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Deliverable D4.7:
Final models for water quality

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Preface

The deliverable 4.7: Final models for water quality builds on existing models, with the goal of extending the current models to make more complete and accurate water quality predictions. The report describes the CO_2 model, which is an extension of the water quality model developed in AQUAEXCEL^{2020}, as well an extension of an existing pond model. Because the models are completely distinct and not integrated, they will be addressed separately in the current deliverable, with A representing the CO_2 model and B representing the pond model.

CO_2 model

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1A. Objective

The purpose of this document is to describe the functionality and implementation of the CO_2 module in the water quality model (Abbink et al., 2020). The water quality model is one of the main components in the AQUAEXCEL3.0 virtual laboratory, which is developed in Task 4.1 - Virtual Laboratories and modelling tools for designing experiments in aquaculture research facilities.

The objective of the sub-model developed by Abbink et al. (2020) was to develop a generic tool that enables a user of a research facility to predict the water quality in an existing research infrastructure (RI) prior to the start of an experiment and to (re-)design a system which results in the desired water quality for the experiment envisioned. The tools will enable teaching of TNA users, RI technicians and others involved in the principles of water quality control in fish culture units.

2A. Background

Experiments with fish usually involve extensive use of laboratory facilities and run for long periods of time. Both from an ethical perspective (3R's) and from a cost perspective, tools for design and planning of experiments are increasingly important. In aquaculture research as well as other domains, numerical models are increasingly used preparatory to the actual experiments.

One of the main research activities in AQUAEXCEL3.0 is to develop a virtual laboratory system that enables virtual experiments in aquaculture research facilities. This system will feature a framework (Bjørnson et al., 2016 and Bjørnson et al., 2019) that allows the integration of mathematical models of different subsystems in common simulations, replicating the system operation of research laboratories. Abbink et al. (2020) describes the technical implementation and functionality of the water quality model and the energy balance model. This model covers relevant conditions such as feed load of fish/feed, seawater/freshwater, system type, life stage of the fish and treatment systems. A second, thermal model was added to predict requirements for heating/cooling and manage water temperature. This report specifically describes the CO2 module that was added to the water quality model.

3A. Materials and methods - Water quality model

The major part of the water quality model is described in Abbink et al. (2020). This report will focus on the CO2 module. CO2 exists in different forms. In this report, when we talk about CO2, we mean the free form of CO2 (in water or in air). When total inorganic carbon (TIC) is mentioned, all different forms of carbonates, including free CO2 is meant.

3A.1 Design

The design of the CO2 module in the water quality model is shown in Figure 1. The fish produce CO2, which increases the CO2 concentration in the tank. From the surface of the tank, CO2 can evaporate to the ambient air. Water from the tank goes to the biofilter, where CO2 is removed. Before the water is returning to the tank, some water is exchanged with fresh water and thereby also some CO2 is removed.

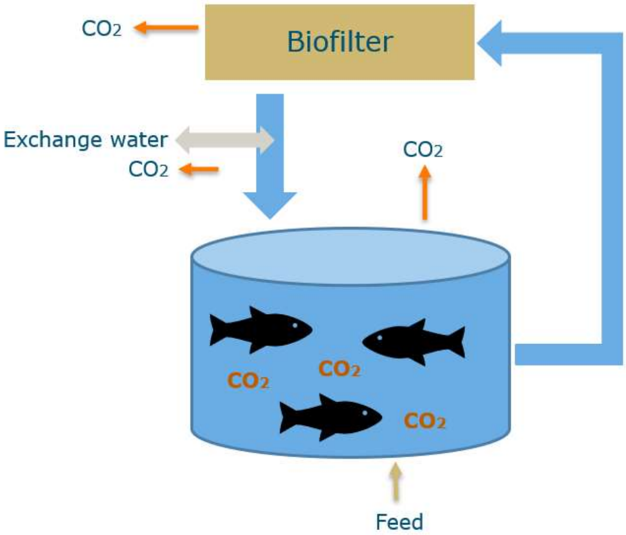

Figure 1: The design of the CO_2 module of the water quality model. Orange arrows indicate where CO_2 is lost or removed from the system.

CO_2 production from nitrification in the biofilter was not considered, since nitrification results in a change in equilibrium between the different forms of CO_2 in water and does not result in an absolute change in Total Inorganic Carbon (TIC), see box below.

Nitrification takes place in two steps: 1) the conversion of ammonium into nitrate and 2) the conversion of nitrate into nitrate:

$NH_4^+ + 3/2\ O_2 \rightarrow NO_2\text{-} + H_2O + 2H+$

$NO_2^- + ½\ O_2 \rightarrow NO_3^-$

The formed H^+ binds to HCO_3^- to form H_2CO_3, that forms an equilibrium with CO_2 and H_2O:

$H^+ + HCO_3^- \leftrightarrow H_2CO_3 \leftrightarrow CO_2 + H_2O$

Also, a small amount of biomass ($C_5H_7NO_2$) is produced. Therefore, the overall equation is as follows (Eding et al., 2006):

$NH_4^+ + 1.86\ O_2 + 1.98\ HCO_3^- \rightarrow 0.020\ C_5H_7NO_2 + 1.88\ H_2CO_3 + 1.04\ H_2O$

3A.2 Input

The water quality model requires input from the user for the fish production plan and the related waste production (Annex 2.1 from Abbink et al., 2020). Here, only the input parameters for the CO2 module are described.

From the fish production plan, the following input parameters are relevant to the CO2 module:

- Initial body weight (BW) of the fish (g)
- Initial number of fish (#)

- Mortality (%/day)

- Specific Growth Rate (SGR) (% BW/day)

Different from the original water quality model, feeding level (%BW/day) is not an input, but it is calculated based on the body weight of the fish.

CO_2 production by the fish is calculated based on the respiration coefficient and the O_2 consumption. The oxygen consumption is based on the feeding level.

Input parameters for CO_2 production:
- Respiration coefficient (RQ)

When the model is coupled with the growth model, the parameters of number of fish, individual weight, feed per fish, O_2 consumption and CO_2 production is taken directly from the external model and there is no need to calculate intermediate variables.

The model requires input for water quality conditions and system characteristics from the user on the experimental system used.

Water quality conditions:
- Water temperature (°C)
- Water pH
- TIC concentration renewal water (mg CO_2/L)
- CO_2 concentration in ambient air (ppm)

System characteristics:
- Volume tank (fish + water) (L)
- Recirculation flow rate (L/day)
- System exchange flow rate (L/day)
- Total biofilter volume (m^3)
- Specific surface area of biofilter (m^2/m^3)
- Gas:liquid ratio (GLR) of biofilter
- Acid-base equilibria carbonate system (K_0, K_1, K_2)

3A.2 Calculations

TIC balance

In the system, CO_2 is added and removed via different pathways (see Figure 1, Chapter 3.1). The TIC balance can be calculated as follows:

$$TIC\ balance = TIC_{production} - TIC_{evaporation} - TIC_{biofilter} - TIC_{exchange} \qquad (9)$$

Where $TIC_{production}$ is the TIC produced by the fish, $TIC_{evaporation}$ is the TIC that is lost through evaporation from the tank, $TIC_{biofilter}$ is TIC removed by the biofilter and $TIC_{exchange}$ is TIC removed by exchanging water from the biofilter with fresh water, all expressed in mg CO_2/L. The TIC balance should be (close to) zero.

CO_2 production fish

The Total Inorganic Carbon (TIC) produced by the fish is calculated with the following equation:

$$TIC\ production\ fish = RQ \cdot \frac{molar\ mass\ CO_2}{molar\ mass\ O_2} \cdot Total\ feed\ load \cdot O_2\ consumption \qquad (1)$$

Where TIC production fish is the amount of TIC produced by the fish (mg CO_2/d), RQ is the Respiration Coefficient (mole CO_2/mole O_2), molar mass of CO_2 is 44.0 (g/mol), molar mass of O_2 is 32.0 (g/mol), total feed load is the amount of feed consumed by all the fish in the tank (g/d) and the O_2 consumption is the oxygen consumed relative to feed load (mg O_2/g feed).

The total feed load (g/d) is calculated based on the amount of feed per fish and the number of fish in the tank. The amount of feed per fish is calculated based on the feeding level and the individual weight of the fish:

$$Total\ feed\ load = \left(\frac{feeding\ level}{100} \cdot BW\right) \cdot \#fish \qquad (2)$$

Where feeding level is the maximum feed intake (% BW d^{-1}), BW is the individual body weight of the fish (g) and #fish is the number of fish in the tank.

The feeding level (% body weight d^{-1}) of African catfish (*Clarias gariepinusis*) used as an example in the standalone version of the model is calculated based on the body weight of the fish (Eding and van Weerd, 1999):

$$Feeding\ level = FLC \cdot BW^{-0.4} \qquad (3)$$

Where feeding level is the maximum feed intake (% BW d^{-1}), FLC is the feeding level constant, based on the species of the fish (14,705 for African catfish, adapted from Eding and van Weerd), BW is the individual body weight of the fish (g) and #fish is the number of fish in the tank.

In the coupled version of the model, these variables are calculated and imported from the growth model.

Evaporation from the tank

The evaporation of CO_2 from the tank is calculated with the surface area of the water and the flux of CO_2 from the surface:

$$CO_{2_{evap}} = A_{exposed} \cdot j$$

Where $A_{exposed}$ is the surface area of the water that is exposed to the atmosphere (m^2) and j is the flux of CO_2 from the surface (mol m^{-2} s^{-1}).

The surface of the tank is calculated based on the volume of the tank and the depth of the water:

$$A_{exposed} = \frac{V_{tank}}{D_{water}*1000} \qquad (4)$$

Where V_{tank} is the volume of the tank (L) and D_{water} is the depth of the water (m).

The amount of CO_2 that evaporated from the surface of the fish tank is calculated based on Hafner et al. (2023):

$$j = h(\frac{a}{H} - c) \qquad (5)$$

Where j is the flux of CO_2 from the surface (mol m^{-2} s^{-1}), h is the mass transfer coefficient of CO_2 (0.0012 m s^{-1}, Hafner et al., 2023), a is the activity of species at the surface of the tank (mol kg^{-1}, in this study we assumed that this was the same as the concentration in the tank), H is Henry's law constant for CO_2 (aq:g, m^3 kg^{-1}) and c is the gas-phase concentration of CO_2 in the ambient air (mol m^{-3}).

Henry's law constant for CO_2 is calculated based on Hafner et al. (2013):

$$\log K_H = 108.38578 + 0.01985T + \frac{-69\ \ .530}{T} - 40.45154 \log T + \frac{669365}{T^2} \qquad (6)$$

Where K_H is Henry's law constant (m^3 kg^{-1}, which can be converted to m^3 kg^{-1} by multiplying by RT, where R is the universal gas constant ($8{,}206 \cdot 10^{-5}$ m^3 atm^{-1} K^{-1} mol^{-1}) and T is temperature (K)).

4A. Results and discussion

4A.1 Output

The CO_2 module of the water quality model calculates the TIC concentration before and after the biofilter (Figure 3A) and the CO_2 concentration in the water entering and leaving the fish tank (Figure 3B). Also CO_2 production from the fish, the amount of CO_2 that evaporates from the tank and the amount of CO_2 that is removed by the biofilter is calculated (Figure 4).

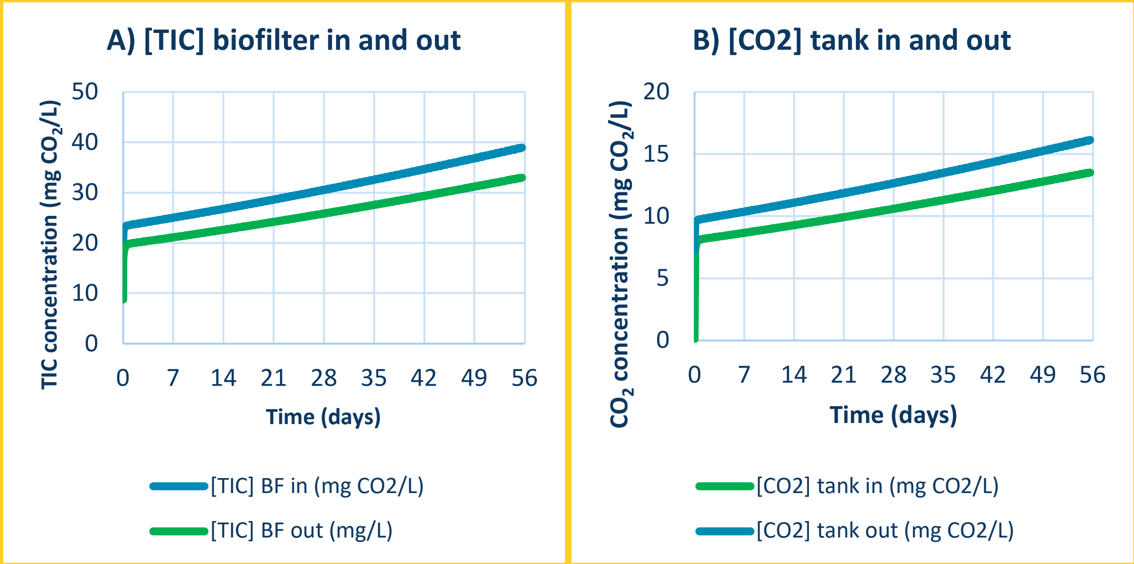

Figure 3: A) TIC concentration of the water before and after the biofilter. B) CO_2 concentration of the water entering and leaving the fish tank.

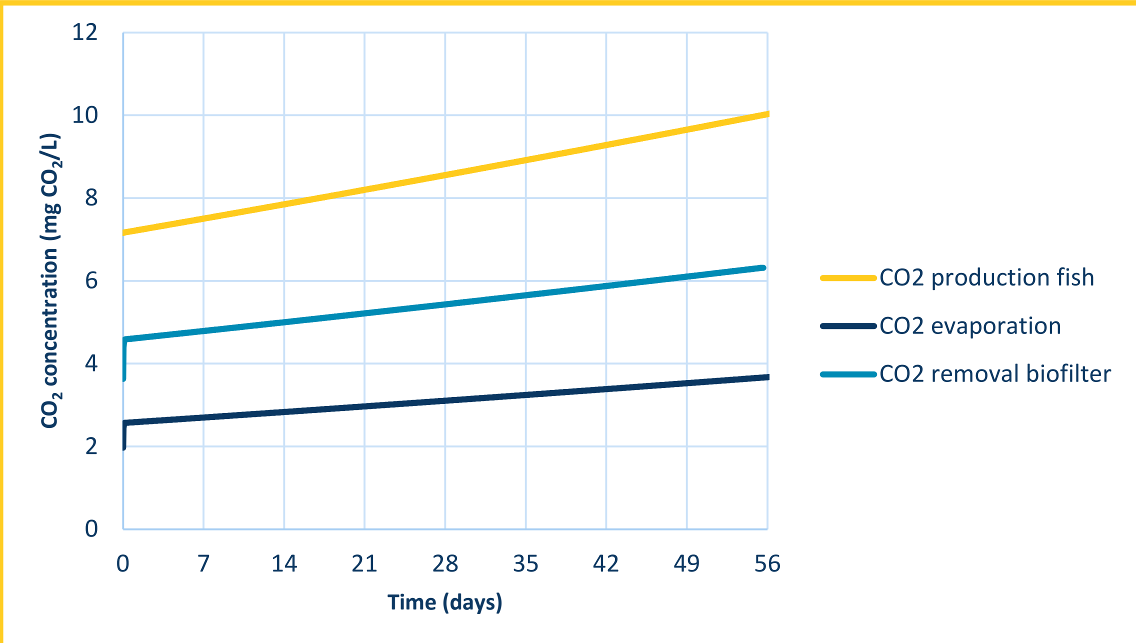

Figure 4: CO_2 production of the fish, CO_2 lost trought evaporation from the fish tank and CO_2 removal from the biofilter.

4A.2 Validation

Initial development of the model was done by using a set of realistic data coming from the experimental fish facilities of Wageningen University and Research (Karimi et al., 2020). These input data for fish and experimental set-up parameters resulted in realistic output data for water quality, including CO_2. Additionally, we used the results from another experiment to validate the calculations of the CO_2 removal from the biofilter (Karimi et al., in preparation).

Karimi et al. (in preparation) used four different fish tanks and the water of all four fish tanks was treated by one biofilter. The model is based on one tank and therefore the inputs are summed or averaged. Input parameters with unit and value can be found in Annex 1. Gas-liquid ratio and pH were varied, resulting in 9 scenario's (Table 1). Only the CO_2 removal of the biofilter was validated, since Karimi et al. (in preparation) showed no data about CO_2 production and evaporation.

Table 1: Gas-liquid ratio (GLR) and pH of the 9 scenario's used for validation of the CO_2 module of the water quality model.

Scenario	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
GLR	2	5	10	2	5	10	2	5	10
pH	6.5	6.5	6.5	7.0	7.0	7.0	7.5	7.5	7.5

Karimi et al. (in preparation) used a low, medium and high CO_2 concentration of the water that was entering the biofilter. The CO_2 concentration of the water in the tank in the model did not completely match with the concentrations from Karimi et al. (in preparation), as is shown in Table 2. The CO_2 concentration of scenario 1, 2 and 3 are in between the measured the low and medium CO_2 concentrations measured by Karimi et al. (in preparation). The CO_2 concentrations in scenario 4, 5 and 6 ware closest to medium concentrations and scenario 7, 8 and 9 to the low concentrations.

Table 2: CO_2 concentration (mg CO_2/L) of the water entering the biofilter. Karimi et al. (in preparation) used a low, medium and high CO_2 concentration.

Scenario	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Karimi et al. (in preparation)									
- **Low**	7,0	6,3	6,3	7,8	8,4	N/a	7,6	7,2	7,3
- **Medium**	16,4	16,7	17,2	15,7	15,8	15,2	16,2	17,8	16,0
- **High**	25,5	26,4	23,2	25,7	25,1	23,5	25,3	23,8	24,5
CO_2 module	10,8	10,1	10,1	13,6	11,2	11,2	7,4	5,6	5,6

The CO_2 removal by the biofilter depends on the CO_2 concentration of the water in the tank. As mentioned before, the calculated CO_2 concentration in the tank is not fully comparable with the measured CO_2 concentrations by Karimi et al. (in preparation). Therefore, in Figure 5, both low and medium CO_2 concentrations are shown.

The absolute CO_2 removal of scenario 1, 2 and 3 (low pH) was higher compared to the measurements from Karimi et al. (in preparation) with low CO_2 concentration in the tank, but lower with high CO_2 concentrations in the tank. This is in line with the CO_2 concentration in the tank, which was in between the low and medium concentration measured by Karimi et al. (in preparation). The absolute CO_2 removal of scenario 4, 5 and 6 (medium pH) was also in between the removal measured by Karimi et al. (in preparation) with low and medium CO_2 concentrations in the tank but tends more towards the removal with medium CO_2 concentrations. This was also in line with the CO_2 concentrations in the tank (Table 2). The absolute CO_2 removal of scenario 7, 8 and 9 (high pH) was comparable with the removal measured by Karimi et al. (in preparation) with low CO_2 concentration in the tank, which is in line with the CO_2 concentrations from Table 2. The relative CO_2 removal with a GLR of 5 or 10 (scenario 2, 3, 5, 6, 8 and 9) was slightly higher than measured by Karimi et al. (in preparation). The other scenario's (GLR 2) are comparable based on the CO_2 concentration in the tank (Table 2). Overall, the results are within the range of acceptable deviation.

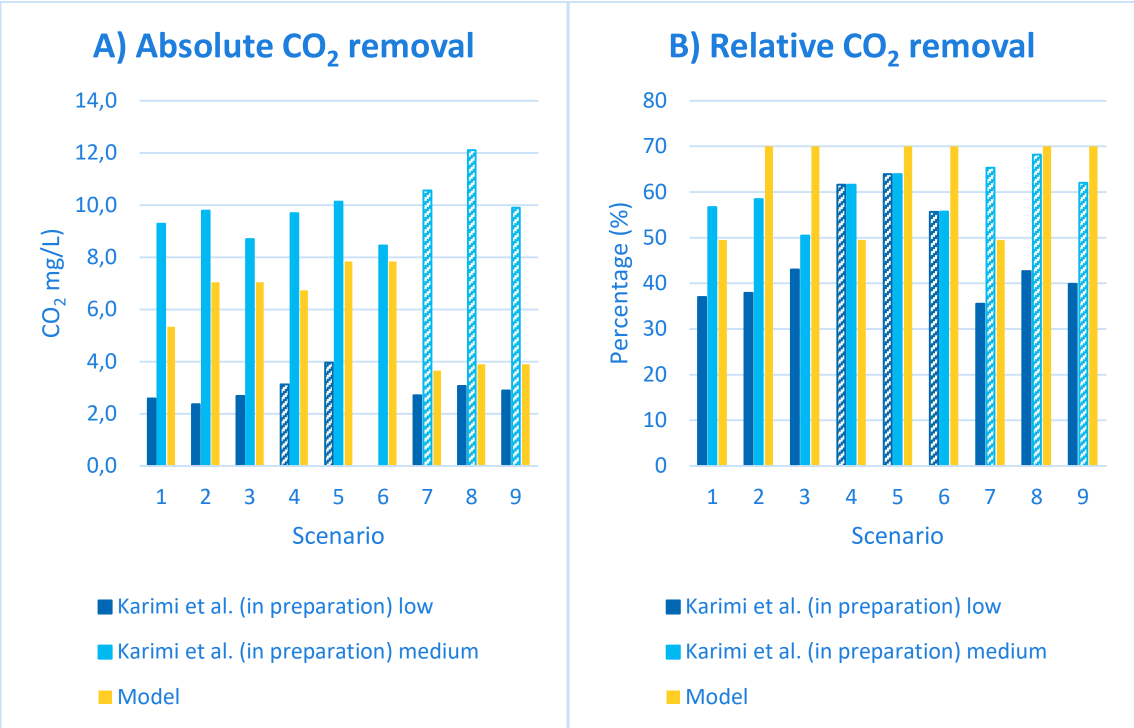

Figure 5: A) Absolute CO_2 removal (mg CO_2/L) and B) relative CO_2 removal (%) in the different scenarios from Karimi et al. (in preparation) with low and medium CO_2 concentration in the tank and the CO_2 module of the water quality model.

To get an indication about the effect of the CO_2 removal by the biofilter on the CO_2 concentration in the fish tank, a sensitivity analysis was done. Figure 6 shows the CO_2 concentration in the fish tank calculated by the CO_2 module of the water quality model when the biofilter removes 10, 20 or 30 percent more or less CO_2 for the different scenarios. This range is compared to the CO_2 concentration in the fish tank measured by Karimi et al. (in preparation). For all scenarios the CO_2 concentration in the fish tank increased with decreasing CO_2 removal by the biofilter and the other way around. However, the CO_2 concentration in the tank increased more than the decrease in the removal by the biofilter.

The CO_2 concentration in the fish tank has an impact on the welfare and growth of the fish (Ellis et al., 2016). Ellis et al. (2016) proposed a range of safe CO_2 limits for recirculating aquaculture systems of 10 – 40 mg CO_2/L. However, already with a CO_2 concentration of 3 mg CO_2/L the metabolic rate is affected and when the CO_2 concentration exceeds 15 mg CO_2/L growth is induced. The CO_2 concentration in the tank calculated by the CO_2 module of the water quality model is within the range of safe CO_2 limits for all the scenarios.

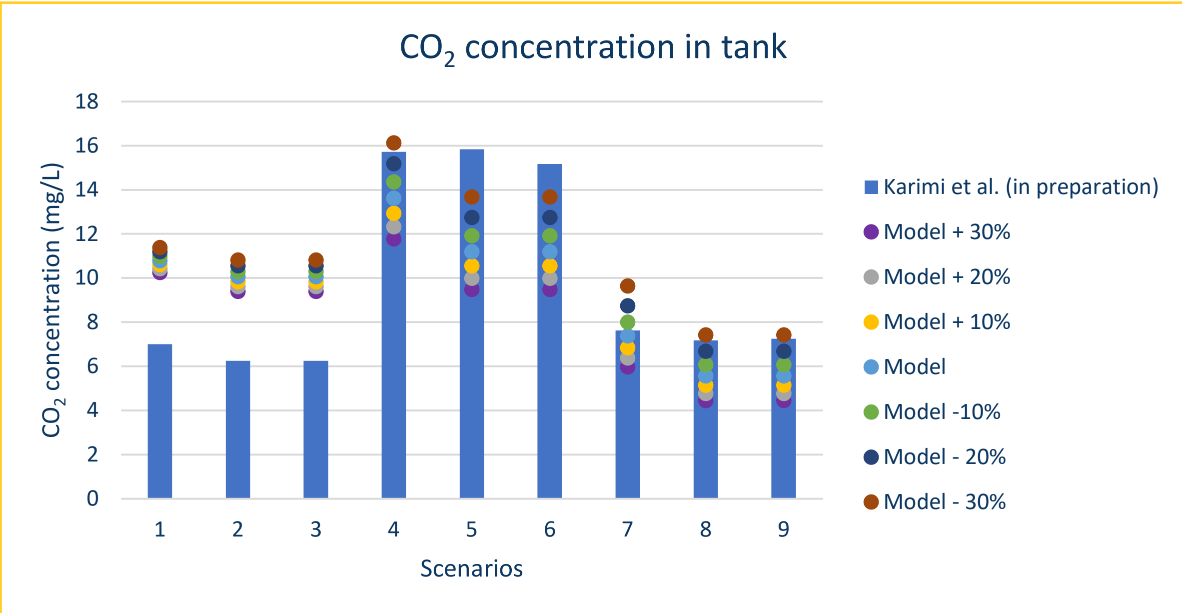

Figure 6: CO_2 concentration in the fish tank when CO_2 removal in the biofilter is varied (-30% to +30%) compared to the CO_2 concentration in the fish tank measured by Karimi et al. (in preparation). For scenarios 1, 2, 3, 7, 8 and 9 the results with low CO_2 concentrations entering the biofilter were used and for scenarios 4, 5 and 6 the medium concentrations were used (based on Table 2).

5A. References

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Pond model

Gergő Gyalog (MATE)

1B. Objective

The overall objective of this work was to ***refine a previously developed and validated reference*** biophysical ***fishpond model*** (Varga et al. 2020) such that it can be applied for simulating the outcomes of carp experiments managed under widely different feeding, stocking, manuring strategies and water management regime.

The reference pond ecosystem model was able to provide reliable simulations on fish growth, but it had low explanatory power for water quality variables (including zooplankton, algae, suspended and sedimented detritus, dissolved nitrogen, phosphorus and oxygen concentration). Our ***primary specific objective*** during this project ***was to improve the theoretical understanding*** of some processes (for instance detritus sedimentation, cyanobacterial growth) that regulate ***dynamics of water quality*** variables. Consequently, model simulations during the planning phase of experiments can inform researchers about major tendencies in water quality variables under different nutrient and stock management scenarios, enabling the user to safeguard the environment and avoid critical levels of sediment accumulation, sub-optimal dissolved oxygen, cyanobacterial blooms by adequate input management.

A ***second specific objective*** of this development ***was to reduce the need for intensive data*** on initial conditions of the pond ecosystem (Day 0 of the experiment). The reference model was very sensitive to input data on initial conditions of algae, zooplankton, nitrogen and phosphorus concentrations, but during refinement of model functionalities, the robustness of the model was increased, resulting in reliable explanatory power under a wide range of assumptions on initial water quality.

2B. Background

The model presented here builds on a previously developed fishpond model by Varga et al. (2020) in the ClimeFish project for assessing effects of climate change on fishpond aquaculture. It is hereafter referred to as the "***reference model***". A simplified ***food web with predator-prey interactions*** involving common carp, bighead carp, zooplankton, phytoplankton, benthos, and detritus was mapped by the medium complexity dynamic process model. The model considered the presence of ***dissolved oxygen, nitrogen, and phosphorus*** in the pond water, in addition to a solid mass of manure and feed (maize). Although the reference model provided robust simulations based on fishpond management practices and climate change simulations, the model had some limitations ***due to the limited availability of data*** useable for training and validation:

- The reference model was validated on data from intensively managed carp pond, with high stocking densities and feeding rates and low manuring rates. Therefore, there was ***a need to refine*** model equations and ***parameters related to nutrient cycling and plankton production***, and this required datasets on water quality dynamics with temporal resolution good enough to train and validate the new model.

- The reference model was trained on data sourced from fish ponds manured at low intensity, and the model ***did not perform well under higher manuring rates***, yielding unrealistically high detritus levels. For this reason, the detritus levels in the reference pond model were restricted to a narrow range. To increase robustness from this aspect, ***sedimentation and resuspension*** processes were needed to be refined. This step required datasets from intensively manure ponds.
- In certain cases, in addition to organic manure, fishponds are treated with ***inorganic fertilizer*** to increase the availability of inorganic forms of nitrogen for algae and enhance the overall productivity of the system. Nutrients from inorganic fertilizer ***were not represented*** in the reference model. In order to account for inorganic fertilizer and ***improve*** model equations describing ***inorganic nitrogen*** flows, data were needed from ponds fertilized with nitrogen fertilizer.

Other data-related limitations of the reference model development included the lack of some important site-specific meteorological data such as solar radiation and humidity – estimates were used from other Hungarian datasets. They called for the need of validating the model with data on weather.

3B. Methodology

3A.1 New data generated for model refinement

In order to parameterize and validate the model field data were generated from experimental fish ponds of HAKI, which ponds are part of TNA calls of Aquaexcel3.0. Information was gathered on food web dynamics, carp rearing experiments were conducted in closely monitored fishponds during the seven-month growing season in 2021 and 2022, from 1 April to 31 October. The experiments were coordinated at the Hungarian University of Agriculture and Life Sciences (Institute of Aquaculture and Environmental Safety, Research Centre for Aquaculture and Fisheries, MATE AKI HAKI, Szarvas, Hungary), the experiments were carried out in earthen ponds with a surface area of 10,000 m2 and a depth of two meters. In 2021 and 2022, two (CS6, CS7) and three (CS2, CS3, CS6) ponds were stocked with second year common carp. Throughout the production season, the ponds were operated under different feeding and fertilization schedules to monitor the effects of different nutrient management scenarios on the pond food web. The raw measurement data, along with the comprehensive feed and fertilizer input for five fishponds, can be found in “RawData_2021.xlsx” and “RawData_2022.xlsx” respectively, which are located in the “Measured_Data” folder of the Mendeley database (Sharma et al., 2024). The process for gathering the data is outlined below:

• Water samples from the ponds were collected twice a week, and analyzed for ammonium (mg/dm3), nitrate (mg/dm3), nitrite (mg/dm3), orthophosphate (mg/dm3) and chlorophyll-a (mg/dm3) using to standard analytical methods;

• In 2021, dissolved oxygen (mg/dm3) and water temperature (°C) were both measured manually twice a day, using multi-parameter water quality meter. In 2022, sensors (Aquaread AP7000) were placed in the fishponds to measure these parameters hourly.

• Zooplankton biomass (cm3/100 dm3) was monitored twice a week using a 50 µm mesh plankton net. For each sample, 100 dm3 of pond water was filtered and concentrated to 100 cm3. All samples were preserved in formaldehyde, then settled in a centrifuge tube and biomass was measured after 24 h.

• Meteorological data, including air temperature (°C), wind speed (m/s), precipitation (mm/day), and solar radiation (W/m2), were collected from the Agromet Solar automatic meteorological station, located approximately 1 km away from the ponds in Szarvas.

• Detailed information on the schedule and amount of feed (in kg) supplied to the ponds was recorded throughout the production period;

• Strategy (date and quantity) for adding organic manure and/or inorganic fertilizer in each pond was recorded. Additionally, laboratory measurements for the manure composition were recorded;

• We recorded the number and weight (in kg) of the fish that were stocked and harvested, as well as the increase in weight, determined through fish sampling under different pond managerial practices.

3A.2 Detailed description of model refinement

The reference model had poor performance when it was forced with high manuring rates. These model-runs simulated a rapid increase in detritus concentration, elevating water turbidity, inhibiting photosynthesis, consequently phytoplankton biomass production was low, and oxygen levels were dropped down. Due to the low phytoplankton concentration, zooplankton began to feed on detritus (a food source alternative to phytoplankton). In the simulations, reduced O_2 levels prevented normal anabolic activity of fish, and this had an overall negative effect on fish production.

We identified that poor performance of the model at the detritus and sedimentation related component was limitedly addressed in the reference model. Thus, inspiring from the above malfunction, this limitation of the reference model was addressed based on the data from the 2022CS6. The model was further improved by extending the *prototype programme "prot_t_detritus"* to consider the permanent sedimentation of a certain fraction of detritus together with the associated amount of N and P. The sedimentation rate was directly linked to the amount of detritus and increased proportionally with it. The detailed procedure is explained in the equations below. Eqn. 1 calculated the amount of sedimented detritus and Equation 2 and 3 determine the N and P in the sediment respectively.

$$DSed = -1 * Sed * \max\left((D - D_{min}), 0\right) * Area * DT \tag{4}$$

$$DSedN = \frac{DSed}{D * Area} * ND * Area * 10000 * Depth \tag{5}$$

$$DSedP = \frac{DSed}{D * Area} * PD * Area * 10000 * Depth \tag{6}$$

where:

Area is the surface area of the pond (ha), while 10000 represents the conversion for m2/ha; D is the concentration of available (suspended) detritus (kg/ha); Depth is the depth of the pond water (m); Dmin is the lower limit concentration of available (suspended) detritus (kg/ha); DSed is the amount of sedimented detritus (kg); DSedN is the amount of sedimented nitrogen (kg); DSedP is the amount of sedimented phosphorus (kg); DT is the time step of the model (day); ND is the detritus-related nitrogen concentration (kg/m^3); PD is the detritus-related phosphorus concentration (kg/m^3); and Sed is the sedimentation rate coefficient (1/day).

During the parameterization process (cyclical incremental improvements) the parameters ***Sed and Dmin were set at 0.6 1/day and 132 kg/ha***, respectively.

Manure decomposition process in the model was also refined (prototype program of *"prot_manure_decomp"*) based on the information on actual composition of manure. These improvements include formulation of the following relations:

$$DM = Alpha * M * Area * DT \tag{7}$$

$$DN = DM * Dry * Ncont \tag{8}$$

$$DP = DM * Dry * Pcont \tag{9}$$

where:

Alpha is the rate of decomposition, (Svirezhev et al. 1984), (1/day); Ncont is the concentration of nitrogen in dry manure, based on lab measurement (kg/kg); Pcont is the concentration of phosphorus in dry manure, based on lab measurement (kg/kg); DM is the amount of the decomposed manure (kg); DN is the amount of the decomposed nitrogen (kg); DP is the amount of the decomposed phosphorus (kg); M is the concentration of the manure (kg/ha); and Dry is the dry matter content of the manure, based on lab measurements (kg/kg).

The dry matter (DM) = 0.421 kg/kg, Ncont = 0.139 kg/kg, and Pcont = 0.0526 kg/kg. from laboratory measurements were applied in the simulations and ***after stepwise identification Alpha = 0.2 1/day was verified***. The simulations for the detritus concentrations resulting after the after the aforementioned improvements is shown in Figure 1. As it is seen, suspended detritus suddenly increases after manure is released, but later – fairly reasonably -- it is gradually sedimented, and there is a convergence toward an equilibrium level.

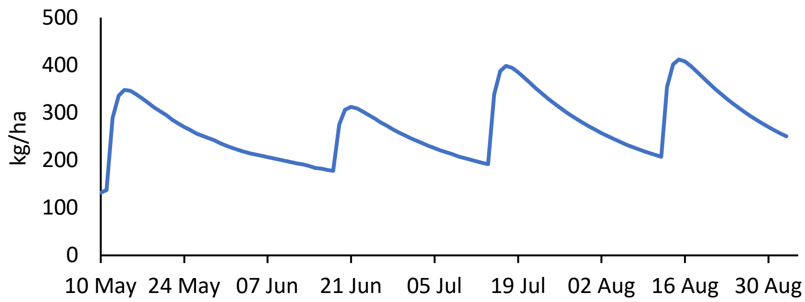

Figure 1. Simulated detritus concentration in one of the experimental ponds.

Simulation with one single algal component (based on the reference model setup)

Simulations after model extension: distinction between eukaryotes algae and cyanobacteria

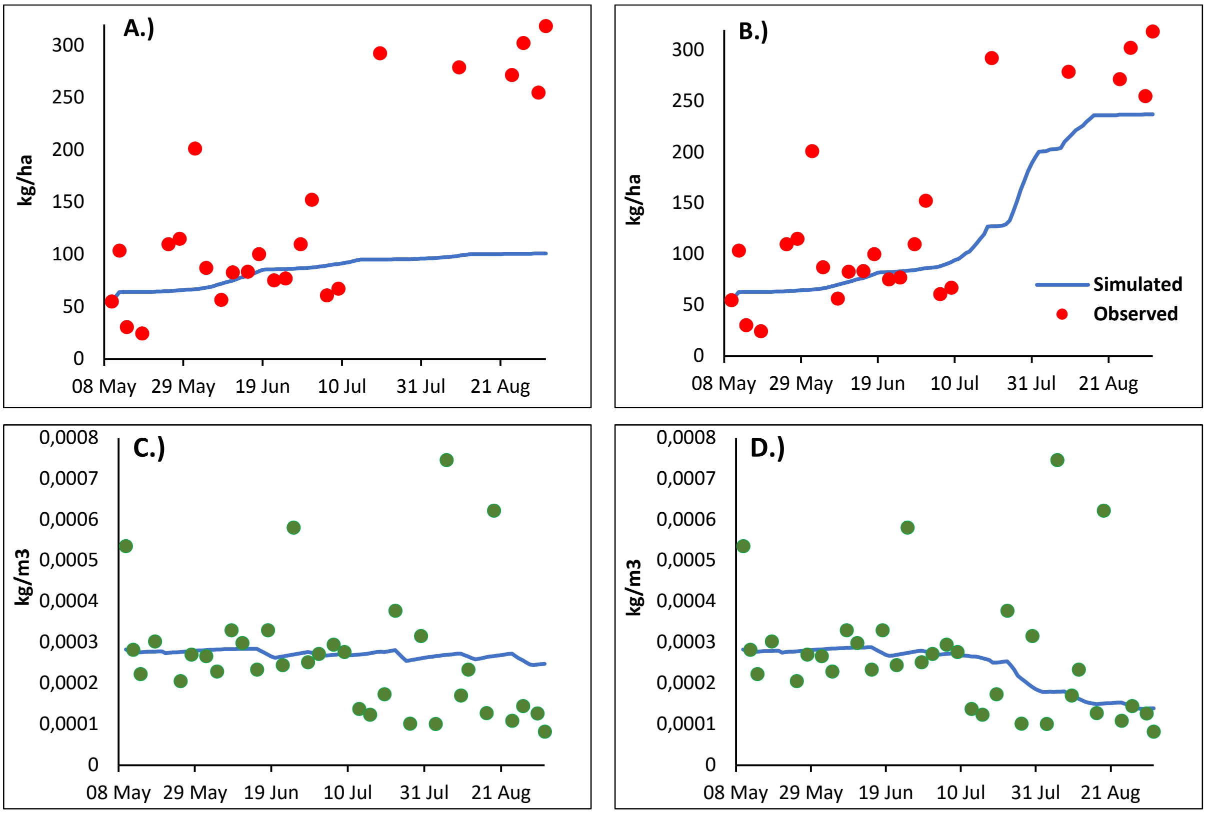

Figure 2. Simulated (blue lines) and measured (dots) phytoplankton biomass (A., B.) and inorganic nitrogen (TIN) concentration (C., D.) in one the experimental ponds before (A., C.) and after (B., D.) model extension. See further explanation in text.

During the validation it was observed that ***the model having one algal component could not capture the rise in chlorophyll-a levels*** toward the end of the production season, as shown in Figure 2A. Measured data on TIN concentration (Figure 2C) suggest that chlorophyll-a peaked when the nitrogen availability was shrinking. It was hypothesized that this algal bloom was triggered by growth of cyanobacterial biomass, which does not require – unlike other algae – dissolved nitrogen in water, as it can utilize atmospheric nitrogen. This called for the need of extending the model and splitting phytoplankton component of the reference model into two taxa: eukaryotes and cyanobacteria. Temperature-dependencies and nutrient requirements (N-P ratio) for cyanobacteria were identified in literature. Compared to eukaryotes (Tmin = 9 °C, Topt = 24 °C, Tmax = 34 °C), the cyanobacteria can develop in warmer temperature window (Tmin = 22 °C, Topt = 28 °C, Tmax = 36 °C). As cyanobacteria can produce toxic compounds, it may also alter further prey-predator relationships in the food web. It is suggested by literature that the presence of cyanobacteria negatively affects the appetite of zooplankton.

Based on the above hypothesis, refinements were made to the process model. This hypothetic extension mainly started with the replacement of state element "s_phytop" by the state elements "s_cyano" and "s_eukar". Accordingly, the transition elements ("t_phytop") and prototype ("prot_t_phytop") were also replaced with the modified code of the transition elements ("t_cyano" and "t eukar") and prototypes ("prot_t_cyano" and "prot_t eukar"), respectively. Based on the estimation by the fishpond experts the initial concentration of the cyanobacteria was set as 0.05%. Systemic identification resulted in the maximum production rate coefficient for eukaryotes and cyanobacteria to be, 20 1/day and 3 1/day, respectively. Furthermore, the prototype program "prot_t_zoop" was also refined based on the new information on the competitive consumption rate kinetics. In the case of eukaryotes, maximum rate was set of 1.6 1/day was set based on an availability ratio of E/(E+C+D), where E, C, and D refer to eukaryotes, cyanobacteria, and detritus, respectively. For cyanobacteria with a maximum rate of 0.2 1/day with an availability ratio of C/(E+C+D) and for detritus with a maximum rate of 0.5 1/day with an availability ratio of D/(E+C+D).

Figure 2B and Figure2D demonstrates that this extension of the model delivered more accurate model predictions.

4B. Results and Discussion

4B.1 Practical useability of the model and its limitations

Although the refined model is capable of simulating ***zootechnical and water quality variables on strategic horizons***, it has to be emphasized that it is not an adequate tool for daily control of water quality, and it is ***not a day-to-day decision support tool***. Carp ponds are complex ecosystems characterized by various food web interactions, chemical and hydrological processes, many of which are influenced by drivers that are not under managerial control, making precise forecasting activity difficult. For instance, trophic interactions may differ from those simulated because of altered photosynthetic activity of algae due to changing atmospheric weather conditions; or hidden presence of unwanted trash fish, being a feed competitor to carps, may unexpectedly reduce carp yields. Therefore, it is particularly important to ***be aware of the limitations when using this tool for decision support.***

Nevertheless, practical applications of the model may include looking at forecasted patterns in water quality during planning of experimental settings. Most notably

- assessing the ***impact of different feeding rates*** on fish growth, detritus formation and sediment accumulations
- assessing the ***impact of different manuring rates*** on simulated patterns in water quality dynamics (algae, zooplankton, oxygen), fish growth and sediment accumulation.
- simulating ***the impact of different stocking densities*** on both water quality and zootechnical performance
- simulating the ***impact of different water management regimes*** (for instance rain-fed pond vs. maintenance of a target water level with intentional water supply) on water quality

Once experiments are started and interim measured data are available, the model can also be used for improving pond management, understanding species interactions, and gathering more knowledge about the actual state of the pond, general ecological relationships, and internal and external factors affecting production to better manage their operations.

The figures below provide graphical representation of model simulations. For instance, simulated datasets in Figure 3. provides guidance on how water quality variables may change in response to manuring interventions. In this case, it is suggested by the simulations that increased detritus levels and consequent lower transparency of water column negatively affects photosynthesis (algae formation) in the short run, which in turn also has impact on carp food (zooplankton) availability.

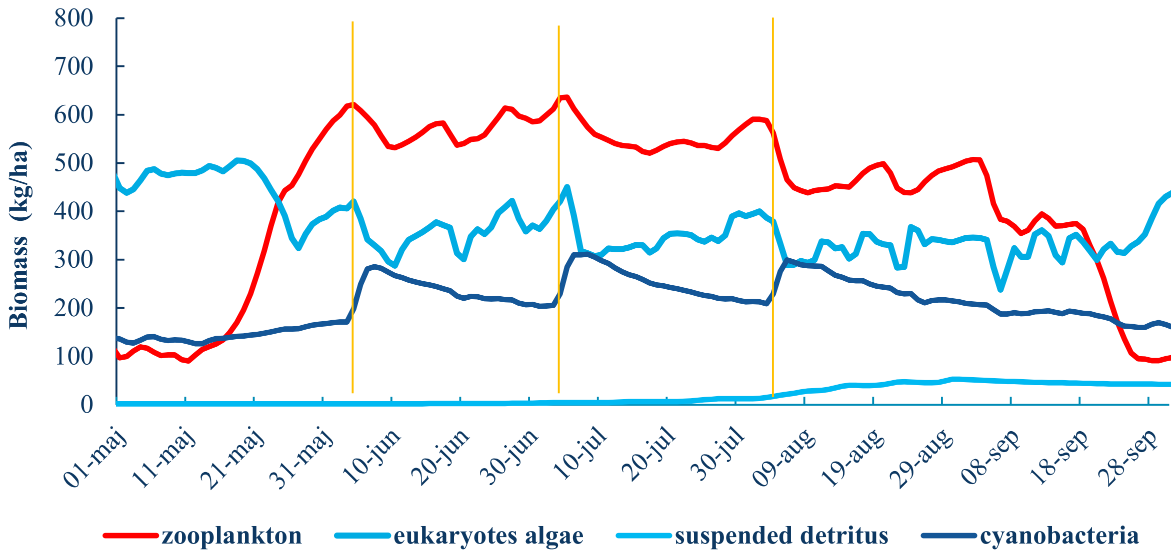

Figure 3. Simulated values for some water quality variables (48 hrs avg) under the following assumption for pond management: stocking density for carp: 300 kg/ha; feeding schedule: daily feed portions corresponded to 0.5; 1; 2; 2 and 1 % of estimated biomass weight in May, June, July, August, and September, respectively; manuring strategy: 4 t/ha preparatory + 5 t/ha supplementary dose in three instalments. Vertical orange lines represent time of supplementary manuring. Food web processes were simulated using recorded meteorological data of the 2017 season.

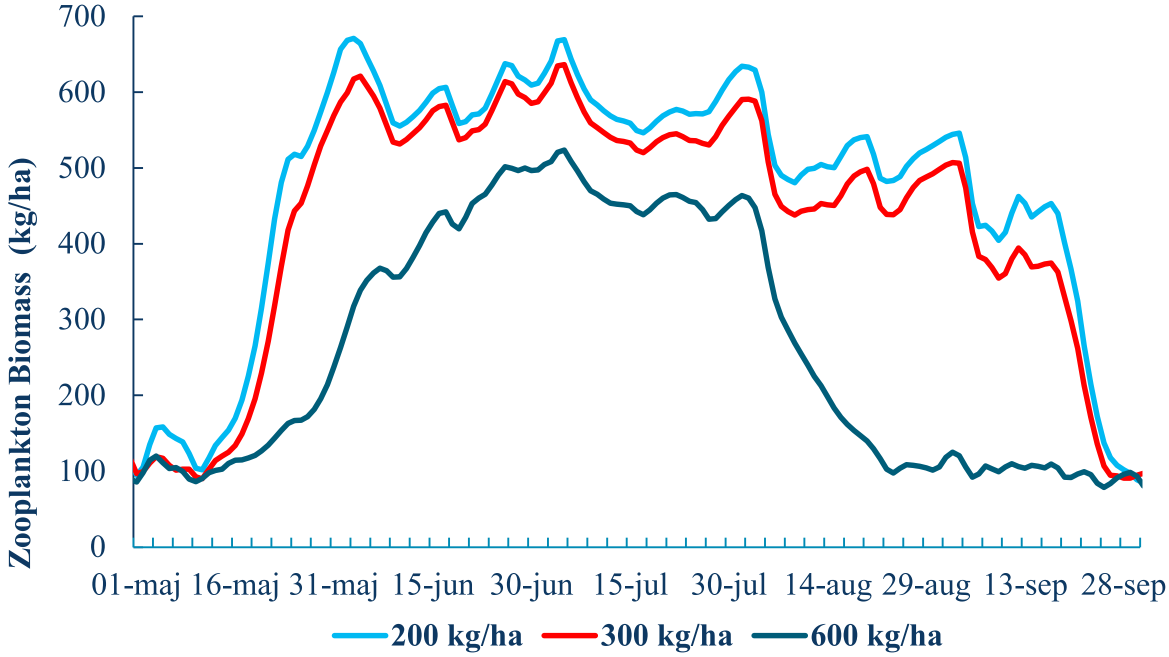

Figure 4. showcases how stocking density might be optimized prior to experiment subject to constraints in water quality in terms of chlorophyll levels. Higher stocking rates result in more intense predation pressure on zooplankton. If zooplankton is overgrazed in the middle of the summer when water temperatures are high, algal blooms are more likely to occur somewhat earlier than otherwise.

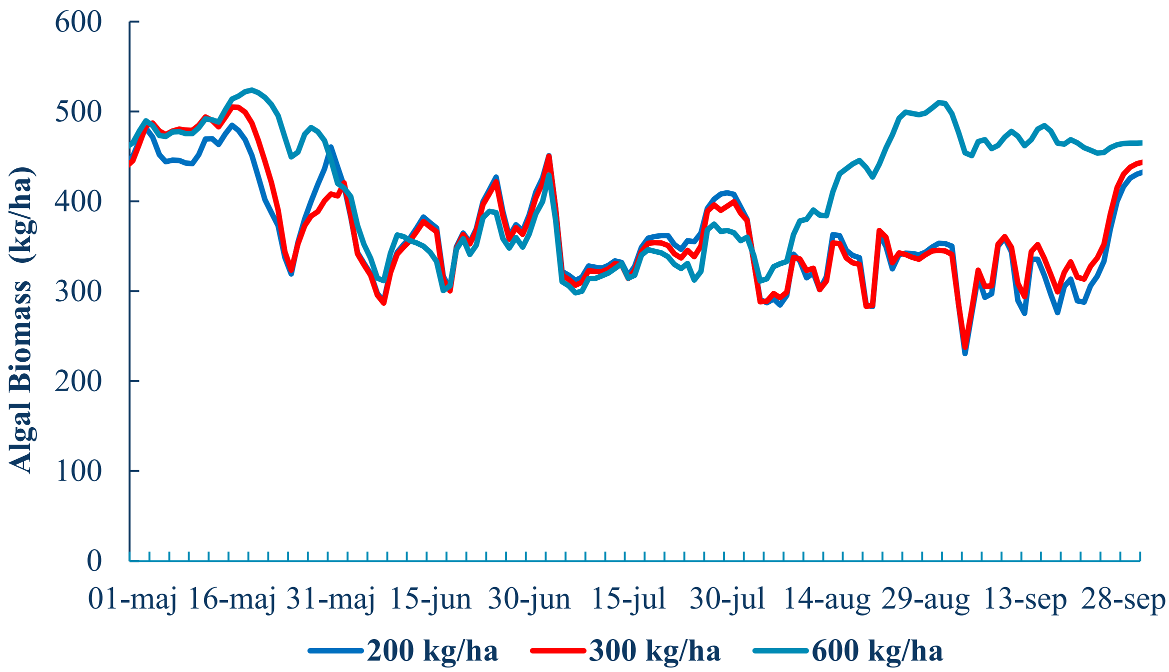

Figure 5. Simulated values for biomass of zooplankton and eukaryote algae under scenarios for carp stocking density. Feeding and manuring strategy are assumed to be the same as in Figure 2. The figure visualizes how different carp biomass impose different predation pressure on zooplankton communities, which in turn impact algal biomass. Further explanation is in the text above.

4B.2 Applied modelling framework

In the current study we applied the Programmable Process Structures (PPS) published and described by Varga and Csukás (2024). PPS generates unified models from one general state and one general transition meta-prototypes, accordingly unified solutions for the implementation and coupled execution of different sub-models can be achieved. The meta-prototypes are configured to represent both additive conservational measures and overwritable signals. In addition to input and output, the meta-prototypes provide a template for defining parameters, as well as temporal and spatial scales. These meta-prototypes are multiplied to explain the process net of the real problem being studied, which is the process of generating the actual models. In fact, a unique net structure is created that describes the nature of the process system under investigation and is made up of the real state and transition elements. The two general meta-prototypes can also be used to derive case-specific functional program prototypes that determine the functionalities within this structure. The locally executable programs are described in these program prototypes. The programs of the corresponding state or transition prototypes compute the real state and transition elements during execution. Uniform connections handle the communication between the state and transition parts, and a general-purpose kernel program executes the resulting model. The PPS framework represents a unified multi-disciplinary methodology to combine holistic structural and local functional characteristics in modeling and simulation-based problem-solving of various process systems. SWI-Prolog, a declarative, logical language is used to implement PPS. In particular, the unification of lists of functors in the logical programming AI language facilitates the efficient (and reusable) generation and execution of the models. The reusable, locally executable code prototypes offer advantages, especially for describing large, multi-scale systems with standardized components. The fact that most variables are local, promotes code reusability and simplifies variable naming within local programs. The model structure, the respective program codes, detailed output simulations for all model-based results from different case studies are available in the Mendeley Data of Sharma et al. (2024a) and Sharma et al. (2024b).

4B.3 Model application

Model inputs have to be provided in the attached excel sheet. As the first step, according to the requirements of the model, the following data must be collected for the planned trial in order to perform accurate and site-specific simulations. While some data are mandatory, other optional inputs may be left at default values unless site-specific information is available.

Pond-Specific Data (Mandatory): in Specific details about the pond where the trial will be conducted must be collected. These details include:

- Pond Area and Dimensions: Input the total surface area of the pond along with the length and width.
- Pond Depth: Specify the depth of the pond.
- Filling and Discharge Schedule:
    - Start date for pond filling.
    - Number of days allocated for pond filling.

- o Discharge water schedule, including the number of days the water will be retained and planned for discharge.

Feed Input Data (Mandatory): For accurate modelling of fish growth and nutrient cycling, following feed related input details must be collected:

- Feed Quantity: Specify the amount of feed planned per hectare per day (kg/ha/day).
- Feeding Schedule: Provide the schedule in terms of the number of feeding days.
- Nutrient Composition: Include data on the nutrient breakdown of the feed (stoichiometric compositions- C, N, P, O, H).
- Moisture Content and Dry Weight: Provide data on the moisture content and dry weight of the feed.

Fish Stocking Data (Mandatory): It is to be noted that the model is designed to account of stocked common carp. In this respect the following information must be provided:

- Planned Stocking Date: Indicate when the fish will be stocked.
- Stocking Density/Total Weight: Enter the density of fish in kg/ha or the total weight of the fish being stocked.
- Number of Fish (pieces): Specify the number of individual fish.
- Average Individual Weight: Provide the average weight per fish (in kg).

Zooplankton and Detritus Data (Optional): If available, input site-specific measurements of zooplankton and detritus from previous trials conducted in similar settings. This data can improve the precision of the model.

Phytoplankton Data (Optional) If available, include Phytoplankton measurements: Site-specific data, particularly for cyanobacteria and eukaryotes, from previous trials or from the water remaining in the ponds prior to filling. This will enhance the model’s accuracy.

The model already contains embedded stoichiometric data for carp, zooplankton, phytoplankton groups. If more precise measurements are available from the site, they can be added. Otherwise, these values can remain at the model's default settings.

Water Quality Data (Mandatory): If site-specific input water quality data from previous studies or measurements is available, this data can be used to generate more precise site-specific results. his may include: Dissolved oxygen levels, nitrogen, and phosphorus concentrations.

Meteorological Data (Mandatory): The model requires meteorological data from the previous year to simulate realistic environmental conditions. This includes: daily air temperature, wind speed, precipitation, radiation preferably from local weather station. Data from a year with similar weather patterns for the entire trial year, and ensure it covers daily time steps.

Planned fertilizer input related data (Mandatory) You will need to input the planned schedule for fertilizer application, specifying: the fertilizer type: if organic manure or inorganic fertilizer or both to be added. Furthermore, fertilizer composition: nutrient composition (N, P), stoichiometric data (C, H, O) (optional), moisture content, and dry weight of the fertilizer etc.

Macrophyte (Reed) Component (Optional) The model includes a component for emergent macrophytes (reed). This section can be left as default if no specific information is available. Or if better estimates on: the percentage of reed in the pond. usual practices of cutting the reed (amount and timing). These values can also be adjusted in the model.

It must be ensured that all nutrient-related data (including feed, fertilizer, etc.) is converted into kmol/kg units before inputting them into the model.

The more precise the site-specific data provided, the more accurate the model simulations will be. For optional data, using default settings will allow the model to run effectively but may result in less site-specific outcomes.

After obtaining the above listed data from the user, in the second step, the following files are then prepared for PPS model generation:

- Core.pl: file, containing the control parameters of the simulation
- Datasupply.pl: contains the meteorological data, as well as the managerial actions. Content of file typically include:

Year,Month,Day,AirTemp(C),WaterTemp(C),WindSpeed(m/s),Precip(mm/day),ACoeff(nd),WaterSupply(m3/day),Radiation(W/m2),ModeofWaterSuppoly(nd),DepthofPond(cm),ForageSupply(kg/ha/day),FertilizerSupply(t/ha/day),NwithSuppliedWater(kg/m3),PwithSuppliedWater(kg/m3),NwithSuppliedWaterAvg(kg/m3),PwithSuppliedWaterAvg(kg/m3)

- Model_N.pl: textual description of PPS model elements (states, transitions, dlists, as well as connections between the state and transition elements)
- Model_G_prot.graphml: contains the calculating formulas (local programs) of the various model prototypes
- Make_D.pl: contains the initial values and parameters of the model

The raw data in prescribed format can be send to MATE team for further processing, running the model and generating simulations for various desired outputs of the planned trail

5B. References

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Work Participants	WU, WR, NAIK			

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