Process-based Simulation Library SALMO-OO for Lake Ecosystems

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EXTENDED ABSTRACT

Over the past three decades numerous lake ecosystem models incorporating algal population dynamics have been developed and published. However, most of these models have been constructed, calibrated and validated *ad hoc* to suit one specific lake application. Even though many models, including SALMO (Recknagel and Benndorf, 1982), were designed and validated as being generic for a range of lake properties they were always rigid in their process equations and parameter values. This paper discusses the concept, implementation and testing of SALMO-OO towards a more generic simulation library for lakes by taking advantage of object-oriented design and Java programming. A library of four process models for phytoplankton growth have been implemented in SALMO-OO, with one growth model from the library presented here as a case study to demonstrate its increased generality and flexibility for simulations of lakes with different trophic states.

The initial focus was on phytoplankton models that were of the form of ordinary differential equations (ODEs). The phytoplankton growth models were selected from the literature where different combinations of growth equations and classical growth-limiting functions regarding nutrients, light and water temperature were applied. Those models that displayed a similar model rationale to the original SALMO were implemented in the full object-oriented version of the model (SALMO-OO). Combinations of different growth functions were tested within the simulation library. The validation of SALMO-OO was based on comparisons of calculated and measured algal biomass data of two lakes with meso- and hypereutrophic conditions.

The results show that the SALMO-OO model can effectively simulate eutrophic systems very well, and improvements made to parameter values produced significantly improved results, compared to the original SALMO model. The SALMO-OO model does struggle to describe mesotrophic conditions, however the application of a growth model from the simulation library greatly improved this result.

Another area of concern with the original model was that the algal functional groups simulated did not fully reflect the typical seasonality observed in eutrophic or mesotrophic systems. Significant improvements were made to the original SALMO model by adopting the more realistic parameter values from the algal growth model of Hongping and Jianyi (2002) whilst retaining the same structure. Experiments with the new parameter values from this growth model improved simulation results of SALMO-OO for the algal groups: blue-green algae, green algae and diatoms. Five parameter values were adopted from Hongping and Jianyi (2002), the most notable were the maximum growth rate (*PHOTXMAX*), half-saturation constant for P uptake (*KP*) and the preference factor (*PF*) values for zooplankton grazing.

The original SALMO model was developed as a generic model and the new SALMO-OO model aims to strengthen this attribute. By improving the original model through the simulation library, SALMO-OO gained more flexibility for the simulation of a broad range of lakes with different trophic states, which demonstrates its generality.

In addition to the algal growth models, a simulation library for algal grazing is currently being tested. This will further strengthen the flexibility and generality of SALMO-OO. Also a multiple parameter optimisation based on evolutionary algorithms will be integrated in SALMO-OO. This will calibrate parameter values within their range of variance to improve the accuracy of simulation results. It is concluded that the object-oriented implementation of ODE based ecosystem models significantly improves its knowledge base, functionality and accuracy.

1. INTRODUCTION

The development and use of ecosystem simulation models has become a popular method of investigating the complexity of aquatic environments. Indeed, perusing the scientific literature it becomes apparent that in the last several decades numerous models and modelling studies have been published, with a large proportion of those being aquatic models incorporating phytoplankton dynamics. However, most of these models have been constructed, calibrated and validated *ad hoc* to suit one specific lake application. As a result, such models are rigid in their structure, process equations and parameter values.

Algae population dynamics are a core component of aquatic models. Many algal population models are generally similar in structure, although there are many ways to mathematically represent key processes, such as growth and grazing. Investigating the behaviour of these process-based functions may assist in the development of more robust and exploratory ecosystem models.

This paper discusses the concept, implementation and testing of the object-oriented lake ecosystem model SALMO-OO towards a more generic simulation library for lakes by taking advantage of object-oriented design and programming in Java. A library of several process models for algal growth are implemented in SALMO-OO and used as a case study to demonstrate its increased generality and flexibility for simulations of lakes with different trophic states, and to determine the merit of such libraries to the modelling of lake ecosystems.

2. METHODS

2.1. Description of SALMO-OO

SALMO-OO is a dynamic, two-layered model that simulates the epilimnion and hypolimnion of stratified water bodies. The state variables currently simulated by SALMO-OO include orthophosphate, dissolved inorganic nitrogen, phytoplankton, zooplankton, detritus, and dissolved oxygen (Figure 1). Phytoplankton is further divided into three state variables for the simulation of three functional groups: blue-green algae (e.g. *Oscillatoria redekei*), diatoms (e.g. *Asterionella Formosa*) and green algae (e.g. *Scenedesmus quadricauda*). The zooplankton state variable represents herbivorous zooplankton only (e.g. *Daphnia galeata*). Fish and predatory zooplankton are considered indirectly by incorporating their influence on the zooplankton mortality rate. Each of the state variables are described by an ordinary differential equation, which is solved by the fourth order Runge-Kutta method. The model uses daily time steps.

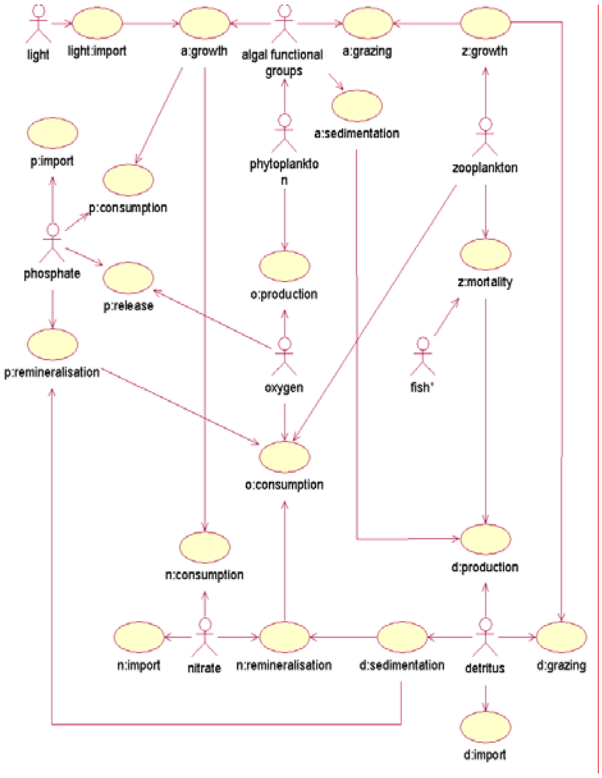

Figure 1. SALMO-OO model structure, including the state variables and corresponding processes simulated by the model.

The majority of the model structure has been generalised as much as possible. Through rigorous and multiple sensitivity analyses using data from a range of conditions, all parameters values are kept constant for all simulations (Recknagel, 1989). The model includes several driving variables, which require time-series data to define important environmental conditions. These include incident solar radiation (J cm^{-2} d^{-1}), water temperature of mixed and stratified layers (°C), external nutrient loads (g Nm^{-3}, mg P m^{-3}), water inflow and outflow from mixed and stratified layers (m^3 d^{-1}), mean and maximum water depth (m) and water body volume (m^3).

2.2. Selection and Analysis of Phytoplankton Growth Literature Models

The development of the SALMO-OO simulation library required an extensive search of the scientific literature for models describing phytoplankton dynamics in aquatic environments. The initial focus was on phytoplankton models that were of the form of ordinary differential equations (ODEs). Those papers that provided sufficient documentation to reproduce phytoplankton dynamics in simulation software were selected for initial experimentation. This eliminated many specific models from being considered, however the overlap between model structures and formulisations ensured that many approaches were well represented. The data that was used for the review and testing of alternative models was from Saidenbach Reservoir (mesotrophic) and Bautzen Reservoir (hypereutrophic), Germany.

In order to review and test many alternative phytoplankton growth models, a simple testing framework was established using the visual simulation software STELLA v 6.0.1. This included the development of a series of phytoplankton ODEs to represent three functional groups of algae (blue-greens, green algae and diatoms). Each functional group had the same model structure and only the parameter values were distinctive. The grazing process was simplified and standardised for all models tested. Zooplankton and phosphate measured data was used to drive the model, rather than using simulated state variables. Water temperature, solar radiation and mixing depth were additional driving variables included as measured data specific to each database tested.

Each growth model, that is photosynthesis and respiration, was tested within this framework, with the output being the phytoplankton biomass (cm^3/m^3). This was compared to the phytoplankton biomass produced by the SALMO growth function and phytoplankton measured data. Those models that displayed a similar model rationale and performed comparably with the original SALMO were implemented in the full object-oriented version of the model (SALMO-OO).

2.3. Implementation of the Process-based Simulation Library in SALMO-OO

From the experiments undertaken within the testing frameworks four models for phytoplankton growth were included within the complete SALMO-OO simulation library. Using Java a new class was created following the object-oriented design format established for SALMO-OO. `SalmoLibrary.class` contains methods and fields for each new phytoplankton growth model, thereby, reducing the need to change code within the original model, and not compromise its structural integrity. Each growth model can be inserted into SALMO-OO and replace the original growth functions. Combinations of SALMO-OO and different growth models were then tested to determine how they might affect the structure of SALMO-OO and how effectively the measured data was simulated. Regression analysis was performed to compare the effectiveness of each modelling experiment in describing the measured data.

3. RESULTS AND DISCUSSION

The results discussed within this paper will focus on the outputs from the SALMO-OO model and subsequent improvements made by two growth models from the simulation library. Table 1 gives an outline of the growth process equations (equations 1–10) and parameter values used in the SALMO-OO model, designated as SALMO-OO 1. SALMO-OO 2 refers to the change in parameter values only and applied to the same structure as SALMO-OO 1. The parameter values have been taken from the growth model of Hongping and Jianyi (2002). SALMO-OO 3 refers to a case study from the simulation library, where a growth model (equations 11–17) from Arhonditsis and Brett (*in press*) is used to replace the growth process equations in SALMO-OO and run with the same parameters as given by SALMO-OO 2 (Table 1).

3.1. Improvement of Original SALMO-OO

The original SALMO model was developed using the FORTRAN programming language (Recknagel and Benndorf, 1982). Since its initial development in the 1980s the main problems associated with the model have been with its lack of flexibility and problems with maintenance and testing. Adoption of the object-oriented modelling paradigm has addressed many of these problems. Modularisation of the models structure has allowed more flexibility for adapting or introducing new model components, and Java's web capabilities have improved the models accessibility. The technical details of the object-oriented version of SALMO-OO will be discussed elsewhere in a future paper.

Figure 2 shows the results obtained by the three case studies simulated by SALMO-OO for two trophically different lakes. Figure 2a refers to results achieved using Bautzen Reservoir data, a hypereutrophic system and Figure 2b refers to results achieved using Saidenbach Reservoir data, a mesotrophic system.

The original SALMO-OO model (SALMO-OO 1 in Table 1) produces a good description of the Bautzen measured data for phytoplankton biomass (Figure 2a). The magnitude of the measured data

Table 1. Description of three case studies examined by SALMO-OO, outlining differences between equations for phytoplankton growth and respiration, change in parameter values, parameter definitions and references. Each case study corresponds to the results in Figure 2.

SALMO-OO: 1 Original Parameters and Functions

$$GROWTH = (PHOTX - RX)*X \qquad (1)$$

$$PHOTX = f(I)*f(T)*f(P)*f(N) \qquad (2)$$

$$f(I) = \frac{IREDZ}{(KI + IREDZ)} \qquad (3)$$

$$IREDZ = IRED*exp(-EPS*z) \qquad (4)$$

$$f\,(\mathrm{T}) = \frac{(PHOTXMAX\text{ - }PHOTXMIN)}{TOPTX*T\ +\ PHOTXMIN} \qquad (5)$$

$$\begin{array}{l} f\,(\mathrm{NS}) = f\,(\mathrm{P}) \text{ for N/P} \geq 0.0072 \\ f\,(\mathrm{NS}) = f\,(\mathrm{N}) \text{ for N/P} \leq 0.0072 \end{array} \qquad (6)$$

$$f\,(\mathrm{P}) = \mathrm{P/X/}(\mathrm{KP/KXP} + \mathrm{P/KXP} + \mathrm{KP/X} + \mathrm{P/X}) \qquad (7)$$

$$f\,(\mathrm{N}) = \mathrm{N/X/}(\mathrm{KN/KXN} + \mathrm{N/KXN} + \mathrm{KN/X} + \mathrm{N/X}) \qquad (8)$$

$$RXT = (RXTOPT - 0.02)/\,TOPTX*T*0.02 \qquad (9)$$

$$RX = RXT + 0.3*PHOTX \qquad (10)$$

	Diatoms	*Green Algae*	*Blue-Greens*	
PHOTXMAX	1.8	3.5	1.7	Maximum photosynthesis rate (d^{-1})
KP	1.7	9.5	1.7	Half-saturation constant for P uptake by algae ($mg\ m^{-3}$)
VS	0.1	0.1	0.05	Phytoplankton settling velocity (m)
TOPTX	20	25	25	Optimum temperature for phytoplankton growth (°C)
PF	0.3	1.0	0.3	Preference factor for each algae functional group (-)

SALMO-OO: 2 Updated Parameters from Hongping and Jianyi (2002) and Original Functions (described above)

	Diatoms	*Green Algae*	*Blue-Greens*	
PHOTXMAX	2.37	3.3	2.37	Maximum photosynthesis rate (d^{-1})
KP	18	16	27	Half-saturation constant for P uptake by algae ($mg\ m^{-3}$)
VS	0.017	0.016	0.025	Phytoplankton settling velocity (m)
TOPTX	21	23	30	Optimum temperature for phytoplankton growth (°C)
PF	1.0	1.0	0.3	Preference factor for each algae functional group (-)

SALMO-OO: 3 Replaced Equations from SALMO-OO with Growth Model from Arhonditsis and Brett (2005) and Updated Parameters from SALMO-OO 2

$$GROWTH = (PHOTX - RX)*X \qquad (11)$$

$$PHOTX = PHOTXMAX*f(I)*f(T)*f(P)*f(N) \qquad (12)$$

$$f(I) = \frac{2.718*FP}{EPS*z}*\left[\begin{array}{l} exp\left(\begin{array}{l} -\dfrac{I}{Is*FP}* \\ exp(-EPS*z) \end{array}\right) - \\ exp\left(-\dfrac{I}{Is*FP}\right) \end{array}\right] \qquad (13)$$

$$\begin{array}{l} f\,(\mathrm{T}) = \exp\left(\text{- }2.3*\left(\dfrac{\mathrm{T\text{ - }TOPTX}}{T\,max - TOPTX}\right)^2\right) \text{ for T} \geq \text{TOPTX} \\ f\,(\mathrm{T}) = \exp\left(\text{- }2.3*\left(\dfrac{\mathrm{T\text{ - }TOPTX}}{T\,min - TOPTX}\right)^2\right) \text{ for T} \leq \text{TOPTX} \end{array} \qquad (14)$$

$$f(P) = \frac{P}{KP + P} \qquad (15)$$

$$f(N) = \frac{N}{KN + N} \qquad (16)$$

$$RX = RO*exp(0.09*T) \qquad (17)$$

EPS	Total extinction coefficient of light	*RO*	Constant phytoplankton respiration rate (d^{-1})
FP	Photoperiod (d^{-1})	*RX*	Phytoplankton respiration rate (d^{-1})
IRED	I reduced by reflexion ($J\ cm^2\ d^{-1}$)	*RXT*	Basis respiration of phytoplankton (d^{-1})
IREDZ	Photosynthetic active light integrated with depth (z) ($J\ cm^2\ d^{-1}$)	*RXTOPT*	RXT at optimum temperature for growth (d^{-1})
KI	Half-saturation constant of light absorbance by phytoplankton during photosynthesis ($J\ cm^2\ d^{-1}$)	*T* *Tmin*	Water temperature (°C) Minimum temperature for growth (°C)
KN	Half-saturation constant for N uptake by algae ($g\ m^{-3}$)	*Tmax*	Maximum temperature for growth (°C)
KXN	Half-saturation constant of the inverse relationship between photosynthesis and algae biomass limited by N ($g\ m^{-3}$)	*X* *z*	Phytoplankton biomass ($cm^{-3}\ m^{-3}$) Depth of layer (m)
P	Dissolved inorganic phosphorous ($mg\ m^{-3}$)	$f(I)$	Function for light (I) limited growth
PHOTX	Photosynthesis rate of phytoplankton (d^{-1})	$f(NS)$	Function for nutrient (NS) limited growth
PHOTXMIN	Minimum photosynthesis rate (d^{-1})	*Is*	Saturated light intensity ($J\ cm^2\ d^{-1}$)

was well simulated, however, the timing of spring algal growth was not simulated until early summer.

The r^2 value for the total algae biomass is very low ($r^2 = 0.03$), which may be caused by the time lag produced by the original growth equations. Improvement in this area would yield a better fit to the measured data and a higher r^2 value. Simulation of zooplankton biomass and phosphate concentration yielded excellent r^2 values which gives confidence in the original structure of SALMO-OO for these state variables. The greatest area of concern is that the algal functional groups simulated by the model do not reflect a hypereutrophic system (Reynolds, 1984), as blue-green algae are the least dominant functional group and do not contribute much to the total biomass (Figure 2a).

A similar condition occurs when SALMO-OO is applied to Saidenbach Reservoir data (Figure 2b). In this case blue-green algae are far more dominant then would be expected of a mesotrophic system (Reynolds, 1984). The simulation of phytoplankton biomass and phosphate concentration for Saidenbach is poor, with very low r^2 values ($r^2 = 0.01$ and $r^2 = 0.08$ respectively). Simulations of zooplankton biomass is good, but produce a less confident result then for Bautzen simulations (Figure 2a).

Significant improvements were made to the original SALMO-OO model by simply changing key parameter values within the growth model. During the testing of the SALMO-OO simulation library it was found that the growth model taken from Hongping and Jianyi (2002) was very similar in rationale to the original SALMO-OO model. Experiments with these parameter values yielded a more desirable result for SALMO-OO, whilst still keeping the same structure (Figure 2). Five parameters were changed, the most notable were the maximum growth rate (*PHOTXMAX*), half-saturation constant for P uptake (*KP*) and the preference factor (*PF*) values for zooplankton grazing (Table 1).

Due to these changes, phytoplankton biomass simulations were improved slightly, with an increase in the spring peak abundance and improved dynamics during summer. The zooplankton biomass and phosphate concentration simulations produced similar outcomes to the SALMO-OO 1 results. The main improvement in these results was the shift in seasonality of the algal functional groups. Blue-green algae abundances are much greater in summer then in previous simulations, with high green algae abundances in spring and very low diatom abundances throughout the year (Figure 2a).

The same parameter changes were used for Saidenbach simulations, and produced a considerable improvement to the previous results. The algal biomass was significantly lowered providing a better fit to the measured data, although the spring peak is still somewhat low. This has also caused zooplankton biomass to be better simulated in timing and magnitude. However, the phosphate concentration has increased, especially after summer, which is most likely due to the decrease in algae biomass (Figure 2b). The improvement in the seasonality of the algal functional groups has also occurred, with a higher abundance of green algae, and a much lower abundance of blue-greens. Diatom biomass still remains very low (Figure 2b).

The original SALMO model was developed as a generic model, where the constant parameters for all state variables are kept fixed for all simulations. The new SALMO-OO model aims to maintain this approach. By applying these new parameter values it can be shown that not only improvements to the original model can be made, but these changes and improvements can be carried on to simulate other databases of different trophic states. This demonstrates the generality and improved applicability of SALMO-OO to the simulation of different freshwater environments.

3.2 Contribution of the Simulation Library to SALMO-OO

The final case study presented involves experiments with the simulation library (SALMO-OO 3 in Table 1). Exchanging the growth process functions from Arhonditsis and Brett (2005) with the original SALMO-OO growth functions has produced encouraging results (Figure 2). SALMO-OO 3 produced a slightly different seasonal dynamic for algae biomass. This growth model more closely simulated the spring peak, with a distinct shift in the main peak closer to the timing of the measured data. Also, the magnitude of algae biomass during autumn is much lower then SALMO-OO 2 and closer to the magnitude of the measured data, with an improved r^2 value for total algae (Figure 2a).

Simulations of zooplankton biomass with SALMO-OO 3 were greatly improved, with the highest r^2 value achieved ($r^2 = 0.73$). The phosphate concentration has increased, particularly

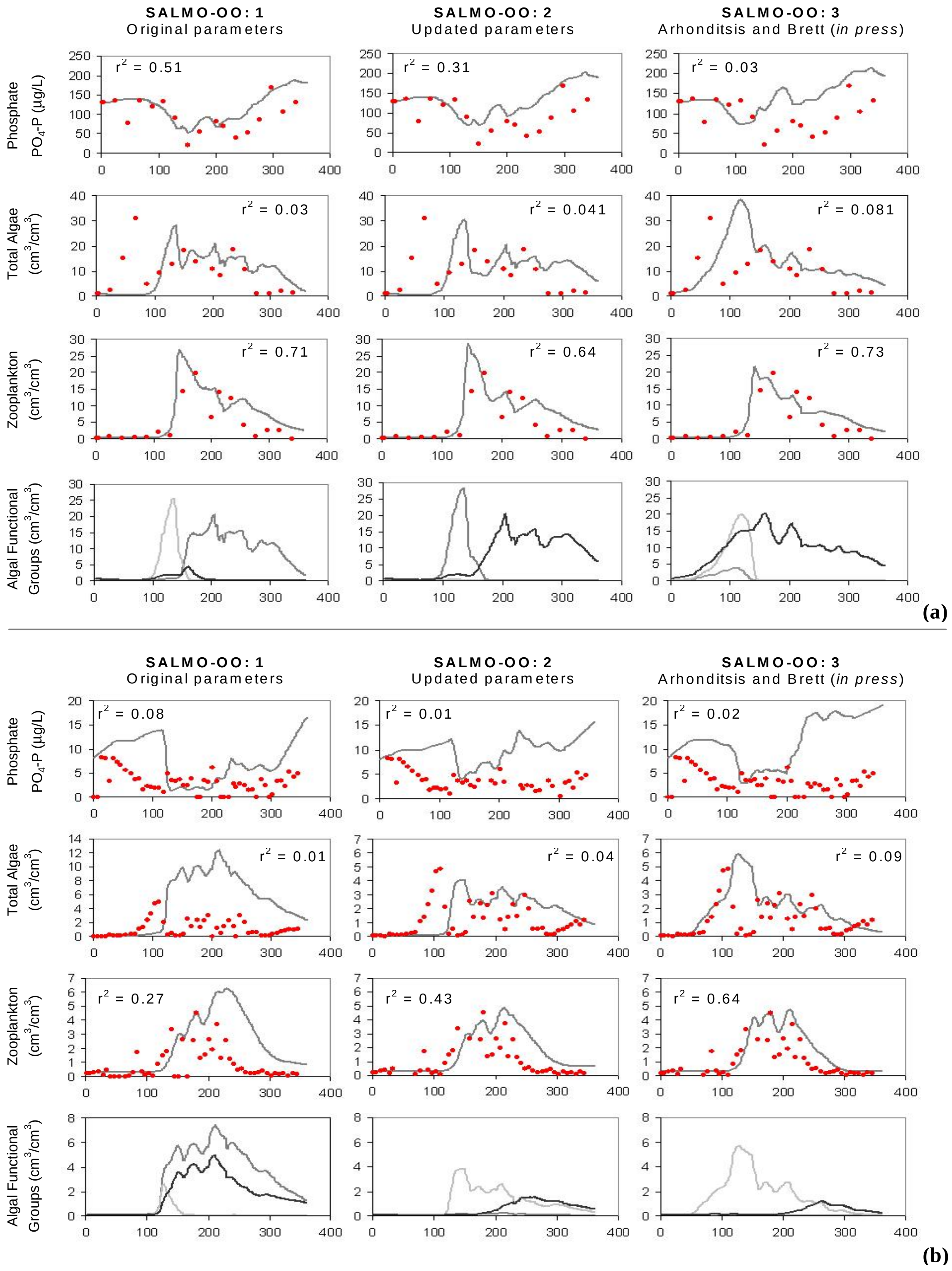

Figure 2. Results from SALMO-OO for three case studies using Bautzen (a) and Saidenbach (b) Reservoir data. X-axis is time in days. Grey lines represent simulated results and the red dots represent the corresponding measured data. For algal functional group graphs: pale grey = Green algae; medium grey = Diatoms; dark grey = Blue-green algae.

during late summer and autumn. As a consequence, the r^2 value has decreased significantly from previous simulations (Figure 2). This may be caused by the lower algal abundances present during these periods, falling off more sharply during autumn then previous simulations (Figure 2b). An improvement has been made to the simulations of the algal functional groups. Blue-green algae are more dominant in abundance then the other functional groups especially during late spring through to autumn. Green algae are less abundant and diatoms have increased compared to simulations from SALMO-OO 2, giving a more realistic description of algal seasonal dynamics.

SALMO-OO 3 has made a significant improvement for simulations of Saidenbach Reservoir data. The trajectories of algae biomass fit the trends in measured data much better then previous experiments with SALMO-OO. The timing and magnitude of the spring peak is simulated well by SALMO-OO 3, producing a slightly improved r^2 value ($r^2 = 0.09$). Zooplankton biomass predictions have improved considerably with the highest r^2 value ($r^2 = 0.64$) produced for the Saidenbach dataset. The seasonality of functional group simulations has changed little compared to SALMO-OO 2, however, green algae dominance is higher then in SALMO-OO 2, contributing more to the total algal biomass, which may describe mesotrophic conditions more effectively.

However, due to the lower abundance of algae biomass in late summer and autumn the phosphate concentration has dramatically increased above the trend exhibited by the measured data, producing a poor r^2 value ($r^2 = 0.02$). It seems that SALMO-OO is unable to simulate the phosphate dynamics in mesotrophic systems as effectively as for eutrophic systems (Figure 2a). Even with the addition of the simulation library, no alternative models have improved this result. This may well indicate the need for a branch within the simulation library for different process models for phosphate dynamics to improve the quantitative results.

4. CONCLUSIONS

Using object-oriented modelling techniques has greatly improved the flexibility of SALMO-OO and has produced a model that is resilient, extendable and reusable. The object-oriented paradigm is well suited to modelling ecological processes as ecological simulations are largely concerned with the way entities interact with each other and their environment. Object-oriented models emulate a natural ecosystem more realistically than models developed as a collection of procedures and routines acting on data, as is the case with conventional programming methods (Sequeira et al., 1997).

The inclusion of a simulation library of alternative phytoplankton growth models has achieved some encouraging results. From these first experiments it appears that the simulation library provides alternative functions that can improve simulations of mesotrophic systems. The library can also give a more detailed understanding of such complex environments through exploring model structure.

The simulation library has also identified areas within the model that need to be improved or expanded upon. Current work is now focused upon the testing of phytoplankton grazing process models, where preliminary results have been promising. This addition may be useful for food web management scenarios.

Another area of focus is the application of multiple parameter optimisation based on evolutionary algorithms. These algorithms will calibrate parameter values within their range of variance for individual lakes in order to improve the accuracy of simulation results. Thus it is expected that a better fit to the measured data, particularly for algal biomass, will be produced. The ability of SALMO-OO to maintain its generic attributes through the simulation library has greatly enhanced the models applicability to a variety of different lake conditions. The options offered by SALMO-OO such as scenario analysis of different management strategies and the simulation library will provide decision-makers with a diversified tool for management of freshwater systems.

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