White paper:

Stream metabolism

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Content

Background

Aquatic ecosystem metabolism refers to the ecosystem-scale rates of organic matter cycling in aquatic ecosystems - namely gross primary production (GPP) and ecosystem respiration (ER) - that form the base of food webs and influence biogeochemical cycling rates (Jankowski et al. 2021). From a management perspective, ecosystem metabolism is interesting as GPP and ER responds to environmental change and disturbances in streams, lakes, wetlands, as well as estuaries (Hoellein et al. 2013, Munn et al. 2020), and can therefore be used as indicators of the ecosystem's health status. Metabolism can be derived from diurnal variations in dissolved oxygen (DO) concentrations based on in-situ sensor measurements. Historically, the cost and level of accuracy of oxygen sensors have limited the widespread application of metabolism. However, recent advances in sensor and modelling technologies now enable routine monitoring of dissolved oxygen (DO) at high quality and low cost, and real-time modelling of aquatic ecosystem function (GPP and ER), including the influence of key physical processes such as gas exchange with the atmosphere. WateriTech has developed a new inverse modelling approach, combining real-time sensor monitoring with machine learning (differential evolution), to deliver cost effective estimates of aquatic metabolism. The method has been tailored for stratifying (lakes and fjords) and vertically mixed (streams) water bodies, respectively. This white paper describes the key concept for deriving metabolism in streams.

About WateriTech & WaterWebTools

WateriTech is a research and consultancy company founded in 2019 by world leading researchers within water quality modelling and data analytics. The company is based in Denmark but offer its services and solutions globally. WateriTech specializes in the development and application of open source hydrological and ecological models, IoT sensor monitoring and advanced data analytics, and focus on digital solutions for addressing water quality, flooding and drought challenges. WateriTech and partners have developed the highly recognized WaterWebTools platform, which is a user-friendly web-platform for live streaming, quality control and postprocessing of sensor data, as well as operationalization of hydrological and water quality models for forecasting purposes. The WaterWebTools platform, which also allows transmission of data to customers own data platform or 3. party platforms, is widely used in Denmark and across Europe by the municipal and water utility sectors, private companies as well as research institutions.

Introduction

The primary drivers of ecosystem metabolism include temperature, light, hydrology, and the quantity and quality of organic matter and nutrients (Battin et al. 2023; Caffrey 2004; Solomon et al. 2013). Metabolic rates can be derived based on different approaches, including isotope analysis, in-situ incubation experiments, field campaigns for monitoring the mass balance of carbon, and sensor technology. Advances in sensor technology during the past 10 years, including improved accuracy and stability and lower cost, has enabled a more widespread use of this approach for deriving metabolism, and this is now the preferred method in most studies (Hall and Hotchkiss 2017). Using one of more sensors installed in-situ, water temperature and oxygen concentration is measured at high frequency (typically 10-30 minute intervals). Using a process-based model that is calibrated to the daily variation in oxygen concentrations, GPP and ER can be estimated for a stream reach for each single day.

The metabolism modelling approach for streams developed by WateriTech is based on a single sensor station, and inspired partly by the *single station open channel diel oxygen* method described by Holtgrieve et al. (2010) and Song et al. (2016), with several new advances, including advanced data quality control for cleaning of sensor data, more accurate numerical integration, use of differential evolution for model parameter optimization, parameter uncertainty estimation, parallel processing of model runs for large datasets, and operationalization of the model via the WaterWebTools portal (Trolle and Nielsen 2024).

While additional data collection can be conducted when estimating metabolism, e.g. using a two-station method, and applying tracer experiments in the field for estimating key model parameters, this greatly increases the cost of metabolism estimates and hamper its application. In practice, several studies (e.g., Bernot et al. 2010; Beaulieu et al. 2013) have showed that the single station method often produces results that are comparable and not significantly different from a two station method – the latter thus providing marginal or no additional benefit for the accuracy. Estimation of key model parameters through automatic parameter optimization algorithms, for example the reaeration constant (K_{20}), as done in the approach by WateriTech, is often also better than using empirical equations for determining K_{20} (Riley at al. 2013). When using different parameter optimization approaches for the single station method, the results are generally still comparable across the different optimization approaches (Grace et al. 2015). Hence, while additional sampling can of course always help

to resolve local heterogeneities in greater detail, the single station method generally produce stable, reliable and affordable estimates of metabolism for a stream reach.

When estimating metabolism, this represents the dynamics of a certain stream reach length. A rough estimate of the distance (D, m) of the upstream reach that contribute to diel DO dynamics in the stream is D = 3v/K, where v is the mean water velocity and K (in a unit of h^{-1}) is the reaeration rate (Reichert et al. 2009). Flow velocities in streams vary at least in a range between 0.1 and 1 m s^{-1} and reaeration coefficients in a range between 0.02 and 5 h^{-1}, which mean that the stream reach length that contributes to diel DO dynamics extends at least from 100 m to 10 km (Reichert et al. 2009).

Data collection

When estimating metabolism in streams, diurnal (e.g., 15 min intervals) water temperature and DO are required for a single station. WateriTech produces sensor stations for this specific purpose (Fig. 1), but data from 3. party can also be linked to the WaterWebTools platform, thereby enabling metabolism estimates for any location on the planet.

Fig. 1. Example of an OPTOD optical oxygen and temperature sensor, which can be installed in a stream station.

Besides in-situ sensor data, local data for incoming radiation and barometric pressure is also required. By default, WaterWebTools will automatically harvest

local data from the ERA5 gridded weather product, which is available globally in near real-time and hourly temporal resolution, and for spatial grids of approx. 30 km spacing. Time series of Secchi depth can also be utilized or alternatively estimated from a cosine seasonal function, and is used to derive photosynthetic active radiation (PAR) as a function of depth and time.

Data pre-processing

A series of pre-processing steps are first conducted to format raw sensor data and weather data into quality assured and quality controlled equidistant time series.

Data cleaning and control

To achieve adequate quality of the in-situ collected data prior to metabolism processing, the raw sensor data is initially harmonized with respect to sampling frequency to create an equidistant time series followed by filtering on sensor-specific error values. Hereafter, outliers are detected with a modified version of the SentemQC approach by van't Veen et al. (2025), which identifies and marks anomalies in the dataset using successive moving windows with varying window sizes. This method has proved efficient for cleaning sensor data, not only for identifying individual outliers, but also clusters of anomalies.

Data resampling and interpolation

After cleaning and control the data is processed further with resampling into half hourly intervals, and then smoothed using a 4-hour running window. These steps are based on experiences and recommendations from the scientific literature, including Staehr et al. (2012), Obrador et al. (2014) and Giling et al. (2017).

Weather and light data

Representative weather and light data are pre-processed according to the following steps:

- Download local weather data including incoming short wave radiation (E, W m^{-2}) and barometric pressure (P, kPa).
- Convert short wave radiation into photosynthetic active radiation at the surface (PAR_0, µmol m^{-2} s^{-1}), where:

  $PAR_0 = E * 4.6 * 0.45$ (Giling et al. 2017).

- The user may choose to use surface PAR_0 in the metabolism model (compatible with the parameterization done in most stream studies), or, optionally, derive and use PAR at the centroid of the mean depth from Secchi depth by following the steps below:
- Calculate Secchi depth (sd, m) for each day from cosine function (which reads maximum sd, minimum sd, and day of the year of maximum sd) or read this directly from external file
- Calculate light attenuation (KD, m^{-1}) from Secchi depth, where:

  KD = 1.7 / sd (Giling et al. 2017)
- Derive PAR (µmol m^{-2} s^{-1}) for each layer depth (z) layer based on Secchi depth, where:

  $PAR(z) = PAR_0 \cdot e^{KD \cdot z}$ (Giling et al. 2017)
- Interpolate PAR and barometric pressure to same temporal resolution as sensor data.

Metabolism modelling

The main body of the metabolism model is a differential equation (Holtgrieve et al. 2010), which describes the changes in oxygen concentration due to gross primary production (GPP), ecosystem respiration (ER), and the oxygen flux due to reaeration between the water surface and the atmosphere (Ds):

$$\frac{\Delta O_2}{\Delta t} = \frac{(GPP - ER + D_s)}{Z_{mix}}$$

Where Z_{mix} is the average mixed layer depth (m) for the stream reach. To be able to solve this equation, each of these terms has to be derived for each day.

Gross primary production

GPP (g O_2 m^{-2} h^{-1}) is calculated based on the approach in Song et al. (2016) and derived from $\mathbf{P_{max}}$, the maximum photosynthetic rate (g O_2 m^{-2} h^{-1}) at saturating light, $\boldsymbol{\alpha}$, the photosynthetic efficiency coefficient (g O_2 m^{-2} h^{-1} [µmol photons m^{-2} s^{-1}]$^{-1}$), **temp**, the water temperature (°C), and θ_P, a temperature coefficient for primary production:

$$GPP = P_{max} \cdot tanh\left(\frac{\alpha \cdot PAR}{P_{max}}\right) \cdot \theta_P^{(temp-20)}$$

Where the temperature coefficient (θ_P) is set to 1.036, as in Song et al. (2016). P_{max} and α are two of the four parameters that are automatically calibrated by the model using a differential evolution algorithm.

Ecosystem respiration

The ecosystem respiration rate (ER) (g O_2 m^{-2} h^{-1}) is determined for each day from $\mathbf{R_{20}}$, the respiration rate at 20°C (g O_2 m^{-2} h^{-1}), and $\boldsymbol{\theta_R}$, a coefficient for the thermal dependence of respiration:

$$\boldsymbol{ER = R_{20} \cdot \theta_R^{(temp-20)}}$$

Where a temperature coefficient (θ_R) of 1.073 is used, based on Jørgensen and Bendoricchio (2001). R_{20} is automatically calibrated by the model using a differential evolution algorithm.

Atmosphere-water gas exchange

The gas exchange between the water surface and the atmosphere (Ds, g O_2 m^{-2} h^{-1}) is calculated from $\mathbf{K_{20}}$, the gas exchange coefficient of oxygen (m h^{-1}) at 20°C, $\mathbf{O_{2sat}}$, the oxygen concentration (g O_2 m^{-3}) at saturation level at the given water temperature and barometric pressure, and $\boldsymbol{\theta_K}$, a temperature coefficient for reaeration:

$$\boldsymbol{D_s = K_{20} \cdot (O_{2sat} - O_2) \cdot \theta_K^{(temp-20)}}$$

Where the temperature coefficient (θ_K) is set to 1.024, as in Song et al. (2016). K_{20} is automatically calibrated by the model using a differential evolution algorithm.

The overall flux oxygen between water and atmosphere flux can be either positive (i.e. oxygen going into the water from the atmosphere, when water is undersaturated with oxygen) or negative (i.e. oxygen leaving the water due to supersaturation). The oxygen concentration at saturation level is derived from the approach in Song et al. (2016):

$$\boldsymbol{O_{2sat} = e^{\left(-139.3441+\frac{1575710}{temp+273.15}-\frac{66423080}{(temp+273.15)^2}+\frac{12438000000}{(temp+273.15)^3}-\frac{862194900000}{(temp+273.15)^4}\right)} \cdot \frac{Pa \cdot 0.998}{101.3}}$$

Where Pa is the barometric pressure (kPa).

Calibration of model parameters

The metabolism model has been developed in Python, where the four model parameters: $\mathbf{P_{max}}$, $\mathbf{\alpha}$, $\mathbf{R_{20}}$ and $\mathbf{K_{20}}$, are calibrated for each single day. The model user can choose between a series of numerical integration approaches and time steps to solve the metabolism model, but the 4th order Runge-Kutta approach with an integration time step of 0.5 hour is used by default. A differential evolution algorithm is used to optimize the four model parameters, which will automatically compare sensor-based observations with the model estimated oxygen concentrations, and optimize the model fit to observations. The differential evolution algorithm seeks to minimize an objective function (by default set to the root-mean-squared-error) for each single day, and the final GPP and ER estimates are extracted from the calibrated model. Models with several parameters, such as the metabolism model, can exhibit equifinality, where good fits to observed data can be achieved by several different parameter value combinations, some unrealistic (e.g., Appling et al. 2018). The model approach by WateriTech overcomes this by constraining model parameter optimization to realistic ranges, and also by allowing the option to run an ensemble of model parameterizations using different initial parameter seeds for the differential evolution algorithm. The mean and the variation in model parameterization and simulated metabolism can then be extracted. In practice, we have found that even though the metabolism model may exhibit some degree of equifinality, the controlled parameter search results in similar estimates of GPP and ER, and therefore the effect of running ensembles is somewhat limited.

Operationalization and post-processing

WaterWebTools integration

The entire model workflow can be made operational via the WaterWebTools platform, where sensor data is live-streamed and pre-processed according to the steps described previously, local weather data is also harvested, and the metabolism model is executed operationally for each 24-hour time period. Parameter bounds used by the differential evolution algorithm, applied when optimizing the metabolism model, are constrained to value-ranges reported in the literature (e.g. Wilcock et al. 1998, Binzer et al. 2006, also see Appendix), which ensure that the calibrated model parameters are within naturally realistic ranges. The output from the model can be followed live via the WaterWebTools platform (Fig. 2).

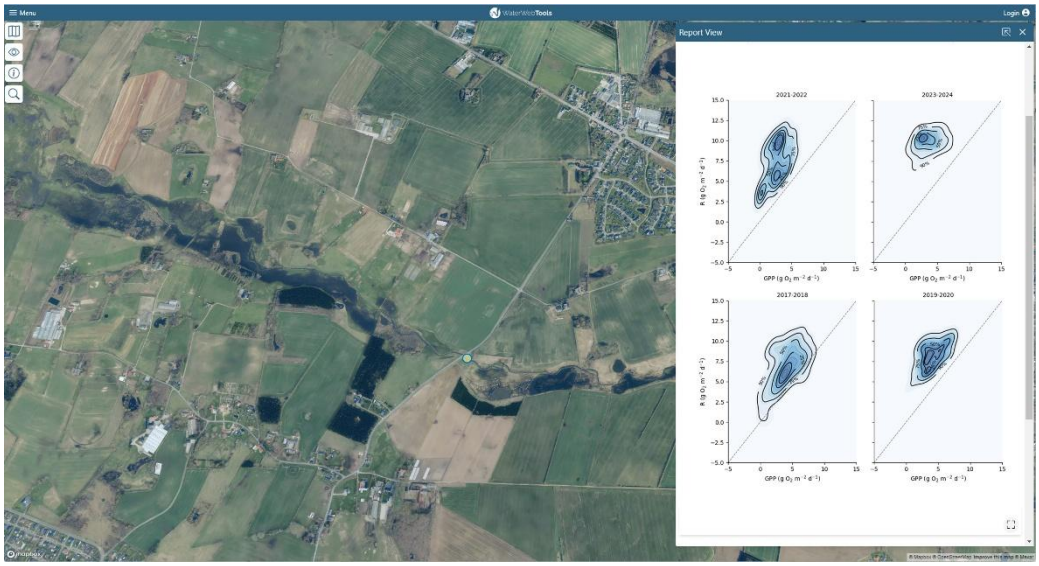

Fig. 2. Example of how metabolic fingerprints have evolved through several years for a stream reach, viewed within the WaterWebTools portal.

The daily metabolism can be used to track potential short-term impacts of for example storm water runoff during cloudburst, where there may be a degradation of the metabolic rates, usually followed by some days or weeks of recovery in the rates.

Metabolic fingerprint

If one or several years of metabolism data is available, we can also derive the metabolic fingerprint of the stream (Bernhardt et al. 2018). This represents the entire distribution of daily estimates of GPP and ER that are observed for a stream, produced through kernel density plots, which allow visualization of peak metabolic rates, the most dominant combinations of GPP and ER, represented by centroid(s) of the metabolic fingerprint, as well as the variance in their ratio (Fig. 3).

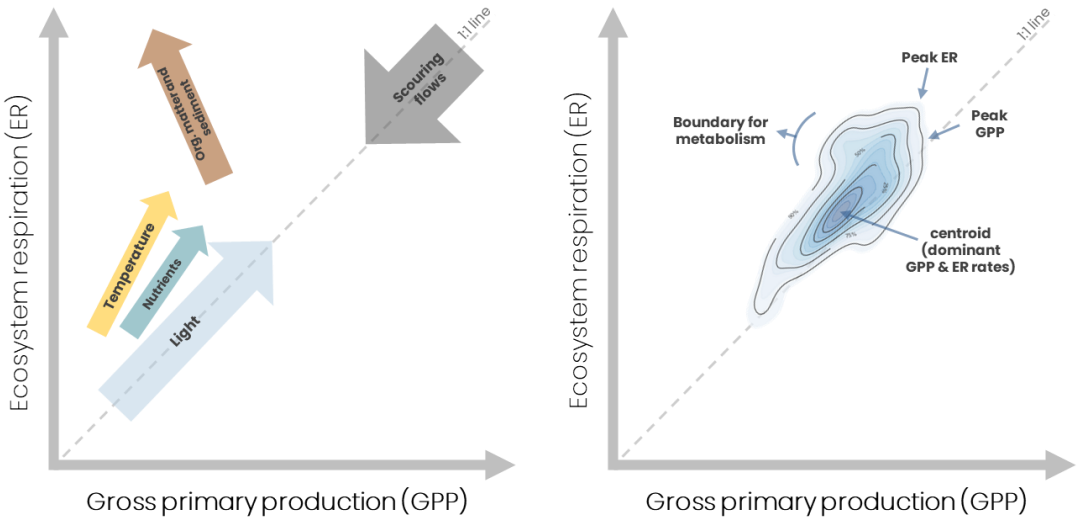

Fig. 3. The metabolic fingerprint (plot to the right) is a diagnostic tool first described by Bernhardt et al. (2018). It can be used for comparing annual patterns of metabolism across streams or across years for the same stream. The "fingerprint" is represented as a kernel density plot of daily estimates of GPP and R rates observed within the stream.

The metabolic fingerprint can be produced for each single year, and then used to follow long-term trajectories of the ecological balance of streams, helping us track changes that can signal stress or improvements in water quality. Is the river responding to improved upstream wastewater treatment, can we see any effects of implementing best-management-practices in nearby agriculture, or does restoration of floodplains or other nature-based-solutions have the expected benefits for the aquatic ecosystem? These are just some of the questions we can try to answer by keeping track of the metabolism.

References

Appling, A., Hall, R., Yackulic, C., Arroita, M. 2018. Overcoming Equifinality: Leveraging Long Time Series for Stream Metabolism Estimation. Journal of Geophysical Research: Biogeosciences, 123(2): 624-645. https://doi.org/10.1002/2017JG004140

Battin, T.J., Lauerwald, R., Bernhardt, E.S. et al. 2023. River ecosystem metabolism and carbon biogeochemistry in a changing world. Nature, 613 (7944): 449-459. https://doi.org/10.1038/s41586-022-05500-8

Beaulieu, J.J., Arango, C.P., Balz, D.A., Shuster, W.D. 2013. Continuous monitoring reveals multiple controls on ecosystem metabolism in a suburban stream. Freshwater Biology, 58(5): 918-937.

Bernhardt, E.S., Heffernan, J.B., Grimm, N.B., Stanley, E.H., Harvey, J.W., Arroita, M., Appling, A.P., Cohen, M.J., McDowell, W.H., Hall Jr, R.O. & Read, J.S., Roberts, B.J., Stets, E.G., Yackulic, C.B. 2018. The metabolic regimes of flowing waters. Limnology and Oceanography, 63: S99–S118, doi:10.1002/lno.10726

Bernot, M.J., Sobota, D.J., Hall, R.O., Mulholland, P.J. et al. 2010. Inter-regional comparison of land-use effects on stream metabolism. Freshwater Biology, 55(9): 1874-1890. https://doi.org/10.1111/j.1365-2427.2010.02422.x

Binzer, T., Sand-Jensen, K., Middelboe, A.L. 2006. Community photosynthesis of aquatic macrophytes. Limnology and Oceanography, 51(6): 2722-2733. http://www.aslo.org/lo/pdf/vol_51/issue_6/2722.pdf

Caffrey, J.M. 2004. Factors Controlling Net Ecosystem Metabolism in U.S. Estuaries. Estuaries, 27: 90–101. https://doi.org/10.1007/BF02803563

Giling, D.P., Staehr, P.A., Grossart, H.P., Andersen, M.R., Boehrer, B., Escot, C., Evrendilek, F., Gómez-Gener, L., Honti, M., Jones, I.D., Karakaya, N., Laas, A., Moreno-Ostos, E., Rinke, K., Scharfenberger, U., Schmidt, S.R., Weber, M., Woolway, R.I., Zwart, J.A. and Obrador, B. 2017. Delving deeper: metabolic processes in the metalimnion of stratified lakes. Limnology and Oceanography, 62 (3): 1288-1306. https://doi:10.1002/lno.10504

Grace, M., Giling, D., Hladyz, S., Caron, V., Thompson, R., Mac Nally, R. 2015. Fast processing of diel oxygen curves: Estimating stream metabolism with BASE (BAyesian Single-station Estimation). Limnology and Oceanography: Methods, 13(3), 103-114. https://doi.org/10.1002/LOM3.10011

Hall, R.O., Hotchkiss, E.R. 2017. Stream Metabolism. Chapter 34 in Methods in Stream Ecology. http://dx.doi.org/10.1016/B978-0-12-813047-6.00012-7

Hoellein, T.J., Bruesewitz, D.A., Richardson, D.C. 2013. Revisiting Odum (1956): A synthesis of aquatic ecosystem metabolism. Limnology and Oceanography, 58(6): 2089–2100. https://doi:10.4319/lo.2013.58.6.2089

Holtgrieve, G.W., Schindler, D.E., Branch, T.A., & A'mar, Z.T. 2010. Simultaneous quantification of aquatic ecosystem metabolism and reaeration using a Bayesian statistical model of oxygen dynamics. Limnology and Oceanography, 55(3): 1047–1063. https://doi:10.4319/lo.2010.55.3.1047

Jankowski, K. J., Mejia, F., Blaszczak, J. R., & Holtgrieve, G. W. 2021. Aquatic ecosystem metabolism as a tool in environmental management. WIREs Water, 8(4). https://doi.org/10.1002/wat2.1521

Jørgensen, S.E. and Bendoricchio, B. (Eds.). 2001. Fundamentals of ecological modelling, 3rd ed. Developments in environmental modelling. V. 21. Elsevier.

Munn, M.D., Sheibley, R.W., Waite, I.R., Meador, M.R. 2020. Understanding the relationship between stream metabolism and biological assemblages. Freshwater Science, 39: 680-692. https://doi.org/10.1086/711690

Obrador, B., Staehr, P.A., Christensen, J.P.C. 2014. Vertical patterns of metabolism in three contrasting stratified lakes. Limnology and Oceanography, 59(4): 1228–1240. https://doi:10.4319/lo.2014.59.4.1228

Reichert, P., Uehlinger, U., Acuna, V. 2009. Estimating stream metabolism from oxygen concentrations: effect of spatial heterogeneity. Journal of Geophysical Research - Biogeosciences, 114, G03016.

Riley, A.J., Dodds, W.K. 2013. Whole-stream metabolism: strategies for measuring and modeling diel trends of dissolved oxygen. Freshwater Science, 32(1): 56-69.

Solomon, C.T., Bruesewitz, D.A., Richardson, D.C. et al. 2013. Ecosystem respiration: Drivers of daily variability and background respiration in lakes around the globe. Limnology and Oceanography, 58(3), 849-866. https://doi.org/10.4319/lo.2013.58.3.0849

Song, C., Dodds, W.K., Trentman, M.T., Rüegg, J., Ballantyne, F. 2016. Methods of approximation influence aquatic ecosystem metabolism estimates. Limnology and Oceanography Methods, 14: 557–569. https://doi:10.1002/lom3.10112

Staehr, P.A., Christensen, J.P., Batt, R.D., Read, J.S. 2012. Ecosystem metabolism in a stratified lake. Limnology and Oceanography, 57(5): 1317–1330. https://doi:10.4319/lo.2012.57.5.1317

Trolle, D., Nielsen, A. 2024. Sundhedstjek af søer, vandløb og fjorde via deres metabolisme. Aktuel Naturvidenskab (Danish popular science journal). https://aktuelnaturvidenskab.dk/find-artikel/nyeste-numre/5-2024/sundhedstjek-af-soeer-vandloeb-og-fjorde-via-deres-metabolisme

van't Veen, S.G.M., Kronvang, B., Audet, J. et al. 2025. SentemQC - A novel and cost-efficient method for quality assurance and quality control of high-resolution frequency sensor data in fresh waters. Open Res Europe, 4: 244 https://doi.org/10.12688/openreseurope.18134.1

Wilcock, R.J., Nagels, J.W., McBride, G.B., Collier, K.J. Wilson, B.T., Huser, B.A. 1998. Characterisation of lowland streams using a single station diurnal curve analysis model with continuous monitoring data for dissolved oxygen and temperature. New Zealand Journal of Marine and Freshwater Research, 32(1): 67-79. https://doi.org/10.1080/00288330.1998.9516806

Appendix

Parameter bounds

Parameter bounds used when running the differential evolution algorithm have been derived from a review of metabolism studies, thereby ensuring that calibrated parameters are within naturally realistic ranges.

Parameter	Unit	Min.	Max.	References
P_{max}	g O_2 m^{-2} h^{-1}	0.01	5.5*	Wilcock et al. (1998), table 2 min. P_{max} = 0.03, max. P_{max} = 1.91 Binzer et al. (2006), table 2 min. P_{max} = 0.34, max. P_{max} = 2.9 Holtgrieve et al. (2010), table 3 min. P_{max} = 0.37, max. P_{max} = 0.45 Beaulieu et al. (2013), table 2 min. P_{max} = 0.0018, max. P_{max} = 0.89 Song et al. (2016), table A1 min. P_{max} = 0.087, max. P_{max} = 0.56
α	g O_2 m^{-2} h^{-1} [µmol photons m^{-2} s^{-1}]$^{-1}$	0.001	0.0115	Binzer et al. (2006), table 2 min. α = 0.001, max. α = 0.0115 Holtgrieve et al. (2010), table 3 min. α = 0.0013, max. α = 0.0025 Beaulieu et al. (2013), table 2 min. α = 0.0011, max. α = 0.33 Song et al. (2016), table A1 min. α = 0.00375, max. α = 0.0021
R_{20}	g O_2 m^{-2} h^{-1}	0.05	2.75	Wilcock et al. (1998), table 2 min. R_{20} = 0.065, max. R_{20} = 1.56 Holtgrieve et al. (2010), table 3 min. R_{20} = 0.28, max. R_{20} = 0.35 Song et al. (2016), table A1 min. R_{20} = 0.082, max. R_{20} = 0.47
K_{20}	m h^{-1}	0.0035	0.4	Wilcock et al. (1998), table 2 min. K_{20} = 0.0035, max. K_{20} = 0.33 Holtgrieve et al. (2010), table 3 min. K_{20} = 0.13, max. K_{20} = 0.27

*Many of the P_{max} values reported in literature are not corrected to 20°C, as many studies ignore the effects of temperature on primary production (i.e. they are more representative of the maximum of the actual growth rate at ambient temperature). The primary production rate in the model by WateriTech is corrected for temperature each time step, and therefore the P_{max} is set to somewhat higher value than those reported in literature (but resulting in an actual growth rate at ambient temperature similar to that reported in literature).