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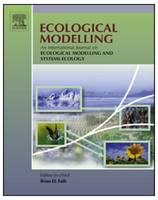

The power of hybrid modelling: An example from aquatic ecosystems

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ABSTRACT

Planktonic communities in ponds and lakes show a high annual dynamic controlled by biotic interactions, nutrients and weather. In recent years, there has been an increase in demand for realistic and accurate lake models to improve ecological management of water bodies and to answer ecotoxicological questions in aquatic risk assessment. Most existing aquatic models are either ecosystem models aimed at describing the overall ecosystem dynamics, but which are incapable of including individual life-cycles and plasticity, or very detailed and realistic individual-based models lacking an appropriate level of environmental complexity. To reconcile these concepts, we present here a modelling approach using an individual-based population model (IBM), integrated within an ecosystem lake model, to link responses at the individual and population levels. We combine an IBM for *Daphnia magna* (IDamP) and a complex biogeochemical lake model (StoLaM), to create the DaLaM (*Daphnia* Lake Model). We use DaLaM to predict population dynamics of *D. magna* and phytoplankton within a simplified, daphnid-dominated food web under field conditions. In DaLaM, relevant variable environmental conditions such as underwater light climate, water temperature, turbulence, and nutrient availability are realistically simulated forced by weather conditions. For model testing we used data from aquatic mesocosm field studies exhibiting variable nutrient and weather conditions and lasting from several months to 2 years. DaLaM gave improved predictions of the overall population patterns of daphnids and phytoplankton in the mesocosms in contrast to its separate submodels. This study is an example of successfully merging individual-based population models with dynamic ecosystem models utilising the accuracy of the former and the dynamic environment of the latter to simulate more realistic field populations.

1. Introduction

In recent years, there has been an increase in demand for realistic and accurate lake models, which are able to address anthropogenic stress factors such as eutrophication and ecotoxicologically relevant pollution, for use in lake management (Jørgensen, 2010; Mooij et al., 2010) and ecotoxicological risk assessment (Galic et al., 2010). Aquatic ecosystems are regulated by a multitude of biological interactions occurring between different trophic levels, known as bottom-up and top-down processes (McQueen et al., 1989). Among these processes, the interactions between primary producers and zooplankton grazers are key processes in pelagic freshwater food webs (Perhar et al., 2013; Persson et al., 2007; Zhao et al., 2008). Modelling these fundamental interactions requires knowledge about relevant factors such as weather conditions and nutrient dynamics controlling phytoplankton biomass and species-specific dynamics of the grazing population.

Several models integrating hydrodynamics and ecological processes have been developed (Jørgensen, 2010) to account for the dynamic physical properties of lakes (e.g., temperature, light and turbulence in the water column) and their variation with meteorological forces (e.g., Bruce et al., 2006; Mooij et al., 2010; Zhao et al., 2008).

In aquatic ecosystem models, nutrient dependency of primary and secondary producers is often described by detailed nutrient cycles (Mooij et al., 2010). Model realism can additionally

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be improved by integrating the concept of ecological stoichiometry (Sterner and Elser, 2002), which deals with the relative ratio of carbon and multiple chemical elements (mostly nitrogen and phosphorus) in food web interactions (Elser and Urabe, 1999). The stoichiometric concept distinguishes between mostly homeostatically regulated consumers and autotrophic organisms with variable nutrient content due to their ability for nutrient storage (Sterner and Elser, 2002). Constant C:N:P stoichiometry of herbivorous organisms can be maintained only by modifying their growth corresponding to the most constraining element in the diet as per Liebig's "law of the minimum" (Andersen et al., 2004). Phytoplankton as autotrophic organisms often have lower nutrient contents compared to the needs of herbivorous consumers (Sterner and Elser, 2002), frequently leading to an imbalance in the C:N:P stoichiometry between food and consumers. This can affect the population dynamics of consumers, e.g. a direct limitation of the growth rates of herbivorous organisms by the lack of nutrients (Urabe and Watanabe, 1992). In addition, the rate of consumer-driven nutrient recycling via excretion of surplus nutrients influences the nutrient content and growth of phytoplankton. Sterner and Elser (2002) pointed out that a combination of predator-prey interactions with biogeochemical-controlled conditions in explicit stoichiometric models leads to a more realistic representation of these processes. Both food quantity and food quality for herbivore consumers have a significant impact on the development of zooplankton and phytoplankton populations.

Although the dynamic carbon-nutrient stoichiometry of algae has long been known (e.g. Droop, 1974), the ecological stoichiometry for higher trophic levels has been rarely taken into account in complex ecosystem models (Jørgensen, 2010; Persson et al., 1999). In several simple strategic models, stoichiometric principles were considered for algae-herbivore interactions (e.g., Andersen, 1997; Diehl, 2007; Hessen and Bjerkeng, 1997; Loladze et al., 2000; Touratier et al., 2001), whereas only few lake models integrated stoichiometric principles (e.g., Perhar et al., 2013; Strauss, 2009; Zhao et al., 2008).

So while ecosystem models deal with nutrient dependencies and cycles, they ignore variability between individuals and adaptive strategies which can be very important for ecosystem dynamics (e.g. Grimm and Railsback, 2005). In contrast, individual-based population models (IBMs) have the potential to simulate the variability between individuals of the same population in terms of life history characteristics and how they change with environmental properties and adaption to different conditions (e.g. food availability, predation, temperature; Forbes et al., 2008; Preuss et al., 2009). The population properties in the IBMs (e.g., abundance, population growth rate, and age/size structure) emerge directly from the interaction of individuals with each other and their environment (Forbes et al., 2008; Grimm and Railsback, 2005). While the density dependence of interspecific interactions is already an important component of ecosystem models with unstructured populations, intraspecific effects such as crowding (Gergs et al., 2014; Preuss et al., 2009) or cannibalism (Strauss et al., 2016) as well as size selective predation (e.g. Gergs et al., 2013) can only be represented by structured population models. Life processes and food web interactions often vary depending on age, size, or developmental stage of the particular species. Among the structured population models, individual-based population models typically have the highest resolution in these properties, and are able to describe the population structure with respect to all these different properties simultaneously, based on tracking of each individual within a population (Cao et al., 2016). IBMs are particularly well-suited when ecotoxicological effect models such as toxicokinetic-toxicodynamic models are coupled with population models, since they can both simulate the individual accumulation of a toxin over time and are able to take into consideration different size-specific sensitivities (Gergs et al., 2015).

Hybrid modelling is a promising approach that integrates models with different scales and organisational levels to extend the questions a single model can deal with (Breckling et al., 2005). On the one hand, IBMs increase the potential of ecological models to describe complex interactions more precisely (Breckling et al., 2005), and on the other hand, ecosystem models can provide a more realistic environment for the individual-based population models. First examples of coupling IBMs to aquatic ecosystem models acting as dynamic environments are given in (Batchelder et al. (2002), vertical migration of copepods in marine upwelling systems) and (Makler-Pick et al. (2011), fish impact on lake food webs).

In this study we emphasized the realism of the modelled physical lake properties, the stoichiometric interactions within the food web, and the advantages of individual-based modelling of a grazer population, in providing realistic predictions of *Daphnia* population dynamics in the field. For this purpose we coupled two existing process-based ecological models: an individual-based population model for *Daphnia magna* (IDamP; Preuss et al., 2009) and a complex stoichiometric biogeochemical lake model (StoLaM; Strauss, 2009). The combination of both models is called DaLaM (*Daphnia* Lake Model) and is used in the present study to predict population dynamics of *D. magna* and phytoplankton in outdoor ponds under realistic weather and nutrient field conditions.

Our aim is to explore the feasibility of connecting IBMs to ecosystem models, and to see whether the predictive power of such hybrid models has been increased relative to the separate models, for extrapolating from individual-level endpoints observed in laboratory tests to populations-level responses in the field. To this end, we compared the use of structured and unstructured population models for *Daphnia* within an ecosystem model framework under similar conditions with reduced food web complexity.

2. Material and methods

2.1. Model description

DaLaM was constructed by combining the two existing, mechanistic models: IDamP and StoLaM. The model description follows the rationale of the ODD protocol (Grimm et al., 2006, 2010), but due to reasons of space limitation only a summary description of the most important elements is given in this chapter. A full ODD description of IDamP as well as a detailed description of StoLaM is provided in the Supplementary Information S1.

2.1.1. Purpose

The purpose of the DaLaM model is to predict population dynamics of *D. magna* under realistic and dynamic environmental field conditions, by considering algal growth in relation to nutrient resource dynamics as well as variable temperature and light conditions. The focus of developing DaLaM was not to include all the food web complexity of real ecosystems, but to capture their essential components relevant for a daphnid-dominated planktonic ecosystem while keeping the model robust and tractable.

The simulated environmental scenario in this paper is as follows: The type of waterbody is represented by aquatic mesocosms without inflow; the trophic state is mesotrophic to eutrophic depending on the sediment phosphorus release rates, and the weather conditions in Aachen, Germany, were used.

2.1.2. Entities, state variables and scales

A flow chart describing the relations between the individual submodels within DaLaM is shown in Fig. 1.

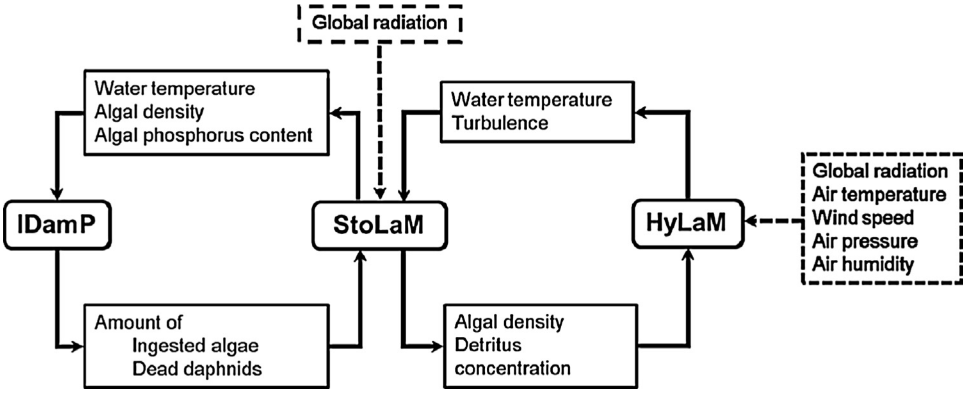

Fig. 1. Relations between the submodels IDamP and StoLaM (including the hydrodynamic module HyLaM) within DaLaM. The submodels are indicated in rounded rectangles, and the simulated variables, which are transferred to the respective interfaces, in square boxes. Dashed arrows indicate the impact of dynamic forcing variables (weather conditions).

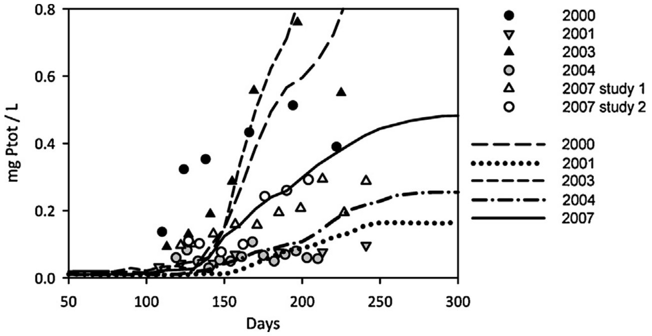

Fig. 2. Simulated and measured total phosphorus dynamics in the mesocosms (study B, 2000–2007). Symbols indicate the measured data for the different years and lines the model simulations. In 2007, two studies (study 1 and 2) were available.

2.1.2.1. The lake model StoLaM and food web structure. StoLaM (Strauss, 2009) is a biogeochemical and ecological lake model that predicts nutrient cycling, plankton succession of several zooplankton and phytoplankton taxa, and water quality in standing waters. In DaLaM, StoLaM describes the dynamic environmental and food conditions for the modelled *Daphnia* populations.

Within StoLaM, a one-dimensional vertical structured hydrodynamic module (HyLaM) allows high resolution of the lake internal physical environment which is required for simulating the nutrient and plankton dynamics in detail. Temperature determines the speed of many biological and chemical processes. In order to accurately predict ecosystem dynamics it is essential to also predict water temperature data precisely. However, most readily available weather data comes from meteorological weather stations, with which HyLaM (Strauss, 2009) is able to simulate water temperature in the water column and sediment as well as vertical turbulence. The ecological part of StoLaM simulates the under-water light climate, the dissolved nutrient dynamics in the water, algal growth and biomass, the phosphorus and nitrogen cell quota in the algae, and detritus dynamics (Figs. 1 and 2 in the Supplementary Information S1). In the present study, only phosphorus is considered as nutrient for algae and *Daphnia*, assuming that nitrogen was not limiting the phytoplankton development in the simulated mesocosm case studies, which are aimed at water bodies in agricultural areas typically rich in nitrogen. Thus, algal growth depends on water temperature, light conditions and the internal cell quota of phosphorus. The carrying capacity of the phytoplankton population is determined by the phosphorus availability, and the stoichiometric constraints are based on the C (expressed as wet weight):P ratio.

For this study, the food web implemented in StoLaM was reduced to only one phytoplankton species, green alga *Desmodesmus subspicatus*. The zooplankton is only represented by the individual-based *Daphnia magna* population model (IDamP) for the cladoceran species *D. magna* (Fig. 2 in the Supplementary Information S1). The models for both organisms were previously validated at the population level with laboratory data (Preuss et al., 2009; Section 5 in the Supplementary Information S1).

2.1.2.2. The IDamP model. The population dynamics of *D. magna* is modelled using the IDamP model. IDamP is an individual-based population model (IBM) that predicts *D. magna* population dynamics from life-history characteristics observed in laboratory experiments with different feeding conditions and temperatures. IDamP is structured in three ecologically relevant hierarchical levels – individual, population and ecosystem – represented by three corresponding objects in the IDamP. The state variables in IDamP are defined on the individual level (Preuss et al., 2009). Each individual daphnid is modelled by its life-cycle, and is characterized by its actual filtration rate, body size, spent juvenile development and lifetime. Reproduction is calculated by the brood size and the spent embryo-development (see Preuss et al., 2009). At the population level, IDamP counts the total number of individuals and the number of dead and newborn organisms per day. In addition, the number of organisms per age or size class is calculated. On the ecosystem level, the exchange of environmental state variables such as phytoplankton density and phosphorus content as well as water temperature between IDamP and the StoLaM model was implemented (Fig. 1).

2.1.2.3. Temporal and spatial scales. The simulation time step used in StoLaM and HyLaM is five minutes. IDamP is synchronized to StoLaM using the same time step of five minutes for the filter feeding of the daphnids and the resulting change in algal biomass and phosphorus concentration in the water. However, the properties of the *Daphnia* population are updated within the IDamP model on an hourly basis. The water volume in IDamP was adjusted to ten litres. Higher volumes do not change the results, whereas lower volumes increase the risk of stochastic extinction of the population. In this study, the vertical structure in DaLaM is divided into two equal vertical layers, which is the minimum number required for the hydrodynamic module. A total water depth of 1 m was used, and the daphnids were assumed to be homogenously distributed in the simulated pond.

2.1.3. Process overview and scheduling

HyLaM simulates the water temperature and turbulence from measured weather data (i.e. standard meteorological data) depending on the turbidity of the water column. StoLaM simulates the under-water light conditions for the phytoplankton growth, the

Table 1
Start values of the state variables (StoLaM) and population properties (IDamP).

Submodel	Description	Value	Unit
StoLaM	Dissolved inorganic phosphorus (*ortho*-Phosphate)	(based on the specific experimental scenario)	mg P L^{-1}
	Dissolved organic phosphorus (DOP)	0.01	mg P L^{-1}
	Detritus biomass	0	mg wet weight L^{-1}
	Detrital phosphorus	0	mg P L^{-1}
	Phytoplankton biomass	0.9	mg wet weight L^{-1}
	Phosphorus cell quota of algae	0.001	mg P mg wet weight^{-1}
HyLaM	Water temperature	4	°C
IDamP[a]	Number of daphnids	11	–
	Size range of the daphnids	0.8 ± 0.2	mm

[a] for the complete list of state variables see Preuss et al. (2009).

nutrient release from the sediment and the phytoplankton development, which is controlled by these environmental factors.

In IDamP, the following processes are executed in this order: First the feeding of the individual daphnids is calculated in dependence of the algal concentration and water temperature delivered by StoLaM. Then, the available water volume per daphnid (the reciprocal of the density) is calculated so that the effect of crowding can be accounted for. Each daphnid undergoes its life-cycle processes, which depend on the ingested amount of algal cells (determined as a function of temperature fluctuations and phytoplankton density), the algal phosphorus content and the water volume per daphnid. Finally, dead daphnids are subtracted from the population and new-borns are added to the population.

In DaLaM, the independent models StoLaM and IDamP exchange information with each other at every time step (Fig. 1). First StoLaM delivers the water temperature as well as the algal biomass and its phosphorus content to IDamP, which simulates the change in *Daphnia* abundance and size structure. During this step, it is calculated whether a phosphorus limitation of the daphnid's growth by phosphorus-depleted food occurs. Afterwards, IDamP returns the biomass of dead and alive daphnids to StoLaM together with the total amount of ingested algae.

In StoLaM, the ingested algae are subsequently subtracted from the algae biomass. The re-excretion of surplus phosphorus of ingested algae by daphnids is then calculated based on the phosphorus content of ingested algae and daphnids, and dead daphnids are added to the detritus pool.

2.1.4. Design concepts

2.1.4.1. Basic principles. In the hybrid model DaLaM, we followed a modular approach: A hydrodynamic-ecological lake model is combined with an IBM for daphnids. Additionally, DaLaM integrates the principles of ecological stoichiometry, which means the changing ratios of nutrients such as phosphorus and nitrogen within the food web and their impact on the growth rates of plankton organisms with respect to nutrient recycling and limitation.

2.1.4.2. Emergence. In DaLaM the predicted population dynamics of the daphnids emerge from the development of individual daphnids, which interact with each other and their environment. The dynamic aspect of the environment in DaLaM is the result of linking the individual based model and the lake model, leading to dynamic algal availability and quality for the daphnids, which in turn results from nutrient dependency, climatic conditions and grazing pressure.

2.1.4.3. Adaptation. The modelled daphnids adapt their life-cycle processes in relation to the ingested algae and the population density, calculated as volume per daphnid. It is known that juvenile development, embryo development, brood size and mortality are affected under crowded conditions (Goser and Ratte, 1994). This "crowding" effect is defined as a density-dependent mechanism due to chemical substances released by the organisms or direct physical contact between the organisms, but independent of food competition (Goser and Ratte, 1994). Crowding is explicitly included in the model: If the volume per daphnid drops below a specific threshold, juvenile and embryo development are slowed down and the brood size is reduced depending on the volume per daphnid and the current food concentration. Similarly, the remaining lifetime decreases if the volume per daphnid falls below a specific threshold (Preuss et al., 2009). Crowding takes place if high *Daphnia* densities result in a volume per daphnid below 50 ml, corresponding to a population density of 20 organisms/L (Preuss et al., 2009).

2.1.4.4. Sensing. The environmental factors sensed by the individual daphnids are the available space, calculated as volume per daphnid, the algal concentration in the water, the phosphorus content per algae, and water temperature.

2.1.4.5. Interaction. The only direct interaction between the individual daphnid and its environment is feeding, which also leads to intra-specific competition among the daphnids. All other processes (growth, development, reproduction, remaining lifetime) are based on the amount and quality of ingested algae and are influenced by temperature and population density.

2.1.4.6. Stochasticity. For each individual daphnid and each state variable a set of individual parameters derived from probability distributions are assigned randomly at birth (for details see Preuss et al., 2009).

2.1.4.7. Observation. For the purpose of DaLaM, the total daphnid abundance was daily counted and recorded for each simulation run. For the environmental conditions, the phytoplankton biomass and its phosphorus cell quota, the phosphate concentration and the water temperature were saved once per day.

The number of conducted Monte Carlo simulations per scenario was fifty simulations over the entire study period (900 days) for study A (a long term study conducted between 2008 and 2010; see section model testing and Fig. 4) and 100 simulations over 365 days for each year of study B (a set of 6 mesocosm pond studies, 2000–2007; see section model testing and Fig. 7). The average, minimum and maximum values of these endpoints were stored daily for all Monte Carlo simulations.

2.1.5. Initialisation

To mimic the mesocosm ponds as used in our studies, the water depth was 1 m as recommended for mesocosm studies (EFSA PPR Panel, 2013). Each simulation run started with 11 neonate daphnids of 0.8 ± 0.2 mm length (mean and standard deviation, Table 1). The simulated water volume for the daphnids was set to 10 L, which enables us to simulate the density of the daphnids down to 0.1 individuals per litre. For the interaction with the lake model the population abundance was converted to 1 L volume. For initial values of nutrient concentrations, algae biomass and water temperature, we used typical values for winter conditions in aquatic outdoor mesocosms (Table 1).

2.1.6. Input data

In DaLaM, case-specific data are needed for the morphometry of the respective water body, the turbidity of the water and the nutrient release from the sediment. Additionally, year-specific weather data with a temporal resolution of at least one hour are necessary for integrating different climatic conditions.

2.1.6.1. Turbidity of the water column. The turbidity of the water column, which influences the penetration depth of solar radiation, is a case-specific parameter needed to calculate the heat budget of the hydrodynamic model as well as the underwater light conditions for the phytoplankton growth. The light attenuation coefficient (decrease of solar radiation with increasing water depth) of the water was set to 0.3 m^{-1} in StoLaM. The additional attenuation caused by algal biomass is calculated dynamically (for details see section 2 in the Supplementary Information S1).

2.1.6.2. Phosphorus release from the sediment. Phosphorus release rate from the sediment depends on the case-specific trophic conditions and therefore varied between the mesocosm field studies due to different sediment types. To simulate the measured nutrient dynamics in mesocosm experiments, we calibrated the coefficient of the temperature-dependent phosphorus release function from aerobic sediments at 20 °C to the mesocosm field data for each mesocosm study.

For the long-term study A, we used five phosphorus release rates: 0.58, 0.61, 0.64, 0.67 and 0.70 mg P m^{-2} day^{-1} (at 20 °C) to account for the variability in phosphorus concentration in the water column.

Three types of sediments with different phosphorus sediment release rates characterized the mesocosm experiments in study B. At 20 °C, the calibrated rates used in StoLaM were 1.7 mg P m^{-2} day^{-1} (in 2001 and 2004), 3.4 mg P m^{-2} day^{-1} (in 2006 and 2007), and 10 mg P m^{-2} day^{-1} (in 2000 and 2003). Using these rates, the measured and simulated total phosphorus contents in the mesocosms at the end of June (Day 190, Fig. 2) show a good correlation with the majority of the mesocosm studies ($r^2 = 0.97$; slope = 0.98; n = 6).

2.1.6.3. Weather conditions. To get realistic and continuous simulations of the physical properties of the water body of mesocosm field studies such as underwater light conditions, turbulence and water temperature, we used data from a meteorological station at RWTH Aachen University with a temporal resolution of 10 min (Schneider and Ketzler, 2000–2010). The meteorological data required are global radiation [J cm^{-2} s^{-1}], air temperature [°C], wind speed [m s^{-1}], atmospheric pressure [hPa], and air humidity [%].

2.1.7. Submodels and interface features

IDamP and StoLaM had been previously independently developed and validated (Preuss et al., 2009; Strauss, 2009). For the coupling within DaLaM, a new interface was implemented.

2.1.7.1. Submodels. IDamP previously demonstrated its potential to predict population dynamics of *D. magna* under different food and density conditions, as well as different initial population size structures (Preuss et al., 2009). Each mechanism in the IDamP model for *D. magna* was parameterized on the individual level and tested on the population level by using laboratory data only (Preuss et al., 2009). In addition to the two forcing functions (ingested food and crowding conditions) of the IDamP model which were previously described in Preuss et al. (2009), the individual daphnids adapt their life cycle processes (somatic growth, development, reproduction and survival) in relation to temperature (details are given in Gabsi, 2014; Gabsi and Preuss, 2014) and phosphorus cell quota.

StoLaM is designed to simulate nutrient fluxes and plankton dynamics for several phytoplankton and zooplankton species as well as annual variations in abiotic conditions (e.g., temperature stratification and oxygen concentration, Strauss, 2009) in different types of lakes. Hence, StoLaM integrates the hydrodynamic lake model HyLaM (Strauss, 2009, modified after Losordo and Piedrahita, 1991). StoLaM was mostly parameterized based on independent data sets from literature and own laboratory studies (Section 2 in the Supplementary Information S1). Only a few lake-specific parameters (e.g., sediment nutrient release, light attenuation of water) had to be adjusted to the respective case studies. The full version of StoLaM was intensively tested on the ecosystem level using field data (e.g. Strauss, 2009). Additionally, the phytoplankton module in StoLaM was tested for *D. subspicatus* under laboratory conditions (section 5 in the Supplementary Information S1). A detailed description of the StoLaM model including the underlying assumptions, equations and parameter values can be found in Strauss (2009) in addition to section 2 in the Supplementary Information S1.

2.1.7.2. Interface. All simulations with DaLaM were conducted using the default parameter sets of IDamP and StoLaM without any fine-tuning or re-calibrations of the case-independent parameters. Only two lake-specific parameters, sediment phosphorus release rate at 20 °C and light attenuation in the water, needed to be adjusted as for any new study design.

StoLaM and IDamP were used without significant changes of their respective processes. However, a few extensions in model parameters and processes were made with respect to the model coupling. Firstly, the minimum water temperature in IDamP was restricted to 4 °C. This restriction was necessary because of the lack of knowledge on the physiological parameters of *Daphnia* organisms at very low temperature values (the tested temperature range in IDamP varied between 4 and 35 °C, see Gabsi, 2014). The second modification related to the amount of phytoplankton consumed by daphnids, as different experimental studies shows that daphnids cannot consume the total amount of suspended algae (see section 4 in the Supplementary Information S1). To reflect this, we implemented a minimum algal concentration of 2600 cells ml^{-1} in the DaLaM, which was not available for the modelled daphnids.

To consider the effects of phosphorus depleted algal food, a potential nutrient limitation of daphnids' growth rate was implemented in DaLaM by a phosphorus limitation factor. This factor reduces the amount of accessible food for the daphnids when the phosphorus cell quota of the algae is below the phosphorus requirements of the daphnids, which are set to 0.0032 mg P mg wet $weight^{-1}$ (details in section 3 in the Supplementary Information S1). If the algal P cell quota exceeds that of daphnids, the surplus phosphorus of ingested algae is assumed to be re-excreted by the daphnids into the water column as phosphate.

The two models calculate the amount of plankton in two different units: StoLaM uses wet weight per litre and IDamP cells per ml, which are converted in both directions at the interface of DaLaM. Also the number of daphnids of different size simulated in IDamP is converted into wet weight per litre for StoLaM (see section 3 in the Supplementary Information S1).

2.2. Model testing

The ability of DaLaM to describe the *Daphnia* population dynamics under field conditions was tested by comparing measured

Daphnia densities from aquatic mesocosm studies with the model outputs which resulted from simulations that explicitly used weather conditions and sediment characteristics from each of these respective mesocosm studies as input. Mesocosm experiments were conducted in artificial outdoor freshwater ponds at the test facilities of RWTH Aachen University and carried out between 2000 and 2010 (data in the Supplementary Information S3). The first dataset was a long-term study conducted from 2008 to 2010 without macrophytes (study A) with four replicated ponds. A second set consists of shorter studies over several months, from 2000 to 2007 (study B) with 3–4 replicated ponds each. In 2002 and 2005, the mesocosm experiments started very late in the year, therefore these data were not considered for this analysis.

Experiments performed in 2008–2010 (study A) as well as in 2000–2003 (study B) were conducted in a mesocosm facility where each pond consisted of a cylindrical glass-fibre reinforced polyester tank, and had a diameter of 2 m. The water depth at the start of the studies was adjusted to 1 m, resulting in a water volume of 3.1 m^3. In 2004–2007 (also study B), a second mesocosm test facility was used, where ponds consisted of cylindrical black PEHD (polyethylene, high density) tanks. These tanks had a diameter of 2.5 m and a water volume of 4.9 m^3. In both mesocosm set-ups, natural sediment was placed on the bottom of the tanks to a height of approximately 10 cm. The experimental mesocosms showed aerobic conditions at any time and depth.

In these mesocosm studies, three daphnid species were present in varying composition, dominated by *D. magna and D. pulex* with the occasional appearance of *D. longispina*. *D. magna* and *D. pulex* are both among the largest species of *Daphnia*, and have quite similar life histories (Gliwicz, 1990). Therefore, we compared the simulated population dynamics of *D. magna* using DaLaM with the measured total abundance of all three species sampled in the mesocosms. These experimental mesocosms were also used to validate the model predictions for phytoplankton dynamics. Data analysis of phytoplankton species' composition in the mesocosms showed that the proportion of the summer phytoplankton in average of both studies A and B (period from 2000 to 2010, analysis based on cell numbers) was often dominated by chlorophyceans (48%), followed by cryptophytes (26%), chrysophytes and diatoms (11% and 8%, respectively). The chroococcale green algal genus *Scenedesmus/Desmodesmus* constituted only 1.3% on average of the total phytoplankton species. In this paper, the simulated population dynamics of the green alga *D. subspicatus* has been compared to the measured phytoplankton community in the mesocosms in terms of total chlorophyll-a concentration despite differences in the taxonomic composition.

2.2.1. *Comparison of DaLaM with its submodels*

To analyse the benefits of using DaLaM for the population modelling of the daphnids, we compared the prediction accuracy of DaLaM (using only the IBM model IDamP for the daphnids) with its single submodels StoLaM and IDamP.

Firstly, we used a standalone version of StoLaM with an unstructured compartment population model for daphnids instead of the IDamP (Strauss, 2009; see also section 2 in the Supplementary Information S1). A conversion factor of 12.5 Ind/mg wet weight was used to estimate the number of daphnids from simulated population biomass. The same modifications that were used in the IBM model in DaLaM were also used with regard to the minimum water temperature for the daphnids (4 °C) and the filtration threshold for ingestible algae (0.15 mg ww L^{-1}), both of which are described in chapter 2.1.7.

Secondly, the standalone version of IDamP was used with a constant daily algal feeding (several scenarios between 0.03-0.5 mg C L^{-1}day^{-1} using a conversion factor for algal biomass of 0.22 mg C/mg wet weight (Siehoff et al., 2009). For both StoLaM and DaLaM, we used weather data from the years 2008–2010 (study A). For IDamP the daily mean water temperature for the same period was calculated in advance by StoLaM.

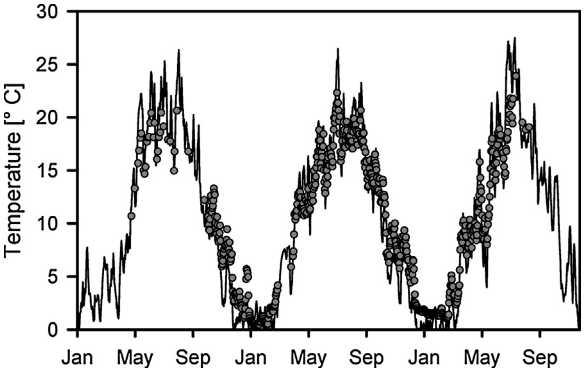

Fig. 3. Simulated and measured water temperatures in the mesocosms (2008–2010). Dots indicate the measured data and lines the simulation results.

3. Results

In the following, model predictions of *Daphnia* and phytoplankton dynamics with DaLaM are first described for the long term mesocosm study A including an analysis of phosphorus limitation and of the use of model approaches of different complexity. Afterwards in study B, we discuss the results for several shorter mesocosm experiments from different years.

3.1. *Model predictions of the long-term mesocosm experiment (study A)*

The hydrodynamic submodel HyLaM captured the observed fluctuations in water temperature dynamics during the experimental period with high precision (Fig. 3).

The measured dissolved phosphorus concentrations during 2008–2010 (Fig. 4A) increased by temperature dependent sediment release in spring and summer, reaching maximum values of 0.066 and 0.047 mg P L^{-1} at days 298 and 662 at the beginning of autumn, which were accurately predicted by the model (0.069 and 0.055 mg P L^{-1}). In early spring, it showed a subsequent decline reaching a minimum measured concentration of 0.02 mg P L^{-1} due to phytoplankton uptake. Both the timing of these fluctuations and their magnitude could be accurately simulated after calibration of the sediment-specific phosphorus release rate (Fig. 4A). The model predictions deviated from the measured data by only 12% on average (Table S2-1 in the Supplementary Information S2).

Similarly, the measured variation of chlorophyll a was predicted well (Fig. 4B) with an overall deviation between the mean measured and simulated data of 27% (Table S2-1 in the Supplementary Information S2). A peak in chlorophyll a concentration occurred during late winter and early spring in both years, followed by a drop during summers. The timings of the onset of these events (increase and subsequent drop in chlorophyll a concentration) were particularly well captured by the model (Fig. 4B) for both years. Besides, the minimum and maximum concentrations could be overall reproduced, and the model was more successful in predicting the magnitude of the first peak than the second one.

The simulated internal algal phosphorus dynamics (Fig. 4D) showed a high amplitude of variation, with maximum values reaching 0.015 mg P/wet weight in autumn. In late winter and early spring, the internal phosphorus content of algae was below the threshold for daphnids (0.0032 mg P mg wet weight^{-1}; red line in Fig. 4D), indicating that *Daphnia* growth was limited by lack of phosphorus.

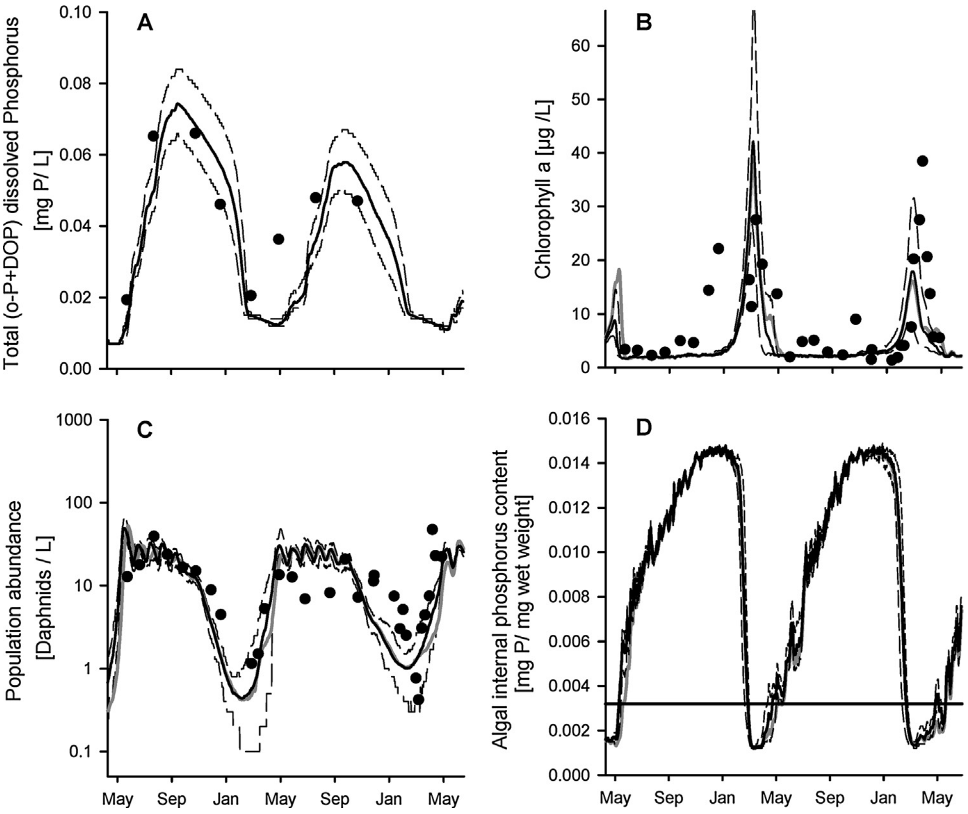

Fig. 4. Simulation results for the mesocosm study A. A, B, C: Comparison of the predicted dynamics (average of 50 Monte Carlo simulations) in the total dissolved phosphorus concentration (A), chlorophyll a (B) and *Daphnia* population size (C) with the measured data in mesocosm studies during 2008–2010. The simulations started on 01 January 2008. Dots indicate the measured data (mean of 4 replicates). Solid black lines show the simulations without P-limitation of the daphnids, the grey lines indicate simulations including P limitation. Dashed lines represent the minimum and maximum values (simulations without P-limitation).D: Simulated dynamics of the internal phosphorus content of algae. The phosphorus limitation threshold (0.0032 mg P mg wet weight^{-1}) for the daphnid's growth is indicated by the horizontal line..

Model simulations including phosphorus limitation (black line) showed a slightly delayed drop in chlorophyll a concentration in spring by 7 days (Fig. 4B). Overall, the deviations to the measured data during spring decline did not exceed 35% on average (calculated for the spring of both years).

The measured *Daphnia* population dynamics had two distinct phases: it increased in spring and then decreased again after summer to reach minimum abundances in winter. DaLaM was able to predict the variations in the *Daphnia* population size over the entire study period (Fig. 4C) with a mean deviation to the measured data of 4.7% (Table S2-1 in the Supplementary Information S2). The minimum abundance of *Daphnia* observed during late winter coincided with the peak in chlorophyll a, whereas the increase observed in *Daphnia* populations in early spring resulted in the observed drop in chlorophyll a. The model successfully predicted these different patterns for *Daphnia* abundance concomitantly to chlorophyll a concentration. Not only the timing of increase in the population size was successfully captured by the model but also its magnitude (maximum of 47 individuals per litre in summer, Fig. 4C) was predicted with a mean deviation to the measured data during summer of only 22%. The timing of the subsequent declining in population abundance, including the minimum abundance reached were also

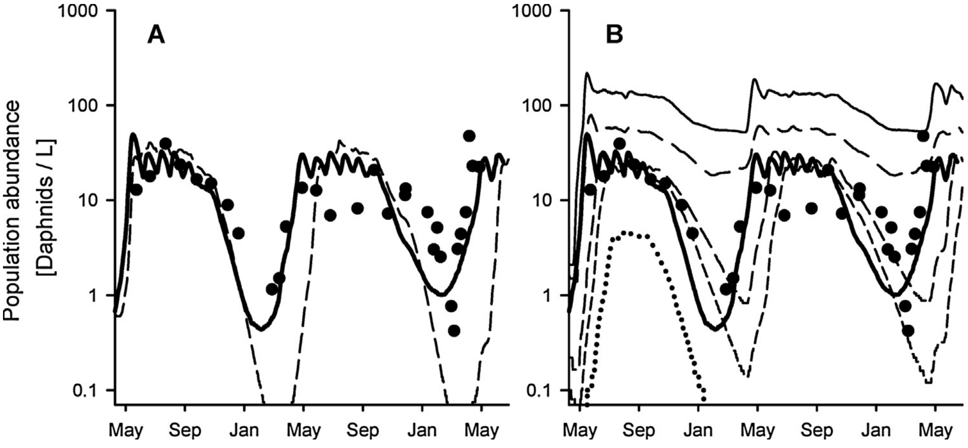

Fig. 5. Comparison of average population abundances in measurements (dots) and simulations (lines) using three different model approaches. A: DaLaM (thick solid line), StoLaM with an unstructured *Daphnia* module (dashed line). B: DaLaM (thick solid line), IDamP with five feeding scenarios (0.03–0.04–0.05–0.1–0.5 mg C L^{-1} d^{-1}, thin lines).

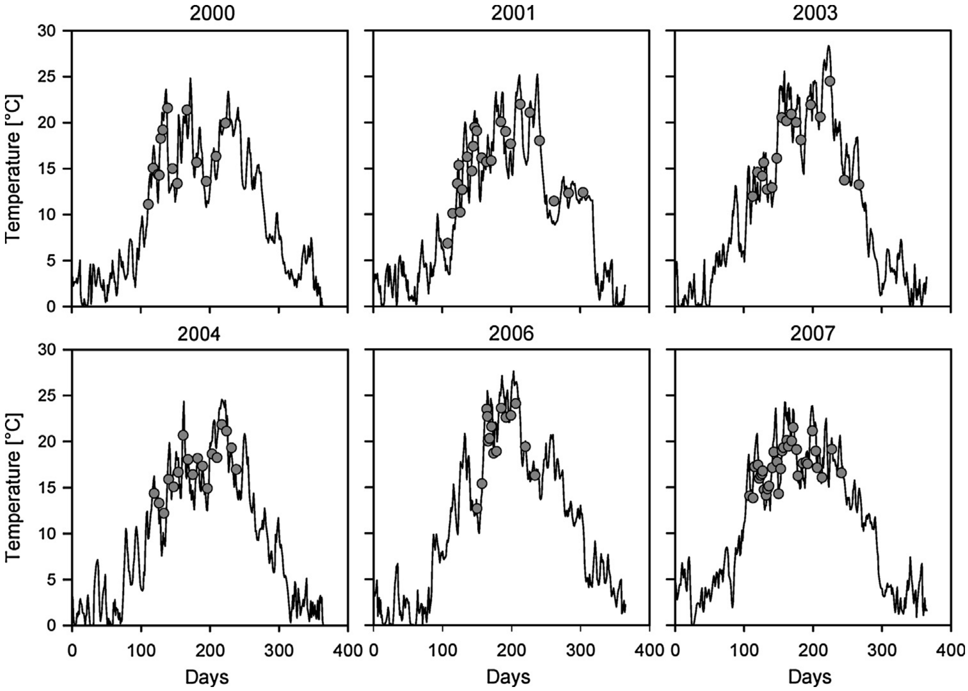

Fig. 6. Simulated and measured water temperatures in the mesocosm experiments (study B, 2000–2007). Dots show the measured data, lines indicate the simulation results.

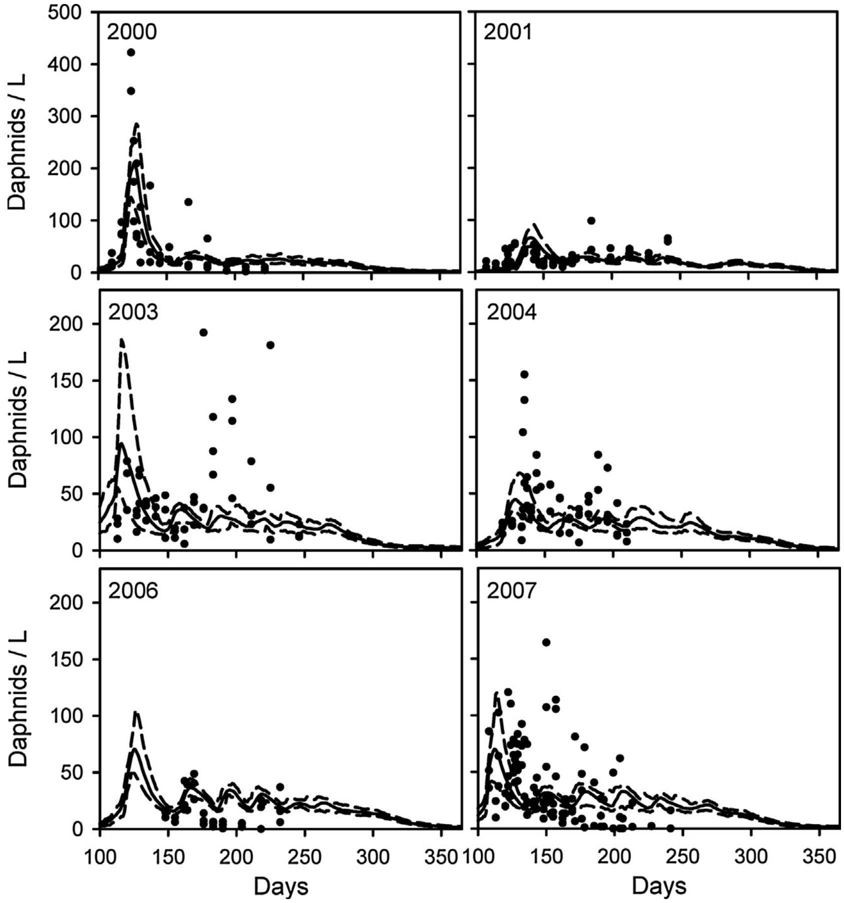

Fig. 7. Simulated and measured *Daphnia* population dynamics in the mesocosm experiments (study B, 2000–2007). Dots indicate the measured density of the daphnids. The simulations started on 01 January (day 1) of each year. Solid and dashed lines show the simulation results: average of 100 Monte Carlo simulations and the 95%-confidence limits, respectively.

well described by the model (with a minimum measured abundance of 1.1 and 0.4 individuals per litre, compared to 0.6 and 1.5 individuals per litre for the simulations, respectively in March 2009 and March 2010). The inclusion of phosphorus limitation of the daphnids (black line, Fig. 4C) in the simulations showed a similar pattern for *Daphnia* dynamics, with a short but distinguishable delay (7 days) in population increase occurring every spring.

3.1.1. *Comparing different model approaches for* Daphnia *population modelling*

Compared to the DaLaM results using the IDamP for the simulation of the daphnid dynamics, the unstructured *Daphnia* module in the standalone version of StoLaM showed unrealistic low densities during winter, and a significantly delayed development in spring (Fig. 5A; see also Fig. S2-1 in the Supplementary Information S2). For the independently used IDamP, we had to test different constant feeding scenarios because the phytoplankton densities dynamically simulated by StoLaM were conceptually not available as input variables. The output of the IDamP covered a large range of *Daphnia* densities depending on the feeding scenario used: i) at low algal concentration, the start of daphnid development in spring was clearly delayed; ii) below 0.04 mg C L^{-1} d^{-1} most of the simulated populations became extinct; iii) at medium algal concentrations (0.1-0.5 mg C L^{-1} d^{-1}), the model reached densities that were too high when compared to the field situation (Fig. 5B). In contrast, simulations with DaLaM showed a slightly premature decrease in *Daphnia* density during autumn, but the best overall match with the outdoor measurements including summer as well as the timing of spring development (Fig. 5). IDamP achieved a similar prediction accuracy as DaLaM with only some of the tested feeding scenarios (e.g. approx. 0.05 mg C L^{-1} d^{-1}). But, in contrast to IDamP, which requires a daily food supply from outside the system, the available food for the daphnids is an emergent property of DaLaM and does not have to be artificially regulated.

3.2. *Model predictions of population dynamics in study B*

As a second step, we tested the DaLaM on a dataset for six individual mesocosm studies (study B, 2000–2007), in which the population dynamics of *Daphnia* as well as phosphorus concentration exhibited different patterns within the vegetation periods in different years. The good agreement between measurements and simulated water temperatures from 2000 to 2007 in the mesocosms and model predictions, demonstrates that the hydrodynamic submodel HyLaM was able to capture year-specific weather conditions (Fig. 6).

The measured mean chlorophyll a concentrations in the mesocosms during late spring and summer from 2000 until 2006 (1.7-5.4 μg/L) were in the range of the simulations (2.2 μg/L, Table S2-3 in the Supplementary Information S2). The only year showing a substantial discrepancy between simulations and measurements was year 2007, when higher phytoplankton densities occurred in the outdoor ponds than those predicted by the DaLaM. This was probably caused by reduced grazing pressure at partly lowered daphnid abundances between days 150 and 200 (Table S2-2 in the Supplementary Information S2). Overall, these results indicate that DaLaM was able to give a realistic prediction of outdoor phytoplankton densities under varying condition during the study periods in spring and summer by taking into account the grazing pressure by the daphnids. In general, the average simulated daphnid population size in spring and summer matched the observations from the mesocosm studies quite well (Fig. 7). This was also true for the timing and magnitude of the variable spring peaks (day 120–140) as well as for the equilibrium conditions during the summer months (day 140–240, with an average of 30 daphnids/L in the mesocosms). Differences between the simulations and measurements in the mean daphnid population density were 19% during spring and 28% during summer (for details see Table S2-2 in the Supplementary Information S2), and DaLaM mostly underestimated the population density slightly in both periods. In the year 2000, the particularly high *Daphnia* densities during spring as a result of specific weather conditions and higher phosphorus concentrations were accurately reproduced by the model (Fig. 7). In 2001, the opposite situation with low phosphorus release and at water temperatures during April, that averaged 3 °C below those in April 2000, could also be well simulated. It should be born in mind, that in the years 2000 and 2001, the mesocosms were free of macrophytes and filamentous algae (metaphyton), which were regularly present in the studies conducted in 2003–2007. However, remarkable deviations between model predictions and measured data could be observed in study B for the four data sets in 2003–2007. For instance, in 2003, the steep increase of daphnid abundance during early summer (days 150–200) was not observed in the other studied years and could not be predicted by DaLaM (52% deviation in the mean population size in summer, Table S2-2 in the Supplementary Information S2). In contrast, in 2006 and 2007, the abundance of daphnids was relatively low during summer compared to the other years, especially for 2007 where daphnids have even become extinct in some of the replicates after day 180.

4. Discussion

DaLaM was created by coupling an IBM (IDamP) with a stoichiometric lake model (StoLaM) which includes a hydrodynamic submodel (HyLaM) to simulate population dynamics of *D. magna* under realistic environmental conditions, particularly for eutrophic, fish-free ponds. Within this concept, StoLaM calculates the dynamic of algal resources including *Daphnia*-algae interactions, and provides outputs for food quantity and quality over time depending on phytoplankton productivity with respect to nutrient availability and weather conditions. The use of the hybrid model DaLaM offers clear advantages over its separate submodels (Fig. 5): On the one hand, the standalone version of StoLaM using an unstructured compartment model for daphnids, which did not include any individual physiological adaptations or intra-specific interactions, did not perform as well as the IBM approach, especially during autumn and winter. This confirmed the findings of Rinke and Vijverberg (2005) that unstructured compartment models are less suitable for simulating population dynamics under variable field conditions compared to IBM approaches, which include demographic effects.

On the other hand, the standalone IBM model IDamP shows high accuracy for individual daphnids and population dynamics under laboratory conditions (Preuss et al., 2009), but provides no dynamic modelling of the algae. Phytoplankton is the key driver for *Daphnia* population dynamics (Schalau et al., 2008), and owing to the missing simulation of primary production in the IDamP model, a simplification of assumptions about phytoplankton availability is required, e.g. fixed feeding scenarios (IDamP, Fig. 5B), or a constant carrying capacity for phytoplankton is needed (e.g. Schalau et al., 2008). In real ecosystems, the environmental carrying capacity of algae and daphnids varies over time and depends on nutrition and other environmental parameters. Hence, the use of simplified assumptions for the phytoplankton availability leads to high uncertainty regarding the relevance of the simulation results for *Daphnia* populations under specific trophic conditions in the field.

In DaLaM, algal productivity and carrying capacity emerge from the dynamically simulated specific environmental scenario, which enables the realistic and dynamic modelling of both algae and individual based daphnids, and their interactions. By combining an ecosystem modelling approach, which takes into consideration relevant physical-biogeochemical processes, and an IBM approach, DaLaM resolves the structural shortcomings of both individual models, StoLaM and IDamP.

From a conceptual point of view, model complexity should arise from the research question and the relevant ecological scenario and this will influence the number of implemented processes required. As a rule, simple models will not be useful in predicting the behaviour of specific systems and, thus, cannot be empirically tested against data from a particular system (Evans et al., 2013). In most cases, models must be complex to make good predictions about real ecological systems (Evans et al., 2013), and therefore should include the most relevant ecological processes of the respective environmental scenario to be modelled. Complex, system-specific models are needed as tools to predict both the current behaviour of systems for model testing, and their future behaviour (Evans et al., 2013; Zhao et al., 2008). If models are built for making predictions for specific systems, then increasing complexity will usually increase generality (Evans et al., 2013). It is important to note that more realistic and complex models with a higher number of parameters do not inevitably exhibit a higher parameter uncertainty than more minimal models as is often assumed when only a low number of parameters have to be calibrated (Mooij et al., 2010), and when the model sensitivity for the added parameters is low or their values are well known.

4.1. *Model performance*

In the present study, the implemented complex food web in DaLaM was reduced to only two trophic levels and two species, the green alga *Desmodesmus subspicatus* and the zooplankton species *Daphnia magna.* Here, it was not our aim to simulate complex food webs in natural lakes, but to combine models for these two organisms under realistic outdoor conditions keeping the modelled food web structure as simple as possible. Despite the deliberately simplified food web in DaLaM, a sufficiently detailed ecosystem model for the simulation of fundamental environmental processes was maintained, with which it was possible to predict the overall dynamics of daphnid populations in good accordance with the seasonal variation of phytoplankton density and phosphorus concentration in several mesocosms studies under different weather and nutrient conditions.

Temperature fluctuations have direct consequences on both population dynamics and ecosystem processes (e.g. Benndorf et al., 2001), but generally only meteorological data is easily available so it is important to predict the water temperatures experienced by the aquatic organisms. The StoLaM predictions indicate that the simulation model generates a realistic physical environment for the plankton organisms in the mesocosms in terms of underwater light climate, water temperature and turbulence. Phytoplankton biomass production is mainly limited by phosphorus uptake from the water column, which in turn depends on phosphorus release from the sediment as well as phosphorus excretion by the daphnids. Hence, a realistic simulation of nutrient availability and the resultant phytoplankton growth is essential for determining the carrying capacity of the modelled daphnid population. In addition, DaLaM integrates the principles of ecological stoichiometry, which allows a more accurate description of nutrient cycling in ecosystems. The consideration of the potential phosphorus limitation of the daphnid's growth can be important for this genus because of its relatively high phosphorus requirements compared to other crustacean zooplankton species (e.g. mean phosphorus-to-dry weight ratio was 1.56% for *Daphnia,* but only 0.68% for the cladoceran *Bosmina longirostris* and 0.38% for the copepod *Eudiaptomus gracilis*; see DeMott et al., 1998). Hence, a phosphorus shortage can limit more likely the growth of the daphnid population than other zooplankton groups.

In our long-term mesocosm study A, the algae are top-down regulated by the grazing of daphnids during summer without phosphorus limitation. In contrast, during spring, phosphorus was the limiting factor for the phytoplankton (bottom-up control), and subsequently delayed the onset of first spring peak of the daphnids for a couple of days compared to simulations without P-limitation. These simulation results have two main implications. On the one hand, populations in more nutrient rich lakes can probably be simulated without accounting for nutrient limitation of daphnids due to usually higher seston P:C-ratios in eutrophic lakes (Persson et al., 2007), which is advantageous as a simpler model approach could also be used. On the other hand, DaLaM can be used to predict the daphnid dynamics also under conditions with lower phosphorus concentrations in agreement with the theory of ecological stoichiometry (according to Sterner and Elser, 2002).

4.2. *Limitations by the simplified food web*

Using *D. magna* as a representative for the most effective planktonic filter feeders and *D. subspicatus* as a surrogate species for the phytoplankton community (both frequently tested species in ecotoxicological laboratory experiments according to OECD test guidelines (OECD, 2004, 2008, 2011)), DaLaM's capacity to capture the main dynamics of the pond ecosystems simulated indicates that in most instances, the essential mechanisms and main drivers of the system have been correctly integrated in the DaLaM approach. Nevertheless, the discrepancies between the observed and simulated *Daphnia* population dynamics in several mesocosm experiments (study B, Fig. 7) could be partly related to food web interactions, which are not covered by our simplified two-species model system.

Predation pressure is one of the main factors, next to feeding conditions and temperature, that controls individual level processes and population dynamics (Mooij et al., 2003). In the present simulation study, predators were not included. In field situations, invertebrate predators such as water bugs (e.g. *Notonecta*) and *Chaoborus* larvae may be able to reduce the daphnids abundance. The year 2006 witnessed high densities of *Notonecta maculata* in the experimental mesocosms. This water bug is known to be an effective predator on daphnids (Gergs et al., 2013), and its presence might explain the observed relatively low abundance of daphnids during summer (Fig. 7) compared to the other years, hence justifying the deviations between model predictions and observations.

Competition by conspecifics is integrated in the DaLaM via the density dependence effects on the life cycle of individual daphnids (Preuss et al., 2009). However, daphnid populations in the mesocosms are exposed to a variety of interspecific competitors (e.g. rotifers and copepods) which are susceptible to limit the access to common food resources (Bengtsson, 1986; Connell, 1983). In addition, different potential food sources for *D. magna* in the mesocosms, such as primary producers (e.g. periphyton, Siehoff et al., 2009) and bacteria (e.g. bacterial biomass due to the decomposition of filamentous algae in summer 2003, Fig. 7) which can stabilize and increase the daphnid population density if phytoplankton is scarce, were not included in DaLaM.

The sharp decrease in the *Daphnia* population size in 2007 (Fig. 7) can be attributed to the very high biomass of the macrophyte species *Elodea canadensis* and filamentous algae (*Cladophora* sp.) which occurred in some of the replicate mesocosms. Burks et al. (2000) reported that dense stands of macrophytes can affect the daphnid population growth by reducing the open water area as well as inhibiting the daphnid growth due to their released infochemicals.

Brett et al. (2000) also pointed out that a potential P-limitation by coccale green algae, which are often not representative for the total algal food composition for daphnids in natural ponds, could be compensated by the consumption of other food items of higher P content.

Also based on the example of a *Daphnia*-algae system, Murdoch et al. (1992) discussed the problem of modelling many-species systems. They recommended testing the model at reduced complexity first without considering *Daphnia*'s predators and without inedible primary producers, before more model components be subsequently added to the food web. Thus simplifying the modelling problem seems to be applicable when data from appropriate case studies is available. In our paper we follow the same approach: Despite the simplified food web, DaLaM was able to predict those population patterns of *Daphnia* in daphnid-dominated planktonic communities, which are free of primary producers such as macrophytes and filamentous algae (long-term study A as well as the years 2000 and 2001 in study B). Using these case studies, the DaLaM model concept was confirmed. In the other years presented in this paper, macrophytes and/or filamentous algae as well as invertebrate predators such as *Notonecta* presumably contributed to the high variability of *Daphnia* densities measured in the outdoor mesocosm ponds, which was not covered by the model structure used. Hitherto, food web components for such primary producers have not been commonly used in ecosystem lake models. However, for specific ecological questions or different food web scenarios, missing model components can easily be integrated within this ecosystem modelling approach either to support (other food resources) or inhibit (predators, competitors) the population growth of daphnids.

5. Conclusion

A robust, case-independent parameterisation of the models plays a key role in the success of this modelling approach. In IDamP, all biological processes related to the *Daphnia* life cycle are based on laboratory data at the individual level. Both coupled models (IDamP and StoLaM) were used as they are, with only a few additional extensions to the model interface, and parameter recalibration was limited to the study-specific sediment phosphorus release. Thus, the simulation results in this paper have emerged from the previously implemented mechanisms of the relevant processes, rather than being artificially forced by restructuring or new parametrisation of the models.

Although IDamP was developed to model populations under laboratory conditions, as soon as it was linked with StoLaM and received realistic inputs about food supply and water temperature, it was also able to make robust predictions of the overall population dynamics in the field. This presented hybrid modelling approach is capable of extrapolating single-species data from the laboratory to the field level, which is for instance relevant in environmental risk assessment of plant protection products (Dohmen et al., 2016). More generally, this study reveals that a combination of individual based population modelling and dynamic ecosystem models is a successful strategy for increasing ecological realism as well as decreasing the model uncertainty by including an appropriate level of complexity.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.ecolmodel.2017.09.019.

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