**Instructions for working with Bayesian Metabolic Model (BaMM)**

by Gordon W. Holtgrieve, KathiJo Jankowski, Daniel Schindler

Created April 5, 2009

Revised July 19, 2010 by GWH

Revised Dec, 2016 by KJJ

Revised May, 217 by DES

**Please read and cite**:

Holtgrieve, G.W., D.E. Schindler, T.A. Branch, and Z.T. A’Mar. 2010. Simultaneous quantification of aquatic ecosystem metabolism and reaeration using a Bayesian statistical model of oxygen dynamics. *Limnology and Oceanography* 55 (3): 1047-1063.

Schindler, D.E., K.J. Jankowski, Z.T. A’Mar, and G.W. Holtgrieve. 2017. Two-stage metabolism inferred from diel oxygen dynamics in aquatic ecosystems. *Ecosphere*.

**Table of Contents**

1. Documentation and installation
2. Creating data and input files
3. Running the model
4. Reading and analyzing output
5. Known bugs and issues

**Contact information**

Gordon Holtgrieve

School of Aquatic and Fishery Sciences

University of Washington

Seattle, WA 98195 USA

[gholt@u.washington.edu](file:///C:\Users\Daniel%20Schindler\Downloads\gholt@u.washington.edu)

**Disclaimer**

This software is freely distributed without warranty or guarantee. Please read Schindler et al. (2017) and Holtgrieve et al. (2010) for specifics on model formulation and assumptions. If your specific system does not match the assumptions outlined therein, please do not use BaMM for rigorous analysis. Feel free to contact us with questions in this regard. This manual is specific to the functioning of BaMM and does not address the theory or methodology behind ecosystem metabolism measurements or stable isotopes.

We recommend you familiarize yourself with the theory and assumptions of likelihoods, Bayesian methods, and Markov Chain Monte Carlo before using BaMM. The Ecological Detective (Hilborn and Mangel 1997) and Bayesian data analysis (Gelman et al. 2004) are excellent references. Care should be taken to ensure that posterior estimates meet assumptions of convergence. It is also important to carefully consider the appropriateness of prior information, since it can be a tempting way to influence posterior results. Last, BaMM is a mechanism for fitting a model to data. If the data are dubious or uninformative, so go the results. Please scrutinize your data carefully.

**Documentation and installation**

The current version of BaMM is v1.60 created using win32 bit ADMB v9.0.65, with MinGW g++ 3.4.4 or Borland 5.5.1 at the University of Washington. We have used BaMM with MS Windows and Mac OS. If you would like a copy of the ADMB source code please contact Gordon Holtgrieve.

BaMM was developed using Automatic Differentiation Model Builder (ADMB; <http://admb-project.org>), an open-source software package specifically designed for non-linear statistical modeling. The oxygen and light sub-models are compiled with existing ADMB routines for differentiation and MCMC estimation into a stand-alone executable program.

BaMM.exe is the stand-alone executable program that contains the O2 model and routines for differentiation and MCMC. There is no need to install ADMB application on your computer; simply copy the BaMM.exe, BaMM.cfg, BaMM.pin, and BaMM.dat files into the folder/directory where you would like to perform the analysis. BaMM creates a number of text files while running which (most of the time) will overwrite existing files. It is wise to delete or rename all of the text files from the folder when repeating analyses, especially the BaMM\_mcmc.dat file is not overwritten.

**Notes on the updated version:**

It is no longer possible to use the Excel interface from the original BaMM. However, you can run BaMM without installing ADMB as long as you have the compiled executable file (BaMM.exe) for your operating system (Windows or Mac). The compilation step (BaMM.tpl 🡪 BaMM.exe) requires ADMB be installed. The model can be run through the terminal (on a Mac), the command line (on Windows), or by calls to either the terminal or command line from R.

**Creating Data and Input files**

These instructions assume you will be using the most recent version of BaMM (Schindler et al. 2017). The section below details how to create the data and input files so that they are readable by BaMM.exe. These input files should be created in R using the package “R2admb” so that formatting is consistent with requirements of BaMM.

**Important note: These files can only be edited in a text editor (not Excel).** If you use Excel it alters the file format somehow so that the files can’t be read into the program.

**The following files are required for each individual run of the model:**

1) BaMM.exe -- model executable file (or can use the original model ADMB code contained in BaMM.tpl, which must be compiled by ADMB into executable file first);

2) BaMM.dat – data file; contains diel data, other necessary constants, and environmental information.

3) BaMM.cfg – sets information on priors and bounds for different parameters (on/off, ranges and distributions for priors)

4) BaMM.pin – sets the parameter starting values

**a. Setting model parameters, specifying priors, and initial values**

**Including priors (BaMM.cfg - configuration file)**

*A template for the BaMM.cfg file has been included with the model documentation since there is currently no function that creates this directly in R2admb. This template can be modified using a text editor to suit your analysis*

It is prudent to reiterate that careful consideration should be given to the appropriateness of prior information (“priors”) in the analysis. Options for priors are: uninformative (no prior information), uniform (equal probability within a range of values), normal (following a normal distribution), or constant (fixed at a given value). Ten of the 13 parameters in BaMM allow for user-defined priors. The photosynthesis-irradiance parameters (αP-I, Pmax) and respiration (Rref) are the only uninformed (unbounded) parameters. The others require specification of at least a range of possible values. See Table 4.

For each parameter, the type of prior can be selected by setting the switch in the first row of the column of numbers below each parameter in the BaMM.cfg file. The values under each parameter are 1) the switch specifying how and whether parameter is estimated, 2) log\_e(min), 3) log\_e(max), 4) mean, and 5) std dev. The additional value under the alpha R parameter is the “alpha transform switch: “-1” means the parameter is estimated in normal space and “1” means the parameter is arctan transformed. Specifications for the switch are as follows: “-1” means that the parameter is NOT estimated; “1” means that the parameter is estimated and bounded (uses max and min values); “2” means that parameter is estimated, bounded and has a normal prior (uses mean and std dev values).

Additional values in the BaMM.cfg file of concern for analysis are the following: 1) “Tref” is the standard temperature for estimation of Rref. This is typically the average temperature from each dataset (°C), 2) “Number of time steps for estimating beta” is typically set at 20 when the time step is 10 min, but can be varied to account for O2 sampling resolution or an understanding of the particular system that may cause this value to differ, 3) “Switch for isotopes” specifies whether isotope data are included (“1”) or not (“-1”), and 4) “18O-O2 scale factor” is the isotope weighting factor and is not important if isotope data are not included.

**Starting values (BaMM.pin - initial values file)**

*Code for creating a .pin file using the R2admb package in R has been included with the model documentation. This also can be modified with a text editor after its initial creation. (“Write.pinfile.R”)*

All parameters must be given starting values. These must be specified as log\_e (natural log) values in the BaMM.pin file. These should be reasonable guesses of what might fall within the posterior distribution of the given parameter. If starting values are far away from the posterior region it is possible that the differentiation step might get trapped in a false minimum. It is wise to try the model with many different starting values to make sure you are fully exploring the parameter space.

If starting values are outside of the bounds specified in the priors an error message will appear. If the parameter is modeled as a constant, its value will be fixed as the starting value.

**b. Creating the data file**

*Code for creating the .dat file has been included along with the model documentation (“Write.datfile.R”). This also can be modified with a text editor after its initial creation.*

**Diel data structure and inputting data (BaMM.dat - data file)**

Diel data are included as a text file, “BaMM.dat”, which can be created using the “R2admb” package. Diel data input into the model include O2, 18O-O2 data if available, water temperature, and light (PAR - photosynthetically active radiation). The data file must also include Julian date, Local hour as a decimal (e.g., 7:00am = 7.00, 5:00pm = 17.00), and Time interval (0, 10, 20 minutes = 0, 0.17, 0.33) for each observation of O2.

The model time step is determined by the temporal resolution of the water temperature data. BaMM has been tested with 10 and 15 minute time steps. Performance at larger time steps is unknown. *Day of Year*, *Local Hour*, *Time Interval*, and *Water T* must be provided for each modeled time step. Additional details are given in Table 1.

To estimate parameter values by Bayesian methods it is necessary to provide measured [O2] data and, if available, δ18O-O2. Oxygen data do not need to be at the same temporal resolution as the model input data (water T, Irradiance) or be evenly spaced in time. However, to get accurate parameters estimates requires quantifying as best as possible daytime O2 peaks and nighttime O2 plateaus (Venkiteswaran et al. 2008).

*Irradiance* can be either measured directly or modeled based on geographic position. If using measured irradiance, the data must be complete for all modeled time points (no missing data) and the *Use S Measured* flag set to “1” in the BaMM.dat file. The Use S Measured flag should set to “0” when using modeled data.

**Environmental and Geographic parameters:** See Table 2 for a description of geographic and environmental parameters. Typically this means changing *Altitude*, *Latitude*, *Longitude*, *Time zone*, *DST*, *Depth*, and *Salinity* to the system specific values. *Aspect* and *Slope* relate to the light model and are usually set to a small positive values (i.e., 0.001). If using modeled light data without calibrating it to measured data, set the *Light model scalar* to 1. The default *Transmissivity* is around 0.8. Note that inaccurate irradiance values (too high or too low) will not affect estimates of GPP, CR, or G, but will affect the photosynthesis-irradiance parameters (Pmax and αP-I).

**Light model (specified in BaMM.dat)**

Primary production is typically modeled as either a linear or saturating function of irradiance. A linear function is of the form

where, αP-I is the slope if the photosynthesis-irradiance curve. The most common form of light saturating production is the hyperbolic tangent model by Jassby and Platt (1976)

where Pmax is the photosynthetic rate at light saturation. Although not described in Holtgrieve et al. (in review), we have also included a Michaelis-Menten formulation of light-saturating production based on Uehlinger et al. (2000).

The light model can be specified in the BaMM.dat file. “0” specifies the linear light model, “1” specifies the Michaelis-Menten model, and “2” specifies the hyperbolic tangeant formulation. See Holtgrieve et al. (in review) for methods to evaluate the best production model using an information theoretic approach.

**Running the model**

After setting the priors and starting values, the user must specify the total *Number of draws to save* and *Thinning* rate for the MCMC chain. It is recommend that you start with short runs with at a low thinning rate to make sure the model is behaving as desired. Check the “bamm.rep” and “bamm.cor” files to see if the model is giving reasonable results (see the next section). Once you are confident the model is doing what you want, set the *Num Iterations* to greater than 100,000 and the *Number of draws to save* to 1,000 or more. To be certain of model convergence, you may need to increase the number of iterations (e.g., at least 1,000,000; see below) and some set of the initial iterations may need to be discarded (“burn-in”).

To generate an MCMC chain from the command line in Windows:

* 1. Open a MSDOS command window (run cmd), and navigate to the working folder using the "cd" function (e.g., cd C:\Users\Gordon Holtgrieve\Documents)
  2. Type the following command into the command line and hit return: "BaMM.exe -mcmc **NumIteration** -mcsave **NumSaved** > BaMMmcmclog.txt" (no “”). Where, **NumIteration** is the total length the MCMC chain and **NumSaved** is the total number of those draw to save. For example, if you want to save every 1000th iteration (draw) in the chain for a total of 1000 saved draws, **NumIterations** would be 1000000 (= 1000\*1000) and **NumSaved** would be 1000.
  3. When the MCMC chain finishes (in a few seconds to many hours), type "BaMM.exe -mceval" and hit return. This will create the Bamm\_mcmc.dat file which contains the results of your run.

To generate an MCMC chain from R on a Mac:

1. Open R and navigate to the working folder by setting the working directory using the setwd() function (e.g., setwd(“/Users/Gordon Holtgrieve/Documents”)
2. To run the model without the mcmc, type the following command into the command prompt and hit return: system(“./BaMM”). This will generate the maximum likelihood estimate for each parameter.
3. To run the full mcmc, type the following into the command prompt: system(“./BaMM -mcmc **NumIteration** -mcsave **Save every Xth value**”). Where, **NumIteration** is the total length the MCMC chain and **NumSaved** is the interval at which those draws should be saved. For example, if you want to generate 1000 saved draws, **NumIterations** would be 1000000 and **NumSaved** would be 1000.
4. When the MCMC chain finishes (in a few seconds to many hours), type system(./"BaMM -mceval") and hit return. This will create the Bamm\_mcmc.dat file which contains the results of your run.

Upon initiating the BaMM-ADMB code you will see that ADMB will first calculate the Hessian matrix of partial derivatives. If the Hessian cannot be found the script will halt (usually with 10 seconds). If this happens, try adjusting starting conditions and priors. If the Hessian matrix is determined, a number of text files generated and used by ADMB will appear in the folder.

After the Hessian step, BaMM will initiate the MCMC chain. The command window will remain open and display information about the objective function and acceptance rate during the MCMC. The acceptance rate should be greater than 0.2 and ideally around 0.3. This can take from 30 minutes to more than 8 hours depending on the number of modeled data points, thinning rate, and number of draws to save. **See Section 4 in regards to interpreting these data.**

**Analysis of [O2] data only (no δ18O-O2)**

To perform a Bayesian analysis of diel [O2] data without corresponding δ18O-O2 data, it is necessary do the following: 1)set the *Switch to estimate isotopes* to -1 (BaMM.cfg file), 2) fix *alphaR*, *δ18O-H2O*, *Starting δ18O-O2*, and *Sigma δ18O-O2* as constants (i.e., no prior information; BaMM.cfg file), and 3) provide reasonable starting values for these parameters (BaMM.pin file). Starting values do not need to representative of the specific system, only within what may be observed in nature. It is also necessary to place at least one dummy data point in the δ18O-O2 section of the BaMM.dat file. The model will generate predicted δ18O-O2 curves based the provided starting values, however these predictions and the dummy data will not be considered when calculating the total likelihood of the model and thus not contribute to ecosystem metabolism estimates.

**Reading and analyzing output**

1. **Data structure**

BaMM produces a text file of MCMC output named “BaMM\_mcmc.dat” (See Table 5). Each row is a saved draw from the thinned MCMC chain. Data within each column are the posterior distribution of the individual parameters. Identifiers are in the column to the left of the data. Model predictions for O2 concentration and δ18O-O2 for each model time point (i.e., for the diel cycle) are identified as *est\_O2conc* and *est\_delta\_18O\_O2*. This output occupies as many columns as there are modeled data points. Similarly, *P*, *R*, and *G* are the model predicted instantaneous production, respiration, and O2 mass flux by air-water gas exchange for each modeled time point. *Integrated PP*, *CR*, and *G* are the estimated 24 hour average of primary production, community respiration, and gas exchange respectively.

The first row across all columns of this file (MCMC iteration 1) is the maximum likelihood estimate (MLE): values for each parameter that minimizes the objective function (i.e., maximizes the likelihood).

1. **Testing for convergence**

The MCMC algorithm used by BaMM approximates the full posterior distributions of the individual parameters. Longer chains will generally better reflect the underlying ‘true’ distribution. Similarly, it is important to ensure the chain has evenly sampled the full range of the distribution. Testing the adequacy of MCMC output in describing the true distribution – termed ‘convergence’ – is an active area of research and there is no one single metric.

At a minimum, the user should check for autocorrelation among MCMC samples [C(t)=corr(x(t), x(t+1)]. Autocorrelation < 5% for all parameters and the objective function is an indicator of convergence. In addition, traces of MCMC output should be examined for a lack of trend. The CODA package in R (R Foundation for Statistical Computing, <http://www.r-project.org>) provides a number of graphical and statistical tests for analyzing MCMC output. Also refer to Plummer et al. (2006).

1. **Calculating posterior distributions**

If the MCMC chain has converged, the data within each column comprise the estimated posterior distribution for each parameter or modeled time point. Distributions can be plotted as histograms or densities. It is also common to report the range of posterior values as mean/median, 2.5%, and 97.5% credible limits. Similarly, error around model fits to the data can be shown by plotting the mean/median value for each modeled time point along with the 2.5% and 97.5% credible limits.

1. **Other relevant data files**

The text file “bamm.rep” contains the maximum likelihood estimates for all the parameters and modeled time points (same as iteration 1 of the BaMM\_mcmc.dat file). It also contains input data including modeled or measured irradiance, water T, Local hour, etc. This file is produced once the software has found the partial derivatives of the function (hessian matrix) and is useful for error checking without having to wait for an entire MCMC chain to finish.

The “bamm.cor” file contains the correlation matrix among parameters. High correlation between two or more parameters will significantly increase the range of values within the posterior distributions.

BaMM produces a number of other files during the differentiation step that can largely be ignored.

**Known bugs and issues**

1. **δ18O-H2O**

Testing has shown that BaMM is relatively uninformative with respect to δ18O-H2O. Estimates of δ18O-H2O using a uniform prior have broad posterior distributions. We recommend that, whenever possible, a measured δ18O-H2O value be incorporated as either a constant or with a normally distributed prior. Measurement error on the δ18O-H2O is generally very small and as a result, the informed prior will essentially fix this parameter near the measured value unless there is strong evidence in the O2 data to the contrary.

**References**

Gelman, A., J. B. Carlin, H. S. Strern, and D. B. Rubin. 2004. Bayesian data analysis. Chapman & Hall/CRC.

Hilborn, R., and M. Mangle. 1997. The ecological detective: confronting models with data. Princeton University Press.

Jassby, A. D., and T. Platt. 1976. Mathematical formulation of the relationship between photosynthesis and light for phytoplankton. Limnology and Oceanography **21:** 540-547.

Plummer, M., N. Best, K. Cowles, and K. Vines. 2006. CODA: Convergence diagnosis and output analysis for MCMC. R news **6:** 7-11.

Uehlinger, U., C. Konig, and P. Reichert. 2000. Variability of photosynthesis-irradiance curves and ecosystem respiration in a small river. Freshwater Biology **44:** 493-507.

Venkiteswaran, J. J., S. L. Schiff, and L. I. Wassenaar. 2008. Aquatic metabolism and ecosystem health assessment using dissolved O-2 stable isotope diel curves. Ecological Applications **18:** 965-982.

Table 1 – Diel data

|  |  |  |  |
| --- | --- | --- | --- |
| **Name** | **Description** | **Complete data (y/n)** † | **BaMM file** |
| Day of Year | Julian day of year; integer value. | y | BaMM.dat |
| Local hour | Local time of sampling with units of decimal hours (not Excel time format). | y | BaMM.dat |
| Time interval | Time from first sampling in decimal hours. First time interval is 0.00. | y | BaMM.dat |
| S measured | Measured irradiance in microEinsteins m-2 s-1, if available. | n\* | BaMM.dat |
| Water T | Water temperature in degrees Celsius. | y | BaMM.dat |
| O2 conc. | Observed dissolved oxygen concentration in mg L­-1. | n | BaMM.dat |
| δ18O-O2 | Observed isotopic ratio of dissolved oxygen in delta units vs. SMOW. | n | BaMM.dat |

†Complete data requires a measured value for each time point being modeled with no breaks

\*If irradiance data is incomplete the user must set *Use S measured* switch (cell B18) to FALSE

Table 2 – Environmental data

|  |  |  |
| --- | --- | --- |
| **Name** | **Description** | **BaMM File** |
| Altitude | Altitude of study location in meters. | BaMM.dat |
| Aspect | Aspect of water body in degrees; must be greater than 0; default = 0.001. | BaMM.dat |
| DST | Daylight savings time; -1 = yes, 0 = no. | BaMM.dat |
| Latitude | Latitude of study location in decimal degrees. | BaMM.dat |
| Longitude | Longitude of study location in decimal degrees; west is negative degrees. | BaMM.dat |
| Slope | Slope of water body in degrees; must be greater than 0; default = 0.001. | BaMM.dat |
| SolConst | Solar constant; 1367 Watts m-2. | BaMM.dat |
| Time Zone | Time zone of study location relative to GMT. | BaMM.dat |
| Transmissivity | Relative transmissivity of the atmosphere; default = 0.8. | BaMM.dat |
| Light model scalar | Scalar to fit modeled light data to measured light data. | BaMM.dat |
| Area | Area of water body if total flux is desired; use 1 for standard units of mg m-2 hr-1. | BaMM.dat |
| Depth | Depth of mixed layer in meters. | BaMM.dat |
| Salinity | Salinity of water body in ppt. | BaMM.dat |

Table 3 – Analysis options and settings

|  |  |  |
| --- | --- | --- |
| **Name** | **Description** | **BaMM File** |
| Prior distribution | Switch allows user to select type of estimation and prior; -1 = not estimated, 1 = uniform prior, 2 = normal prior | BaMM.cfg |
| Lower bound | Lower bound of uniform prior. Also applies to constant prior. | BaMM.cfg |
| Upper bound | Upper bound of uniform prior. Also applies to constant prior. | BaMM.cfg |
| Mean | Mean of the prior distribution. Applies to normal priors only. | BaMM.cfg |
| Std. Dev | Standard deviation of the prior distribution. Applies to normal priors only. | BaMM.cfg |
| Starting Values | Initial starting values for differentiation and MCMC; must be logged values. | BaMM.pin |
| Number of draws to save | Total number of MCMC draws to save as the posterior distribution. 1,000-5,000 is recommended. | Specify at model run (-mcsave) |
| Initial 'Burn in' | Number of MCMC iterations before draws start to be saved. 5,000-20,000 is recommended. | Can remove after model run |
| Num Iterations | Total number of MCMC iterations between saved draws. For ADMB model this should be between 100,000 and 5,000,000 depending on model convergence. | Specify at model run (-mcmc) |
| Weighting factor for δ18O-O2 | Relative weighting of O2 concentration data versus δ18O-O2 data in the total likelihood. Value of 1 is equal weight while 0 means the δ18O-O2 does not contribute to the likelihood at all. | BaMM.cfg |
| Use S measured | Switch to specify if the model is to use measured light data. | BaMM.dat |
| Light model | Pull down menu to specify the production model. Options are linear, hyperbolic tangent, and Michaelis-Menten. | BaMM.dat |
| Transform alphaR | Switch to specify if the model will use an arctangent transformation when estimating alphaR. The transformation may help in estimating alphaR by expanding the uniform prior. When estimated values are close to the boundaries (i.e., 0.970 or 1) the transformation tends to skew results towards that boundary. No transformation is suitable in most cases. | BaMM.cfg |

Table 4 – Priors

|  |  |
| --- | --- |
| **Parameter** | **Information about priors** |
| Pmax | Uninformative prior only |
| alphaP-I (αP-I) | Uninformative prior only |
| Rref | Uninformative prior only |
| Eb | Can be modeled with a uniform or normal prior. Default is set to theoretical average - 0.65 eV. |
| Ep | Can be modeled with a uniform or normal prior. Default is set to theoretical average - 0.32 eV. |
| Beta | Can be modeled with a uniform (-1000 to 1000) or normal prior (Schindler et al. - mean = 1.61, sd = 0.5). |
| k20 | The gas transfer velocity can range widely depending on the system and local conditions. Measurements of k20 by tracer addition are common. In addition, empirical models have been developed that predict k20 based on wind speed (lakes, oceans) or discharge/velocity (streams, rivers). These sources of prior information can be incorporated as a normal prior. Both measured and modeled estimates of gas transfer have a high degree of uncertainty and it is important to accurately quantify the error around these values and include that in the prior. Given the uncertainly it is not recommended that k20 be fixed as a constant. |
| alphaR (αR) | Observed values range from 0.978 – 1.0. It’s possible to measure alphaR with incubation experiments of water or sediment slurries, and it may be appropriate to incorporate such a measurement as prior information. However, one should consider if this is truly an accurate measurement of in situ processes or if the incubation methodology potentially skews the results. |
| δ18O-H2O | Please refer to section 5a of this document. This is an easy measurement to make and we suggest using a prior (constant or normal). Note that δ18O-H2O is typically measured by either the CO2 equilibration method (IsoPrime) or laser spectroscopy (LGR) and there can be differences between methods in terms of both accuracy and precision. |
| starting O2 conc. | Initial O2 should be modeled with a uniform prior and a range that encompasses O2 observations. It is not recommended that this parameter be fixed because this forces the model to start a particular place without error. |
| starting δ18O-O2 | Initial δ18O-O2 should be modeled with a uniform prior and a range that encompasses δ18O-O2 observations. It is not recommended that this parameter be fixed because this forces the model to start a particular place without error. |
| sigma O2 conc. | The standard deviation of the likelihood can be quantified directly by repeated measurements under identical conditions or estimated directly from the diel data. If estimating from the data, use a uniform prior with a relatively wide range (approx. <0.01 to 5). |
| sigma δ18O-O2 | The standard deviation of the likelihood can be quantified directly by repeated measurements under identical conditions or estimated directly from the diel data. If estimating from the data, use a uniform prior with a relatively wide range (approx. <0.01 to 5). |

Table 5 – BaMM\_mcmc.dat (MCMC data)

|  |  |
| --- | --- |
| **Name** | **Description** |
| MCMC iteration | Index of saved MCMC trails |
| obj\_fun | Objective function – negative log-likelihood of model fit to the data with the current parameter draw (row) |
| Pmax | Maximum rate of photosynthesis at light saturation |
| alpha\_P\_I† | Slope of photosynthesis-irradiance relationship |
| Rref | Respiration rate at reference temperature (°C) |
| Eb | Temperature sensitivity of base respiration (Rb) |
| Ep | Temperature sensitivity of production-based respiration (Rp) |
| beta\_prod | Rate of consumption of previous time steps of production (used for calculation of Rp) |
| k20 | Gas transfer velocity at a reference temperature; typically average of dataset (°C) |
| alphaR | Fractionation factor for respiration |
| delta\_18O\_H2O | Isotopic value of water |
| init\_O2\_conc | Initial O2 concentration |
| init\_delta\_18O\_O2 | Initial δ18O-O2 |
| sigma\_O2\_conc | Standard deviation of the likelihood function for O2 concentration |
| sigma\_delta\_18O\_H2O | Standard deviation of the likelihood function for δ18O-O2 |
| est\_O2conc\* | O2 concentration for each modeled time point in the diel cycle |
| est\_delta\_18O\_O2\* | δ18O-O2 for each modeled time point in the diel cycle |
| Integrated PP | Estimated daily GPP in mg O2 m-2 d-1 – calculated as 24hr moving average through the modeled data |
| Integrated CR | Estimated daily CR in mg O2 m-2 d-1 – calculated as 24hr moving average through the modeled data |
| Integrated G | Estimated daily G in mg O2 m-2 d-1 – calculated as 24hr moving average through the modeled data |
| Integrated Rp | Estimated daily Rp in mg O2 m-2 d-1 – calculated as 24hr moving average through the modeled data |
| Integrated Rb | Estimated daily Rb in mg O2 m-2 d-1 – calculated as 24hr moving average through the modeled data |
| P\* | Instantaneous P for each modeled time point in the diel cycle |
| R\* | Instantaneous R for each modeled time point in the diel cycle |
| G\* | Instantaneous G for each modeled time point in the diel cycle |
| Rb | Instantaneous Rb for each modeled time point in the diel cycle |
| Rp | Instantaneous Rp for each modeled time point in the diel cycle |

†Included under light saturating assumption

\*Number of columns varies and depends on the number of modeled time points