P., Schopf, P.S., & Casey, N.W. (2003). Phytoplankton and iron: validation of a global three-dimensional ocean biogeochemical model. *Deep Sea Research Part II: Topical Studies in Oceanography, 50*, 3143-3169

Gregg, W.W., & Rousseaux, C.S. (2017). Global Trends in Ocean Phytoplankton: A New Assessment Using revised Ocean Color data. *Remote Sensing Letters*

Rienecker, M.M., Suarez, M.J., Gelaro, R., Todling, R., Bacmeister, J., Liu, E., Bosilovich, M.G., Schubert, S.D., Takacs, L., & Kim, G.-K. (2011). MERRA: NASA''s Modern-Era Retrospective Analysis for Research and Applications. *Journal of Climate, 24*

Rousseaux, C.S., & Gregg, W.W. (2012). Climate variability and phytoplankton composition in the Pacific Ocean. *Journal of Geophysical Research, 117*, C10006

Werdell, P.J., & Bailey, S.W. (2005). An improved in-situ bio-optical data set for ocean color algorithm development and satellite data product validation. *Remote Sensing of Environment, 98*, 122-140