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A short review of contemporary developments in aquatic ecosystem modelling of lakes and reservoirs

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1. Introduction

A special issue of Environmental Modelling and Software (Gal et al., 2014) listed “key challenges” in aquatic ecosystem modelling and collated case studies that applied novel modelling tools and approaches to address these challenges. These challenges were:

A. Model development and integration of models
   1. Selection of most suitable modelling approach
   2. Identification of appropriate degree of complexity
   3. Improvement of accuracy of model process representation (model structure) given our prior biophysical and ecological understanding of the system
   4. Integration of models
   5. Improved sharing and coupling of models

B. Model reliability
   1. Definition and quantification of impacts of uncertainty and sensitivity of complex models on their results
   2. Delineation of appropriate application of models (i.e. improve our ability to select the most suitable model for an application at hand)
   3. Improved model assessment

C. Model implementation and usage
   1. Incorporation of emerging rich data sources
   2. Providing timely predictions to facilitate operational management through near-real time and forecasting models
   3. Using complex models to increase ecosystem understanding
   4. Enhancement of model coupling with management tools to increase integration into the decision making process

Recently, 35 modellers from nine countries gathered in Brisbane, Australia, to discuss these challenges and the progress that has been made over the past few years. Of the challenges identified by Gal et al. (2014), we, the authors, identified the following nine areas in which significant progress has been made in either addressing or further elucidating these challenges:

1. Model development
2. Model facilitation
3. Model parameterisation
4. Model structure
5. Optimising model practice
6. Model integration
7. Data and data repositories
8. Advancing transdisciplinary global networks
9. The value of modelling

Our aim in this paper is not to provide a comprehensive literature review, but to stimulate discussion on deficiencies in methods and model development, as well as on how to overcome some of the identified deficiencies. Our focus is on aquatic ecosystem models (AEMs), but most subjects discussed are applicable across a broad range of environmental models.

AEMs quantify the state of an aquatic ecosystem based on internal or external forcing of that system (sensu Janssen et al., 2015). Most AEMs consider water column transport and transformations of one or more major nutrients (typically nitrogen, phosphorus and/or carbon), together with aspects of plankton ecology and sometimes other ecosystem components (Robson, 2014a). Mooij et al. (2010) compare a range of AEMs; Janssen et al. (2015) provide a comprehensive list of AEMs that are currently in use in the supplementary material in their paper.

2. Model development

In recent years there has been a strong drive by modellers to adopt open source approaches to enhance model development, facilitating interactions with model code by a broader subset of the aquatic ecosystem modelling community. Online model repositories are the standard for open source models (e.g. https://github.com), allowing for version control and a standardised documentation process. However, open source code also presents challenges. For example, technical issues may arise when there are different branches of a model, requiring a custodian or overseeing group to decide on whether new or modified algorithms should be incorporated into the parent code, and the point in time when this should occur.

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The aquatic ecosystem modelling community has also tended to divide into three specialist groups: model designers, programmers and users (Robson, 2014b). Typically, only a small proportion of modellers contribute to code development. Several studies have shown that scientific models are improved by coding collaboratively and cross-cutting disciplinary areas (e.g., through interactions amongst software engineers, scientists and practitioners), and that it leads to higher quality of software in terms of algorithm accuracy and relevance (Storer, 2017). By contrast, a single programmer may act as a custodian of the model code and disseminate it upon evaluating requests to develop and use it. The community development approach may be sustained by funding for a research coordination network or researcher cluster, while the single programmer model generally requires funding to be sustained by a local group. The latter approach can be limited by the continuity of research support at a local scale, by the workload required for model documentation and bug-checking, and by sharing knowledge with users about model limitations and new model developments.

Community models therefore tend to engage a wider cross-section of the aquatic ecosystem modelling community, facilitating increased dialogue and interrogation of approaches, but may require development of protocols and policies that facilitate version control, model development and funding support.

3. Model facilitation: “easing the pain of modelling”

A coordinated community approach is key to improving modelling efficiency and adoption of improved modelling practices and technologies. The move towards open source code allows a broader suite of scientific models and software tools to be developed, used and tested amongst a global modelling community. Making software resources available is important to allow easier entry into the modelling process and for growing the community and engaging researchers globally. Emerging high-volume ecological datasets and efficient computational algorithms have greatly enhanced opportunities for data assimilation (Zobitz et al., 2011) as has the use of advanced visualisation techniques to interpret outputs (Rink et al., 2018). Community efforts supporting software environments such as R or Python have become integral to the development and application of AEMs. For example, the R package “rodeo” (Kneis et al., 2017) facilitates model development by combining the widely used language R with automatically generated Fortran code to achieve high computational performance. Software packages have been designed to handle specific models (e.g., the R package “glmtools”, Read et al., 2016b) and to support generation of figures or animations from NetCDF files, e.g., the R package “OceanView” (Soetaert, 2016) and the Python-based graphical user interface “PyNcView” (https://sourceforge.net/projects/pyncview/).

Virtual laboratories (like the Biodiversity and Climate Change Virtual Laboratory BCCVL, http://www.bccvl.org.au/) provide user-friendly interfaces to allow users to focus on the experimental or synthetic systems created by the model, rather than on code development and runtime issues. They are not yet available for AEMs, but tools like the Database Approach To Modelling (“DATM”; Mooij et al., 2014) can carry out automated translation of information in a database into a model framework. Similarly, the Water Ecosystem Tool (“WET”; http://projects.au.dk/wet/, Nielsen et al., 2017) links climate change and catchment model output scenarios as input to the hydrodynamic-ecosystem model GOTM-FABM-PCLake. These tools help to simplify AEM applications and can be linked to virtual laboratories. Another model interface, GRAPLEr (https://github.com/GRAPLE/GRAPLEr, Subratie et al., 2017), allows a user to utilise distributed computing resources to run large numbers of simulations. Together with parameter databases (e.g., http://shiny.csiro.au/CDM/parameterlibrary/latest/, Robson et al., 2018), code libraries (e.g., LibBi to support Bayesian inference: http://libbi.org/faq.html, Murray, 2013) and statistical packages to support model enquiry such as Monte Carlo simulation and sensitivity analysis (e.g., the R package “FME” by Soetaert, 2016; “PEST”, http://www.pesthomepage.org/Home.php by Doherty, 2015), these interfaces effectively provide a toolbox to promote advanced discussion on parameterisation and calibration of complex models.

4. Model parameterisation

With increasingly rich sources of data, better matching the time and space resolution of our models (Hamilton et al., 2014) it is possible to more thoroughly calibrate and evaluate models (e.g., Adiyanti et al., 2016). Remote sensing and the Internet of Things (IoT) are contemporary fields of research that can greatly enhance data acquisition for AEMs. Recent and planned launches of Sentinel satellites (https://sentinel.esa.int/web/sentinel/home) provide data on an increasing number of optically active constituents, with opportunities to enhance spatial and spectral resolution, suitable for modelling smaller lakes and reservoirs (Toming et al., 2016). AEMs have already been adapted to represent water colour or reflectance at specific wavelengths and align directly with true colour images of the water surface derived from Earth observation missions (e.g., Baird et al., 2016). Cheap sensors and expanding sensor networks will provide a greater spatial coverage of environmental monitoring data, supporting model validation (Hipsey et al., 2015). Efficient algorithms are therefore required to assimilate sensor data for model application (Baracchini et al., 2019).

Collaborations between experimentalists and modellers are important to determine new ways to align or measure parameters that are commonly calibrated through inverse modelling (Flynn, 2005). The need for innovation in measurements to better match what is modelled is an important component of parameter identifiability. This has been considered with respect to zooplankton observations and modelling by Everett et al. (2017), and is an ongoing theme in papers by Flynn et al. (2015, 2016). Few current applications of complex AEMs have dealt with the emerging complexity of species and strain-level diversity being revealed by molecular techniques. Methods that explore differences amongst isolates and strains of species indicate intra-species genetic and phenotypic variability that in some cases can be of similar magnitude to inter-specific variability (e.g., Xiao et al., 2017). Bayesian methods (e.g., Arhonditsis et al., 2007; Couture et al., 2018; Jia et al., 2018), individual-based models (Hellweger et al., 2016) and adaptive trait-based models (Smith et al., 2014) offer methods to explore the inherent variability in biota but these have not commonly been applied at an ecosystem scale.

5. Model structure

Most of the AEMs used today have gained acceptance through a sustained period of development and application that has demonstrated their utility. As a result, many models employ equations based on process understanding that often extends back to the 1960s (e.g., Eppley et al., 1969), with code that was initially written in the 1970s-90s (e.g., Cerco and Cole, 1995; Di Toro et al., 1975; Hamilton and Schladow, 1997; Postma, 1984). Although much of the underlying conceptual understanding still holds today, advances in knowledge may provide either better representations of existing processes or identify entirely new processes that need to be embedded within AEMs. Examples of processes identified in the 1990s but neglected in most AEMs are anammox (Mulder et al., 1995; Van de Graaf et al., 1990), uptake of dissolved organic nitrogen by plants and phytoplankton (e.g., Berg et al., 1997; Glibert et al., 2004; Vonk et al., 2008). Other processes are phosphorus uptake enhanced by alkaline phosphatase production (Prentice et al., 2015) and production of greenhouse gases such as CO_2, CH_4 and N_2O associated with organic matter from different sources and ages (Koehler et al., 2012; Sinsabaugh et al., 2013).

We argue that structural uncertainty needs to be revisited more frequently. The modularisation of models (e.g., the Aquatic Ecodynamics Modelling Library “AED2”, the Ecological Regional Ocean Model “ERGOM”) and multiple algorithm options supported by high frequency observations (e.g., Woolway et al., 2015) make testing, validation and re-coding of processes easier. Structural uncertainty can further be explored by comparing different process representations within a complex model (Frassl et al., 2014; Sadeghian et al. 2018) or output from model ensembles (Trolle et al., 2014a; Van Vliet et al., 2019). Applying models of different complexity and structure (LakeMIP: http://www.unige.ch/climate/lakemip/, Stepanenko et al., 2010) can help with selecting models and modules that are fit for purpose. Applying a single model across a diverse range of lakes with different morphologies, residence times or climates is time consuming but importantly can reveal model structural deficiencies (GLM-MLCP, Bruce et al., 2018).

6. Optimising model practice

Methodological summaries (Bennett et al., 2013; Brown et al., 2011) and modelling guidelines (Jakeman et al., 2006; Pianosi et al., 2016; Wilson et al., 2017) have helped to disseminate best practices within the modelling community. The sheer number and diversity of AEMs, however, make it difficult to choose a suitable model that is fit for purpose (Janssen et al., 2015). An increase in number and diversity has also been observed for supporting tools (e.g., Wolski et al., 2017) and data (e.g., LaDeau et al., 2017). Accessing and finding the right data, tools and models fit for the specific project is essential (Wirtz and Nowak, 2017) and the development of a roadmap for each of these would be of great benefit to the aquatic ecosystem modelling community.

There has recently been a focus on full documentation of model code, simulation experiments and publishing of data sets, which are the cornerstones for reproducibility (Hutton et al., 2016; Nosek et al., 2015). Nevertheless, this initiative is in its infancy for AEMs and there is a need for an agreed standard for both documenting code, e.g., through model repositories and version control, and providing model-relevant outcomes from simulation experiments (e.g., parameter tables). Scientists and model practitioners need to conduct this exercise jointly to develop a framework for benchmarking real and virtual experimental systems to support good model performance. Successful examples of model benchmarking in related disciplines (e.g., Hunter et al., 2008) can serve as a base for benchmarking AEMs. This would help to communicate uncertainties whilst building trust in the models by a broader cross-section of stakeholders. Ideally, a community toolkit of resources and operational procedures could be developed, defining workflows and including model parameterisation and uncertainty assessment.

7. Model integration

Much uncertainty in model results can stem from model inputs adopted as boundary conditions. Limitations of field measurements have led to the practice of integrating AEMs with other environmental models to interpose sparse input data as well as to examine interactions across system boundaries or changing boundary conditions. Fluxes of energy and mass across system boundaries are crucially important for many biophysical models (Goyette, 2017; Krause et al., 2017; Tranmer et al., 2018), and address an important management issue of loss of connectivity within and between systems (Stewart et al., 2018). For example, catchment nutrient fluxes are primary drivers of lake ecosystems, so there is a strong case for coupling AEMs with catchment models. For a recent review on catchment models see Fu et al. (2019). Coupled catchment-lake models can be used to estimate incoming (non-point) loads to lake ecosystems and to simulate the effects of land use change on the lake ecosystem (Bucak et al., 2018; Crossman and Elliott, 2018; Me et al., 2018; Rossel and de la Fuente, 2015). This coupling, however, is hindered by simplistic load generation algorithms used in many catchment models and a mismatch in simulated time scales and model variables (e.g., nutrient speciation, water temperature). Similar issues exist when considering lake-groundwater exchanges.

Improvements in Earth system modelling, resulting in greater spatio-temporal resolution, make it feasible to derive comprehensive input data for AEMs. For example, data from reanalysis (Xue et al., 2015) and weather forecast models (e.g., Valerio et al., 2017) have been used to generate wind fields to drive lake hydrodynamic models. Output from Global Change Models and reanalysis projects can provide boundary conditions for simulating remote, data-sparse water bodies. However, it remains a challenge to derive water quality parameters and obtain validation data for simulations of these systems (Frassl et al., 2018a).

A major hurdle to integrating models is the interoperability of different models and the lack of standards across environmental domains. Voinov and Shugart (2013) emphasised that working collaboratively between disciplines helps to prevent the creation of ‘integronsters’ that hinder model interoperability. That is, sub-modules that were developed and validated for one application may not be meaningful anymore when combined with each other and applied in a different context. Progress has been made in coupling different types of models, like agent-based, stochastic or process-based models, e.g. to understand socio-ecological interactions (Martin and Schlüter, 2015). Technical factors can still be impediments to achieving interoperability and include the need to agree on common interfaces (e.g., Buahin and Horsburgh, 2018), to bridge across different scales, to develop common standards, and to define model variables consistently. We contend that insufficient emphasis has been placed on the importance of boundary conditions in aquatic ecosystem modelling.

8. Data and data repositories

Conducting multi-site or global modelling studies can be a challenge because of issues related to data accessibility and heterogeneity. Preserving data for general accessibility can help to address this challenge, for example by using supplementary information accompanying published articles, by publication in data journals (http://www.forschungsdaten.org/index.php/Data_Journals; Candela et al., 2015) or by storing the data in specific databases and repositories (https://www.re3data.org/). The association with a digital object identifier (doi) makes these data citeable. The use of standardised vocabularies (Cox et al., 2014) also makes them more readily searchable and discoverable. Model inputs as well as model outputs are increasingly being delivered through data services and repositories. Access to these data can be facilitated through open software packages (e.g., Winslow et al., 2018).

Data-intensive scientific applications require that the data are discoverable, accessible and well-described. A recent study has found that only 63% of scientists deposit data or make the data available as supplementary material (Stuart et al., 2018). This is counterproductive because publication of data sets can ‘kick start’ subsequent studies, reducing the time required for data preparation and quality control, and facilitating exploratory studies. Best practices for data storage (Hart et al., 2016) and data management, e.g., through data management plans (DMPs; Michener, 2015) or by following the FAIR Guiding Principles “Findability, Accessibility, Interoperability, and Reusability” (Wilkinson et al., 2016) will improve data availability and support comparative modelling studies including changes with different model versions.

Data delivery via an application programming interface (API) (e.g., OpenDAP, https://www.opendap.org/) and servers (e.g., THREDDS, https://www.unidata.ucar.edu/software/thredds/current/tds/TDS.html) can provide a stable data set with quality assurance/quality control (QA/QC) standards and known provenance. Automated or advanced manual QA/QC procedures (e.g., Campbell et al., 2013; Horsburgh et al., 2015; McBride and Rose, 2018; ‘B3,’ Read et al., 2016b) linked with data assimilation techniques (Hipsey et al., 2015) have the potential to greatly simplify the time consuming process of data preparation.

Data sharing is often associated with building trust (Wolski et al., 2017). Therefore, it is crucial in modelling studies to give credit to the provenance of the data and to work collaboratively with those who collected the data (e.g., Bruce et al., 2018; Frassl et al., 2018b). Agreeing on a data management plan (DMP; Michener, 2015) and clear authorship guidelines (e.g., Brand et al., 2015) are good ways to build trust and facilitate data sharing. Further sharing of pre- and post-processing scripts can result in time savings and greater diversity and quality of model output interrogation.

9. Advancing transdisciplinary global networks

Many of the above mentioned challenges posed in aquatic ecosystem modelling may be more easily addressed through transdisciplinary networks of modellers, scientists and stakeholders. These networks are mostly maintained through funding initiatives and can be fostered through joint workshops (Bloesch et al., 2005), special issues in scientific journals (Fang et al., 2017), international research programs across disciplines (Dohmann et al., 2016; Kottmeier et al., 2016) and team science projects involving the Global Lake Ecological Observatory Network, GLEON (Read et al., 2016a; Weathers et al., 2013). The persistence of these initiatives is an issue, however, and more robust funding frameworks are required based on well organised disciplinary groupings seen in climate modelling (www.wcrp-climate.org).

Past research programs have revealed the value of bringing together water agencies, consultants and scientists. The “Queensland Water Modelling Network” (Lawrence and Riches, 2017) is an example of a new initiative to improve operational water modelling through a coordinated network of model practitioners, models and data sets. The Aquatic Ecosystem Modelling Network (AEMON), a consortium of AEM experts, has been very productive in summarizing the current state-of-the-art of aquatic ecosystem modelling, pointing to gaps in model development and providing useful overviews of AEMs (Janssen et al., 2015; Mooij et al., 2010; Trolle et al., 2012).

AEMON hosts an active user forum which shares knowledge and modelling resources, and supports early career AEM developers and practitioners (https://groups.google.com/forum/#!forum/aquaticmodelling). The AEM community may benefit from considering how to best train the next generation of modellers. Specific training strategies include community-developed, continuously tested and dynamically updated open teaching modules (e.g., the EDDIE project https://serc.carleton.edu/eddie/index.html or https://software-carpentry.org/). Provision of real-world data and easily operated computing infrastructure can help new modellers to focus on the science and later engage in the technical detail whilst ensuring best modelling practices are implemented. A further step would be to conduct international hands-on workshops that make use of diversity in the environmental modelling community. Possible outcomes could be model ensemble studies across different lakes and reservoirs, cross-boundary simulations over entire catchments, or large-scale modelling studies that address global environmental issues like water scarcity or global climate change (e.g., https://www.isimip.org/about/). Currently, regular meetings of the international aquatic ecosystem modelling community are lacking. A possible solution is to strive to consistently include specialist modelling sessions at large aquatic science conferences or to establish regular virtual conferences.

10. The value of modelling

AEMs can inform policy by providing a technical basis for making informed decisions. They can provide quantitative predictions of how aquatic ecosystems respond to pressures like land use change (Bhagowati and Ahamad, 2019; Ménesguen and Lacroix, 2018; Trolle et al., 2014b; Vinçon-Leite and Casenave, 2019), hydropower plant operations (Rossel and de la Fuente, 2015), mining (Salmon et al., 2017) or altered hydrology (Jones et al., 2018; Weber et al., 2017). More broadly, embedding the modelling process into decision-making can increase transparency (Merritt et al., 2017), highlight gaps for further study (Krueger et al., 2012), characterise sources of uncertainty, generate new knowledge and clearly define risks (Refsgaard et al., 2007). Development of coupled natural-human systems models potentially supports decision making by capturing links between water quality and socioeconomic processes such as changes in property values in lake catchments (Cobourn et al., 2018). Further, AEMs are increasingly being linked to up-to-date forcing data to make near real-time predictions to guide water management operations (Bertone et al., 2015; Wang et al., 2016). This can substantially reduce risk (e.g., drinking water contamination) and provide economic efficiencies.

Despite these advantages, AEMs are often poorly integrated into the decision-making process, which can limit their value. Model scenarios may not accurately encompass the management options available, or the implications of model results are “lost in translation” between scientists and managers (Delaney and Hastie, 2007). A greater emphasis needs to be placed on the interactions of the modelling process with the broader aspects of water management (Refsgaard et al., 2007). Structured Decision Making (Gregory et al., 2012) or participatory modelling (Voinov et al., 2016) are examples of concepts that could be used to embed modelling into decision-making. The collaborative nature of these concepts, e.g., through transdisciplinary scenario development (IPBES et al., 2016), can help participants to understand model assumptions, capabilities, uncertainties and the complex relationships in aquatic ecosystems.

An increasing number of AEMs is used to estimate greenhouse gas emissions from lakes (e.g., Stepanenko et al., 2016; Tan et al., 2015). Nevertheless, the potential to support integrated scenario simulations within the framework of both the Intergovernmental Panel on Climate Change (IPCC) and the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES) remains largely unexplored. The need to use this potential is reinforced in the necessity for the aquatic ecosystem modelling community to provide quantitative predictions for the UN sustainable development goals (UN, 2015), particularly Goal 6: to ensure availability and sustainable management of water and sanitation for all.

11. Conclusion

The amount of data, and number of methods and tools used in the aquatic ecosystem modelling community has continued to increase, necessitating a greater level of integration and coordination to exploit the resulting opportunities. Model and equation libraries, processing tools and parameter databases provide a strong basis for model development as well as a focus on the scientific and management implications of model output. Agreed standards to facilitate inter-operability and workflows provide for consistency of modelling practice and can be implemented at early career levels to provide a cohort of skilled practitioners. More than ever, managers require model predictions to support effective and transparent decision making. For model predictions that are used to support policy and have important social and economic implications, reliable and accurate models are critical to avoid compounding error, while at the same time model uncertainties need to be clearly communicated and documented. Trust in models is achieved through progressive model development, ongoing support and funding, as well as identification of data requirements to address parameter uncertainties. We have shown the considerable scope for the aquatic ecosystem modelling community to make further advances that improve both AEMs and the modelling processes. By linking shortcomings with emerging opportunities, this paper provides insight into the current state of the field and, more importantly, highlights ways forward to resolve current issues and address future challenges.

Declarations of interest

None.

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