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OxyPOM and DiaMO: simple FABM models for dissolved oxygen and biogeochemistry

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Software

- Review
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Summary

OxyPOM (Oxygen and Particulate Organic Matter) and DiaMO (Diagnostic Model for Oxygen) are aquatic biogeochemical models that consider key processes for dissolved oxygen (DO), such as re-aeration, mineralization, and primary production, in fresh, transitional and marine waters. Both are implemented in the `Fortran`-based Framework for Aquatic Biogeochemical Models (FABM, Bruggeman & Bolding, 2014) for reusability in a variety of hydrodynamic models, in realistic and idealized applications, and for interoperability with other aquatic process models. With these models, we include an updated light profile implementation and testcases for simulating DO at Cuxhaven Station in the Elbe estuary 2005–2024; for this, we use the hydrodynamic General Ocean Turbulence Model (GOTM, Burchard, 2002) including tides, and `R` and `bash` scripts for including weather and river data from kuestendaten.de.

Statement of need

Dissolved oxygen is a key variable for assessing water quality and ecological state of aquatic ecosystems (European Commission, 2006). Most existing models describe DO dynamics as a side product of more or less complex (a)biotic dynamics. OxyPOM and DiaMO remove much of this complexity and focus on the key processes that produce or consume oxygen.

A predecessor simplified 1D long-channel version of OxyPOM was initially implemented by Holzwarth & Wirtz (2018) for the closed-source UnTRIM-DELWAQ hydrodynamic and water quality system. We elaborated on this earlier work by adding vertically explicit process formulation for re-aeration in rivers and estuaries (Raymond & Cole, 2001), primary production, and light attenuation. We included additional mortality terms related to micro-algae viral infections (Wirtz, 2019), and a step-wise temperature-sensitive micro-algae loss rate (Scharfe et al., 2009). With OxyPOM, we can now demonstrate unprecedented skill in representing oxygen dynamics including hypoxia events in the Elbe river.

Where a complete representation of bio-geochemical dynamics is not needed, DiaMO is an even more simplified model for quick assessments of DO dynamics. All of this is implemented as an open source, findable, accessible, interoperable and reusable (FAIR) modeling system.

OxyPOM: Oxygen and Particulate Organic Matter

The model OxyPOM resolves the dynamics of dissolved oxygen (DO), (semi-)labile particulate organic matter (POM) pools, silicate particles, dissolved organic matter (DOM), inorganic dissolved nutrients, and two micro-algae classes. Oxygen dynamics is based on a mass balance equation:

$$\frac{d\mathrm{DO}}{dt} = \text{Re-aeration} + (\text{Photosynthesis} - \text{Respiration}) - \text{Mineralization} + \text{Nitrification}. \quad (1)$$

Re-aeration occurs in the surface layer as a function of temperature, salinity and wind speed (Weiss, 1970). Photosynthesis is limited by nutrient concentration and light intensity with an exponential saturation (Platt et al., 1980). Respiration includes oxygen consumption for micro-algae. Mineralization and Nitrification is the oxygen consumed to transform matter from organic to inorganic forms and to oxidize ammonia into nitrate, respectively.

POM and DOM have an explicit elemental composition (carbon, nitrogen and phosphorus); POM is present in two qualities, which transition in the sequence labile → semi-labile → dissolved. POM and DOM mineralize to inorganic dissolved nitrogen and ortho-phosphate. Dissolved inorganic nitrogen is the sum of ammonium and nitrate; ammonium transitions to nitrate as a function of DO. Silicate is present in dissolved –bio-available– and particulate mineral forms. The two micro-algae classes (one with dependence on dissolved silicate, thus representing diatoms) have growth rates that depend on photosynthesis; their growth rates depend on dissolved nitrogen and ortho-phosphate concentrations. Micro-algae take up and release dissolved nutrients when they die with a temperature-dependent mortality rate.

OxyPOM shows high skill by reproducing surface DO at the Cuxhaven station in the Elbe estuary (Figure 1).

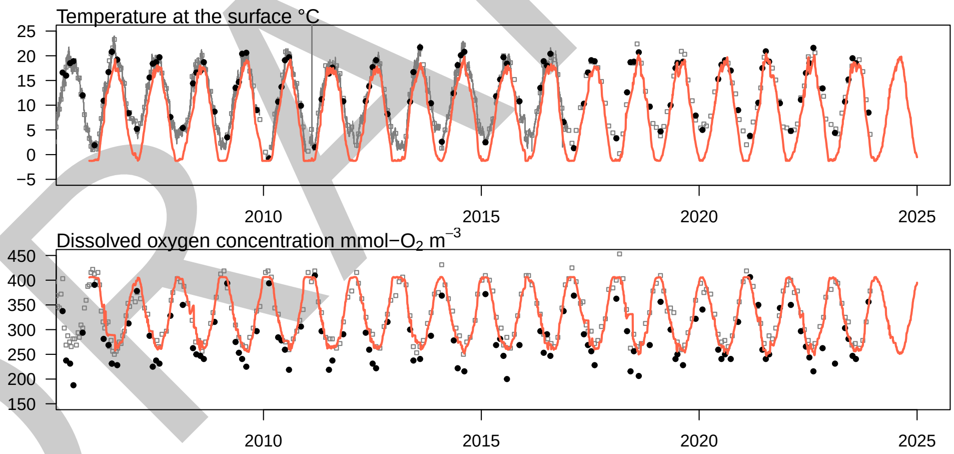

Figure 1: Validation of OxyPOM model with the testcase `estuary` contained in the repository. Model results for temperature (from GOTM, top, red) and OxyPOM DO (bottom, red) are compared to station data (black and grey dots) available from kuestendaten.de

DiaMO: Diagnostic Model for Oxygen

DiaMO resolves the dynamics of DO, living and non-living organic particulate carbon forms (Phytoplankton (Phy) and Detritus (Det), respectively) under the assumption that light, not nutrients, is the limiting factor for photosynthesis; DiaMO is a carbon-only implementation. DO is solved with the mass balance equation of OxyPOM (Equation 1), setting nitrification to zero. The complete system is represented as

$$
\begin{aligned}
\frac{d\text{Phy}}{dt} &= \text{Photosynthesis} - \text{Respiration} - \text{Aggregation} \qquad (2)\\
\frac{d\text{Det}}{dt} &= \text{Aggregation} - \text{Mineralization} \qquad (3)\\
\frac{d\text{DO}}{dt} &= \text{Re-aeration} + (\text{Photosynthesis} - \text{Respiration}) - \text{Mineralization}. \qquad (4)
\end{aligned}
$$

Aggregation rate is a mortality term for phytoplankton (Maerz & Wirtz, 2009). As in OxyPOM, all rates in DiaMO are temperature-dependent. DiaMO was equally validated and shows high skill reproducing surface DO at the Cuxhaven station.

Light in OxyPOM and DiaMO

Together with OxyPOM and DiaMO, this repository includes the model `oxypom/light` as an alternative model to the standard GOTM light model. While the default light model assumes that the photosynthetically active radiation (PAR) in a vertical layer z of thickness Δz is in the centre of the layer, `oxypom/light` calculates PAR in the representative depth $\bar{z}$, which satisfies the mean value theorem, such that PAR evaluated at $\bar{z}$ is the mean PAR intensity in the layer. Since this calculation can be computationally expensive to evaluate, first- and second-order approximations are implemented. The first-order solution is equal to the centre of the layer $z + \frac{1}{2}\Delta z$, and the second-order approximation is

$$
\bar{z} = z + \frac{1}{2}\Delta z - \frac{\alpha}{3}\Delta z^2, \qquad (5)
$$

where α is the light extinction coefficient for the layer, accounting for physical and biological light absorption, assuming an exponential light decay.

Model documentation and license

The models are documented in short form in the `ReadMe.md` section of the repository and a complete description of the science behind OxyPOM is in Holzwarth & Wirtz (2018). Open access data from third parties are not included with the model, and scripts for their download are included. Our own models, scripts and documentations are are released under open source licenses, foremost Apache 2.0, CC0-1.0, and CC-BY-SA-4.0; a comprehensive documentation of all licenses is provided via REUSE Software.

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