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Research Article

A Flexible Water Quality Modelling Simulator Based on Matrix Algebra

Matris Cebrine Dayanan Esnek Bir Su Kalitesi Simülatörü

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Abstract

For the sustainable management of aquatic ecosystems, an integrated approach is required. This is why watershed-based management is becoming an increasingly popular instrument for the improvement of water quality. Water quality models serve as a central part of the watershed management. Predictive water quality models are valuable tools, but they are usually complex infrastructures in terms of both operation and software development. The aim of this study is to develop the water quality simulator of a larger hydro-ecological modelling framework. Since the water quality problems are diverse, development of one water quality kinetics sub-model that would fit to all water quality problems would be an impossible task. This is the reason why; the water quality simulator software code was developed following the open source philosophy, implemented on a high level (yet high performance) programming language, and documented intensively in-line to enhance the code readability. The water quality simulator software, which is designed as a component of HIDROTURK integrated modelling platform, consists of a general transport sub-model, three water quality kinetics sub-models and utilities.

Keywords: *water quality modelling, eutrophication, open source code, generic pollutants*

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Öz

Su ekosistemlerinin sürdürülebilir yönetimi için entegre bir yaklaşım gereklidir. Bu nedenle havza bazlı yönetim, su kalitesinin iyileştirilmesi için giderek daha popüler bir araç haline gelmektedir. Su kalitesi modelleri havza yönetiminin merkezi bir parçasıdır. Su kalitesi tahminleri yapan modeller değerli araçlardır, ancak işletme ve yazılım geliştirme açısından genellikle karmaşık altyapı bileşenleridir. Bu çalışmanın amacı, daha büyük bir hidro-ekolojik modelleme çerçevesinin su kalitesi simülatörünü geliştirmektir. Su kalitesi sorunları çok çeşitli olduğundan, tüm su kalitesi sorunlarına uyacak tek bir su kalitesi kinetiği alt modelinin geliştirilmesi imkansızdır. Bu nedenle; su kalitesi simülatörü yazılım kodlaması, açık kaynak felsefesini takip ederek yüksek seviyede (ancak yüksek performanslı) bir programlama dilinde gerçekleştirilmiş ve kod okunabilirliğini artırmak için kod içi belgelendirmeye önem verilmiştir. Genel bir taşınım alt modeli, üç su kalitesi kinetiği alt modeli ve yardımcı programlardan oluşan temel su kalitesi simülatör yazılımı HİDROTÜRK entegre modelleme platformu için bir bileşen olarak tasarlanmıştır.

Anahtar sözcükler: *su kalitesi modelleme, ötrofikasyon, açık kaynak kodu, genel kirleticiler*

Introduction

Water quality models can be defined as idealized formulations that represent the response of a physical system to external forcing. The impact-effect relationship between loading and concentration depends on the physical, chemical, and biological characteristics of the receiving waterbodies. Predictive water quality models are important tools for water quality management for aquatic ecosystems. In aquatic science and environmental/water resources engineering, water quality models are used to evaluate the potential impacts of external forcings and to understand the functioning of the system (Thomann & Mueller, 1987; Chapra, 1997; Arhonditsis & Brett, 2004). They are useful tools to get a holistic picture of ecosystems, to fill in the gaps in field data or to forecast the systems responses to different external forcings.

Water quality models have been used throughout the history of environmental and water resources engineering. These models evolved from simple equations to sophisticated modelling software following the new concerns related to the problems in the aquatic ecosystems and consequently rising water quality management problems. The early modelling studies mostly focused on the urban waste load allocation problem. The model developed by Streeter and Phelps (1925) on the Ohio River was the first study in the field. The following studies provided the evaluation of dissolved oxygen levels in streams and estuaries (Velz, 1938; Velz, 1947;

O'Connor, 1960; O'Connor, 1967). Bacteria models were also developed (O'Connor, 1962).

In the 1960s, digital computers became available, which led to major advances in both the models and the ways they are applied. Computers allowed analysts to address more complicated system geometries, kinetics, and time variable simulations; however, dissolved oxygen was still the main focus. The computers also allowed a more comprehensive approach to water quality problems. A watershed could be analysed as an entire system, rather than focusing on local effects of single point sources. As tools developed originally in the field of operations, models were used to generate cost effective treatment alternatives (Thomann & Sobel, 1964; Deininger, 1965; Ravelle et al., 1967).

In the 1970s eutrophication was the principal water quality problem addressed. Consequently, more mechanistic representations of biological processes were included leading to the development of detailed nutrient and food chain models (Chen, 1970; Chen & Orlob, 1975; Di Toro et al., 1971; Canale et al., 1974; Canale et al., 1976) incorporating more feedback loops and nonlinear kinetics.

In the 1980s more detailed problems such as the food web and toxic substances were on concern, because they represented an important threat to human and ecosystem health. Solid matter in the transport and fate of toxicants were among the major modelling advances in this period (Thomann & Di Toro, 1983; Chapra & Reckhow, 1983; O'Connor, 1988).

Following the needs and developments in the world, many water quality codes became available. Some of them such as WASP 8.32 (United States Environmental Protection Agency, 2020), QUAL2K (Chapra et al., 2012), QUAL2Kw (Pelletier & Chapra, 2008), HEC-RAS 5 (Brunner, 2016), are free of charge, whereas others such as LAKE2K (Chapra & Martin, 2012), CE-QUAL-W2 4.2 (Wells, 2021), AQUATOX (Park & Clough, 2018) and DELWAQ (Deltares, 2020) are open sourced. These models are mainly developed and used for investigating the conventional water pollution and eutrophication problem.

The number of studies on nutrient based water pollution and eutrophication modelling in Turkey is substantially less than those in the United States and in the European Union. Yet, it is known that the first studies started in the 1980s (Artan, 1983). For river water quality modelling studies in Turkey QUAL2E (Barbaros, 1997; İnkayalı, 2001; Küçükballı, 2003; Özbayrak, 2003) and QUAL2K (Baysal, 2014) models have been used usually. QUAL2E/QUAL2K models take the primary

producers in the ecosystem into account. Although the models meet the needs in many watershed management studies in terms of the processes that they consider, their non-dynamic nature can cause problems, especially if the natural drainage network in the studied watershed contains streams and stagnant waters. This situation restricts the applicability of these models in Turkey where many reservoirs have been built in recent years. Yüceer (2005) developed a fully dynamic version of QUAL2E model, but the relevant model is not suitable for dynamic simulations in river systems where there are deep and stratified lakes and reservoirs, since all segments are fully mixed reactors. One of the models, WQRRS (Water Quality for River and Reservoir Systems), developed by US Army Corps of Engineers, is suitable for the simulation of deep and stratified lakes. WQRRS (United States Army Corps of Engineers, 1978) model's reservoir module was adapted only for Turkey. The model, which assumes horizontally complete mixing, contains many vertical layers. It has been applied several times in Turkey (Öktem, 1996; Genç, 1998; Üstün, 1998). Hasanoğlu (2015) realized dissolved oxygen simulations of Borabey Reservoir by using the more advanced CE-QUAL-W2 model. Instead of using models developed specifically for rivers and standing waters, general-purpose water quality models (suitable for lakes, rivers and estuaries) are also used in the studies in Turkey. Among these models, WASP was used by Yenilmez (2007) and Ekdal (2008), whereas, AQUATOX was used by Karaaslan (2009) and Karami (2017). The main disadvantage of these models is that they allow very rough definition (completely mixed or two-layered) of stagnant water bodies. This makes the calibration of the relevant models inefficient and integration with optimization models become very difficult. PCLake, which was applied to Eymir Lake by Kuzyaka (2016), is a model suitable for shallow lake ecosystem simulations.

Other than the models described above, although some original modelling infrastructures were produced for streams (Yüceer, 2005) and lakes (Aydın, 1993; Davaslıgil, 1998; Koçal, 2006) in Turkey, development of these infrastructure for general purpose applications has not continued.

The aim of this study is to develop an independent water quality simulation code following the criteria as listed below. The next section of the paper will provide more details about their implementation as a water quality modelling software.

- **Criterion 1:** The model should be compatible with Turkey's condition in both: biogeographical diversity and data availability. Turkey's biogeographical condition necessitates a flexible water quality modelling framework so that it can make the application of multiple water quality kinetics sub-models possible. The model should also be

able to cope with irregular data and missing data. It should also be scalable, from simple sub models to more complex ones making the use of simple model input data sets at first and then upgrading to the model inputs for more sophisticated water quality models without repeating the model inputs that define the simple versions of the final model.

- **Criterion 2:** The model should be applicable and operable based on the knowledge in water quality issues and field and laboratory methods as successfully applied in Turkey for decades. The application and operation of water quality models even for simple cases will necessitate a teamwork conducted by a team of field scientists trained in field methods, laboratory infrastructure with trained technicians and modelling experts with broad theoretical knowledge and computer skills.

- **Criterion 3:** The model should be applicable to different waterbodies such as streams and rivers, lakes, reservoirs, estuaries and coastal waters. The transport scheme should be designed considering this criterion. The model should also be aware of the waterbody type of each model box so that different sub-models or assumptions can be programmed for different waterbody types. The hydrodynamic variables (flow rates and turbulent diffusion/longitudinal dispersion if necessary) will be inputs provided by the users by all means necessary.

- **Criterion 4:** The model should contribute to the general knowledge of modelling for the academicians and institutions. This is an important issue, since water quality modelling software for general purposes are already available. However, specific applications of such modelling software with different kinetic sub models are not straightforward and sometimes impossible. In such a case further development of those modelling software may be necessary but can be impossible if the original developers do not have a source code sharing or developmental support policy.

- **Criterion 5:** The model code should be able to incorporate different water quality kinetic sub models and therefore should be easy to study and understand. As stated previously, Turkey's complex biogeography necessitates the application of different water quality kinetic sub models. To develop one infrastructure for making all of the different

water quality sub models is a considerably difficult task, if possible at all. Therefore, the general code of the model should be easy to study and to extend.

Method

As discussed previously, the water quality simulation code consists of a transport code that is solving the transport equation by box model discretization. Three water quality sub-models: 1) a general water quality model for management applications targeting conventional pollutants and eutrophication, 2) an advanced water quality model for more detailed management applications and research, and 3) a generic water quality model with an unlimited number of state variables which are implemented as water quality sub-models.

The Main Transport Equation and Water Quality Kinetics Sub Models

The Transport Equation and its Discretization and its Solution

The transport equation is the advection diffusion equation (Equation 1) considering x and y as the coordinates of any point in lateral directions and z as the coordinate in vertical direction.

$$\frac{\partial C}{\partial t} = -u \cdot \frac{\partial C}{\partial x} + D_x \cdot \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{dy} + D_y \cdot \frac{\partial^2 C}{\partial y^2} - w \cdot \frac{\partial C}{dz} + D_z \cdot \frac{\partial^2 C}{\partial z^2} - v_{set} \cdot \frac{\partial C}{dz} + \sum_{h=1}^{\substack{number\ of\ external\ sources/\ sinks}} S_h + \sum_{k=1}^{\substack{number\ of\ kinetic\ processes}} R_k$$

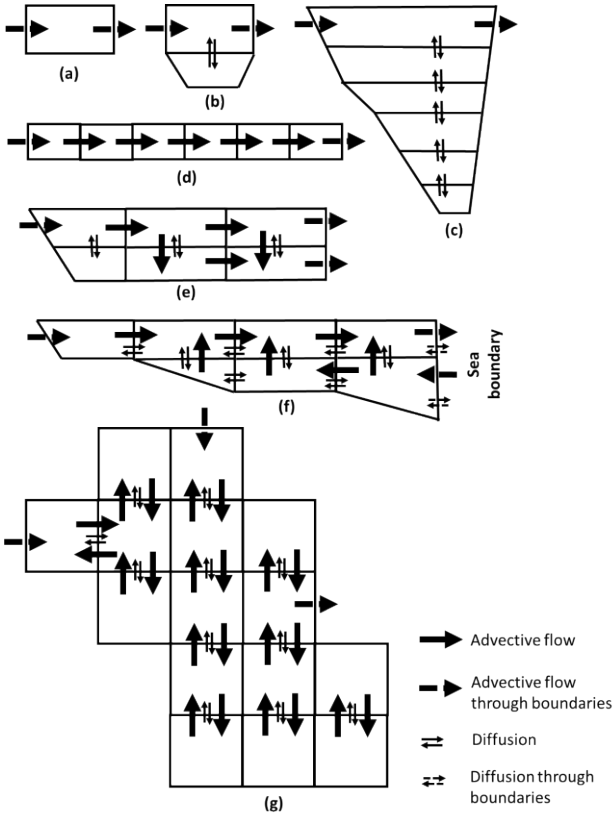
(Equation 1)

Where; C is the concentration of any state variable [$M \cdot T^{-3}$]; t is the time [T]; u, v and z are the velocities in x, y, z directions [$L \cdot T^{-1}$]; v_{set} is the settling velocity [$L \cdot T^{-1}$]; D_x, D_y and D_z are the diffusion coefficients in x, y, z directions [$L^2 \cdot T^{-1}$]; k is the index for the processes related to the particular state variable; R_k is the reaction rate of the process k related to the particular state variable [$L \cdot T^{-3} \cdot T^{-1}$]; h is the index for external mass inflows/withdrawals for a particular state variable; S_h is the inflow/withdrawal rate of the inflow/outflow for a particular state variable [$L \cdot T^{-3} \cdot T^{-1}$].

As discussed previously in the introduction; the equation was discretized into spatial boxes, where each box was assumed to be a completely mixed reactor (Figure 1), which is dynamic in time but homogeneous in space.

Figure 1

The Spatial Discretization into Boxes



(a) A completely mixed pond/lake (b) A two-layer lake (c) A vertical one-dimensional and horizontally fully mixed lake/reservoir (d) A non-dispersive river (e) Two-layer scheme for a narrow and deep reservoir (f) Two-layer scheme for a narrow and deep estuary (g) Top view of a multi-dimensional general waterbody (Only top boxes shown each of the box seen could have several neighbouring boxes in vertical direction)

As seen in Figure 1, a model domain consists of boxes and the model domain consists of any number of boxes. Boxes can have any shape, and transfer water and

through advection and diffusion processes. A box can be connected to any number of other boxes through links. The boxes are vertically grouped into segments. The boxes and segments can have any configuration and shape (Figure 3). The only limitation imposed is that a box cannot be a part of more than one segment.

Figure 2

Boxes and Links

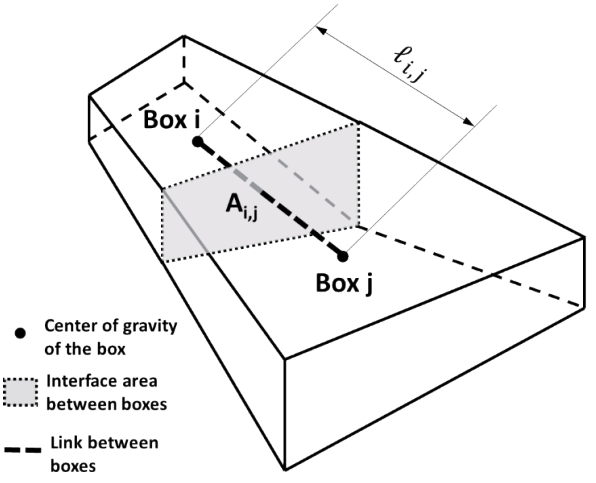
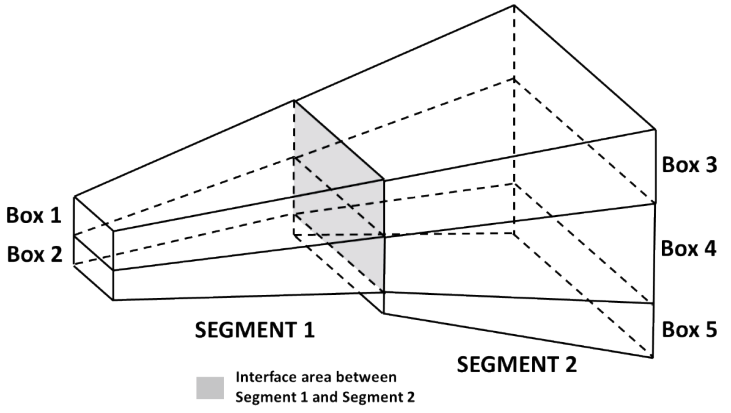


Figure 3

Boxes and Segments



The boxes can be of any shape and the model uses user-entered shape functions for the volume-depth relations of a segment, depth-surface area relations of a segment, depth-interface area relations between two segments and depth-mixing length areas between to segments. Basically, the model calculates the volume of each box and segment (as the sum of related boxes) each time step conducting a water mass balance. The volume is translated to depth and to water surface elevation. This information is then used for each box to calculate the surface area, the interface area and the mixing length between any other neighbouring boxes eliminating the need of user defined time series for these important model inputs. The algorithm conducting these calculations is fairly complex with many intermediate checks and is therefore not given in this paper.

The first step of a modelling study using the described model is to spatially discretize Equation 1 according to box model scheme is to integrate it over the box volumes, box interface areas and box distances. Equation 2 is an example of such an integration considering box i and its link to box j as illustrated in Figure 1.

$$\int_{V_i} \frac{\partial C}{\partial t} \cdot dV_i = \underbrace{\int_{A_{i,j}} \left(-u \cdot \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x} \cdot dx - v \cdot \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y} \cdot dy - w \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \cdot dz \right) \cdot dA_{i,j}}_{ADVECTION} +$$

$$\underbrace{\int_{A_{i,j}} \left(D_x \cdot \int_{\ell_{x,i,j}} \frac{\partial^2 C}{\partial x^2} \cdot dx + D_y \cdot \int_{\ell_{y,i,j}} \frac{\partial^2 C}{\partial y^2} \cdot dy + D_z \cdot \int_{\ell_{z,i,j}} \frac{\partial^2 C}{\partial z^2} \cdot dz \right) \cdot dA_{i,j}}_{DIFFUSION} -$$

$$\underbrace{\int_{A_{i,j}} \left(v_{set} \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \right) \cdot dA_{i,j}}_{SETTLING} + \underbrace{\sum_{h=1}^{\substack{number\ of\\ external\\ sources/sinks}} \int_{V_i} S_h \cdot dV_i}_{EXTERNAL\ SOURCES\ AND\ SINKS} +$$

$$\underbrace{\sum_{k=1}^{\substack{number\ of\\ kinetic\ processes\\ for\ the\ state\\ variable}} \int_{V_i} R_k \cdot dV_i}_{KINETIC\ PROCESSES}$$

(Equation 2)

Evaluating the advection terms

$$\int_{A_{i,j}} \left(-u \cdot \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x} \cdot dx - v \cdot \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y} \cdot dy - w \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \cdot dz \right) \cdot dA_{i,j} =$$

$$-u \cdot \int_{A_{i,j}} \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x^2} \cdot dx \cdot dA_{i,j} - v \cdot \int_{A_{i,j}} \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y^2} \cdot dy \cdot dA_{i,j} -$$

$$w \cdot \int_{A_{i,j}} \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z^2} \cdot dz \cdot dA_{i,j}$$

(Equation 3)

Since

$$u \cdot \int_{A_{i,j}} dA_{i,j} = Q_{x,i,j}; \quad v \cdot \int_{A_{i,j}} dA_{i,j} = Q_{y,i,j}; \quad w \cdot \int_{A_{i,j}} dA_{i,j} = Q_{z,i,j}$$

(Equation 4)

Equation 3 can be rewritten as

$$\int_{A_{i,j}} \left(-u \cdot \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x} \cdot dx - v \cdot \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y} \cdot dy - w \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \cdot dz \right) \cdot dA_{i,j} =$$

$$-Q_{x,i,j} \cdot \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x^2} \cdot dx - Q_{y,i,j} \cdot \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y^2} \cdot dy - Q_{z,i,j} \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z^2} \cdot dz$$

(Equation 5)

Considering that,

$$\int_{\ell_{x,i,j}} \frac{\partial C}{\partial x^2} \cdot dx = \frac{\partial C}{\partial x} \approx \frac{C_j - C_i}{\ell_{x,i,j}}; \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y^2} \cdot dy = \frac{\partial C}{\partial y} \approx \frac{C_j - C_i}{\ell_{y,i,j}}; \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z^2} \cdot dz = \frac{\partial C}{dz} \approx \frac{C_j - C_i}{\ell_{z,i,j}} \quad and$$

$$Q_{i,j} = Q_{x,i,j} + Q_{y,i,j} + Q_{z,i,j}$$

(Equation 6)

$$\int_{\ell_{x,i,j}} \frac{\partial C}{\partial x} \cdot dx = \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y} \cdot dy = \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \cdot dz = (C_i - C_j)$$

(Equation 7)

Equation 5 can be rewritten as

$$\int_{A_{i,j}} \left(-u \cdot \int_{\ell_{x,i,j}} \frac{\partial C}{\partial x} \cdot dx - v \cdot \int_{\ell_{y,i,j}} \frac{\partial C}{\partial y} \cdot dy - w \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \cdot dz \right) \cdot dA_{i,j} = -Q_{i,j} \cdot (C_j - C_i)$$

(Equation 8)

Evaluating the diffusion terms

$$\int_{A_{i,j}} \left(D_x \cdot \int_{\ell_{x,i,j}} \frac{\partial^2 C}{\partial x^2} \cdot dx + D_y \cdot \int_{\ell_{y,i,j}} \frac{\partial^2 C}{\partial y^2} \cdot dy + D_z \cdot \int_{\ell_{z,i,j}} \frac{\partial^2 C}{\partial z^2} \cdot dz \right) \cdot dA_{i,j} =$$

$$D_x \cdot \int_{A_{i,j}} \int_{\ell_{x,i,j}} \frac{\partial^2 C}{\partial x^2} \cdot dx \cdot dA_{i,j} + D_y \cdot \int_{A_{i,j}} \int_{\ell_{y,i,j}} \frac{\partial^2 C}{\partial y^2} \cdot dy \cdot dA_{i,j} +$$

$$D_z \cdot \int_{A_{i,j}} \int_{\ell_{z,i,j}} \frac{\partial^2 C}{\partial z^2} \cdot dz \cdot dA_{i,j}$$

(Equation 9)

by considering Equation 6, Equation 7 and Equation 10; Equation 9 can be rewritten as

$$\int_{A_{i,j}} dA_{i,j} = A_{i,j} \quad and \quad \ell_{i,j} = \ell_{x,i,j} + \ell_{y,i,j} + \ell_{z,i,j} \quad and \quad D_{i,j} = f(D_x, D_y, D_z)$$

(Equation 10)

where f is an arbitrary function depending on the size, shape and positions of the neighbouring boxes i and j

$$\int_{A_{i,j}} \left(D_x \cdot \int_{\ell_{x,i,j}} \frac{\partial^2 C}{\partial x^2} \cdot dx + D_y \cdot \int_{\ell_{y,i,j}} \frac{\partial^2 C}{\partial y^2} \cdot dy + D_z \cdot \int_{\ell_{z,i,j}} \frac{\partial^2 C}{\partial z^2} \cdot dz \right) \cdot dA_{i,j} =$$

$$\frac{A_{i,j} \cdot D_{i,j}}{\ell_{i,j}} \cdot (C_j - C_i)$$

(Equation 11)

Considering the index j as all the neighbouring boxes of i, the advective and diffusive mass flow rate can be written as in Equations 12 and 13 respectively, where M is mass of any state variable. Now, they can be plugged in back to Equation 2 and Equation 14 is obtained.

$$\left(\frac{\partial M}{\partial t}\right)_{ADVECTION} = \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{j,i} \cdot C_j - \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{i,j} \cdot C_i$$

(Equation 12)

$$\left(\frac{\partial M}{\partial t}\right)_{DIFFUSION} = \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} \frac{A_{i,j} \cdot D_{i,j}}{\ell_{i,j}} \cdot (C_j - C_i)$$

(Equation 13)

$$\int_{V_i} \frac{\partial C}{dt} \cdot dV_i = \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{j,i} \cdot C_j - \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{i,j} \cdot C_i + \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} \frac{A_{i,j} \cdot D_{i,j}}{\ell_{i,j}} \cdot (C_j - C_i)$$

$$\underbrace{\int_{A_{i,j}} \left(v_{set} \cdot \int_{\ell_{z,i,j}} \frac{\partial C}{\partial z} \right) \cdot dA_{i,j}}_{SETTLING} + \underbrace{\sum_{h=1}^{\substack{number\ of\\ external\\ sources/sinks}} \int_{V_i} S_h \cdot dV_i}_{EXTERNAL\ SOURCES\ AND\ SINKS} +$$

$$\underbrace{\sum_{k=1}^{\substack{number\ of\\ kinetic\ processes\\ for\ the\ state\\ variable}} \int_{V_i} R_k \cdot dV_i}_{KINETIC\ PROCESSES}$$

(Equation 14)

Considering that the settling term as an advective inflow from overlaying box (indexed as obox) and outflow to underlying box (indexed as ubox) outflow, and taking all the integrals in Equation 14; Equation 15 is obtained. Dividing both sides of Equation 1 by the volume of box i, the final form of spatially discretized transport equation is obtained.

$$\frac{\partial M_i}{dt} = \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{j,i} \cdot C_j - \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} Q_{i,j} \cdot C_i + \sum_{j=1}^{\substack{Number\ of\\ neighbouring\\ boxes\ to\ box\ i}} \frac{A_{i,j} \cdot D_{i,j}}{\ell_{i,j}} \cdot (C_j - C_i) +$$

$$v_{set,obox,i} \cdot A_{i,obox} \cdot C_{obox} - v_{set,obox,i} \cdot A_{i,ubox} \cdot C_i +$$

$$\sum_{h=1}^{\substack{number\ of\ external\ sources\ and\ sinks\\ sinks}} S_h \cdot V_i + \sum_{k=1}^{number\ of\ kinetic\ processes} R_k \cdot V_i$$

(Equation 15)

$$\frac{\partial C_i}{dt} = \sum_{j=1*}^{\substack{Number\ of\ neighbouring\\ boxes\ to\ box\ i}} \frac{Q_{j,i}}{V_i} \cdot C_j - \sum_{j=1}^{\substack{Number\ of\ neighbouring\\ boxes\ to\ box\ i}} \frac{Q_{i,j}}{V_i} \cdot C_i + \sum_{j=1}^{\substack{Number\ of\ neighbouring\\ boxes\ to\ box\ i}} \frac{A_{i,j} \cdot D_{i,j}}{\ell_{i,j} \cdot V_i} \cdot (C_j - C_i) +$$

$$\frac{v_{set,obox,i} \cdot A_{i,obox}}{V_i} \cdot C_{obox} - \frac{v_{set,obox,i} \cdot A_{i,ubox}}{V_i} \cdot C_i + \sum_{h=1}^{\substack{number\ of\ external\ sources\ and\ sinks}} S_h + \sum_{k=1}^{\substack{number\ of\ kinetic\ processes\ for\ the\ state\ variable}} R_k$$

(Equation 16)

If Equation 16 is written for each model box and state variable a system of equations is obtained. The transport related terms related to different state variables are independent from each other; however, the water quality kinetics related terms couple the entire equation system over the state variables. The system of equations can be written in matrix form as shown in Equation (17).

$$\frac{\partial}{dt}\left[\ C\ \right]_{m\,x\,n} = \left(\left(\left[\begin{matrix}Transport\\ Matrix\end{matrix}\right]_{m\,x\,m} x \left[\ C\ \right]_{m\,x\,n}\right) + \left[\ TEI\ \right]_{m\,x\,n}\right) + \left[\ R\ \right]_{m\,x\,n}$$

(Equation 17)

where m is the number of boxes, n is the number of state variables, $\left[\ C\ \right]$ is the concentration of each box of each state variable [ML^{-3}], $\left[\begin{matrix}Transport\\ Matrix\end{matrix}\right]_{m\,x\,m}$ is the transport matrix for each box [T^{-1}], $\left[\ TEI\ \right]_{m\,x\,n}$ is the total external inflows matrix for all boxes and state variables[$ML^{-3}T^{-1}$] and $\left[\ R\ \right]_{m\,x\,n}$ is the kinetic rates for each

box and state variable [$ML^{-3}T^{-1}$] handled by one of the water quality kinetics sub models in the following sections. The transport matrix has the following rules that help developing an algorithm to generate it:

- All outflows are located on the diagonal of the transport matrix, where the row and column indexes should be equal to the box number.
- If there is an advective inflow, then the inflow will be located on the receiving boxes row and on the boxes column from which inflow is received.
- A diffusive mass transfer is considered as two advective inflows one from the relevant box to its neighbour as an outflow and one from the neighbour of the relevant box as an inflow. Since both boxes in this case will get one inflow and one outflow, four elements of the transport matrix will be occupied. Considering i as the relevant box and j as its neighbour, matrix elements Row:i, Column:i, Row:j, Column:j; Row:i, Column:j and Row:j, Column:i will be occupied by the diffusive transport term.

The transport equation is handled in the same way for all of the state variables. The kinetic sub models are represented by the kinetics matrix $\left[\ R\ \right]_{m\,x\,n}$ plugged into Equation 17. The contents of the kinetics matrix are given in the next three subsections.

The numerical solution of Equation 17 is straightforward using the simple Euler scheme as shown in Equation 18,

$$\left[\ C^{t+\Delta t}\ \right]_{m\,x\,n} = \left[\ C^{t}\ \right]_{m\,x\,n} + \left(\left(\left(\left[\begin{matrix}Transport^{t}\\ Matrix\end{matrix}\right]_{m\,x\,m} x \left[\ C^{t}\ \right]_{m\,x\,n}\right) + \left[\ TEI^{t}\ \right]_{m\,x\,n}\right) + \left[\ R^{t}\ \right]_{m\,x\,n}\right) \cdot \Delta t$$

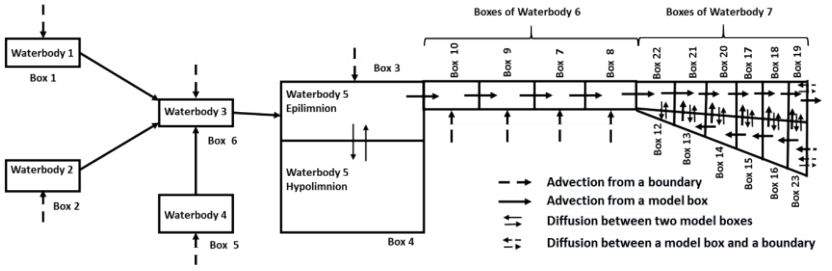
(Equation 18)

where the superscript $t + \Delta t$ represents the next time step and t represents the present time step.

The box model discretization approach provides great flexibility when building a model. Since boxes can be of any shape and configuration, all the waterbodies of an entire watershed could be incorporated into a single model domain (Figure 4).

Figure 4

An Example Model Domain Incorporating Several Waterbodies



In such a configuration, some of the segments (with one or more vertical boxes) could correspond to one waterbody, whereas other segments with their boxes could be assigned into single waterbodies that need to be simulated in more detail. As seen in this Figure, a box could be considered as important as an entire waterbody (such as the boxes 1 to 4 in Figure 4), or a relatively insignificant part of a waterbody (such as box 12 in Figure 4). To provide this flexibility; defining the box shapes is a complex task and the water quality modelling software developed in this study includes the infrastructure that enable to track:

- The water surface elevation of each box depending on its volume
- The horizontal interface area and mixing length of each box pairs depending on their surface and bottom elevations
- The vertical interface area of each box pairs being same segments

Water Quality Sub Model 1

Water quality kinetics sub model 1 (Figure 4) is a conventional water quality model intends for general water pollution problems and eutrophication oriented but not limited to environmental engineering related water quality studies. The model includes 10 state variables and is configured for 4 different complexity levels (Table 1).

As seen in Table 1, the model is designed to be scalable for managing different water quality problems. The interactions among the state variables are illustrated in Figure 5. State variables salinity and total solids are kinetically non-reactive however they are subjected to transport, where salinity is conservative and total suspended solids are subjected to settling. Salinity is used to calculate the saturation concentration of dissolved oxygen and can be used as a conservative tracer. Total suspended solids are used as a common conventional water quality parameter for water quality classification, can be used as ecological state indicator and is usually measured in most of the monitoring campaigns.

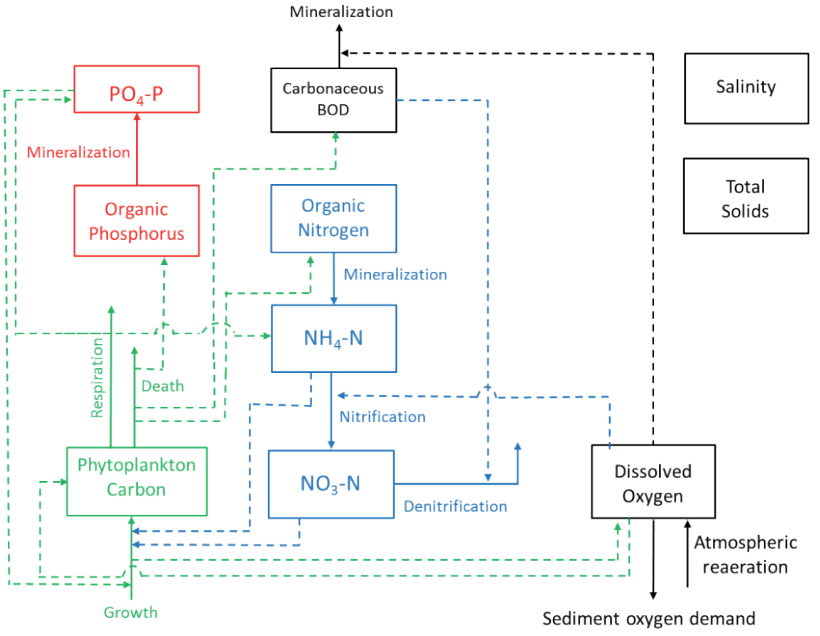
Table 1

State Variables and Complexity Levels of Water Quality Kinetics Sub Model 1

State Variable No	State Variable	Representation in Model	Complexity Level 1	Complexity Level 2	Complexity Level 3	Complexity Level 4
1	Salinity	SALT	✓	✓	✓	✓
2	Total Suspended Solids	TSS	✓	✓	✓	✓
3	Carbonaceous BOD	CBOD	✓	✓	✓	✓
4	Dissolved Oxygen	DOXY	✓	✓	✓	✓
5	Non-algal Organic Nitrogen	ORGN		✓	✓	✓
6	Ammonia Nitrogen	NH4N		✓	✓	✓
7	Nitrate Nitrogen	NO3N		✓	✓	✓
8	Non-algal Organic Phosphorus	ORGP			✓	✓
9	Phosphate Phosphorus	PO4P			✓	✓
10	Phytoplankton Carbon	PHYC				✓

Figure 5

Water Quality Model 1 State Variable Kinetic Interactions



Colour codes: Black: State variables active in model complexity 1, Blue: Additional state variables for model complexity 2, Red: Additional state variables for model complexity 3, Green: Additional state variables for model complexity 4.

The kinetic rates of model state variables are given in the Equations (19-26). Salinity is considered to be conservative and total suspended solids undergo settling that is handled during the solution of the main transport equation only.

$$\frac{dCBOD}{dt} = \underbrace{\left(a_{O2:C,PHYTO} \cdot R_{PHYTO,DEATH}\right)}_{\substack{Gain\ of\ CBOD\ due\ to\ death\ and\ respiration\ of\ phytoplankton.\\ Only\ active\ if\ complexity\ level>3}} - \underbrace{R_{CBOD,MINER}}_{\substack{Loss\ of\ CBOD\ due\ to\ aerobic\ mineralization\ of\ organic\ matter}} - \underbrace{\left(\frac{5}{4} \cdot \frac{32}{14} \cdot R_{DENIT}\right)}_{\substack{Loss\ of\ CBOD\ due\ to\ denitrification.\ Only\ active\ if\ complexity\ level>2}}$$

(Equation 19)

$$\frac{dDOXY}{dt} = \underbrace{R_{REAR}}_{\substack{Gain\ of\ DOXY\\ due\ to\ atmospheric\\ reaeration}} - \underbrace{R_{CBOD,MINER}}_{\substack{Loss\ of\ DOXY\ due\ to\\ aerobic\ mineralization\\ of\ organic\ matter}} - \underbrace{\left(a_{O2:C,PHYTO} \cdot R_{PHYTO,RESP}\right)}_{\substack{Loss\ of\ DOXY\ due\ to\ the\ respiration\\ of\ phtoplankton.\ Only\ active\ if\\ complexity\ level > 3}} +$$

$$\underbrace{\left(a_{o2:C,PHYTO} \cdot pref_{NH4N} \cdot R_{PHYTO,GROWTH}\right)}_{\substack{Generation\ of\ DOXY\ due\ to\ primary\ production\ where\\ NH4N\ was\ uptaken\ as\ DIN.\ Only\ active\ if\\ complexity\ level>3}} +$$

$$\underbrace{\left((1 - pref_{NH4N}) \cdot R_{PHYTO,GROWTH} \cdot \left(a_{o2:C,PHYTO} + \frac{48}{14} \cdot a_{N:C,PHYTO}\right)\right)}_{\substack{Generation\ of\ DOXY\ due\ to\ primary\ production\ where\ NO3N\ was\ uptaken\ as\ DIN,\\ considering\ the\ effect\ of\ three\ oxygen\ atoms\ in\ nitrate.\ Only\ active\ if\\ complexity\ level > 3.}} -$$

$$\underbrace{\frac{SOD}{H}}_{\substack{Loss\ of\ DOXY\\ due\ to\ SOD}} - \underbrace{\frac{64}{14} \cdot R_{NITR}}_{\substack{Loss\ of\ DOXY\ due\ to\ nitrificaiton.\\ Only\ active\ if\ complexity\ level>1}}$$

(Equation 20)

$$\frac{dORGN}{dt} = \underbrace{\left(f_{ON} \cdot a_{N:C,PHYTO} \cdot R_{PHYTO,DEATH}\right)}_{\substack{Generation\ of\ ORGN\ due\ to\ phytoplankton\\ death\ and\ respiration.\ Only\ active\ if\\ complexity\ level > 3.}} - \underbrace{R_{ORGN,MINER}}_{\substack{Loss\ of\ ORGN\ due\ to\ organic\\ matter\ mineralization}}$$

(Equation 21)

$$\frac{dNH4N}{dt} = \underbrace{\left((1 - f_{ON}) \cdot a_{N:C,PHYTO} \cdot R_{PHYTO,RESP}\right)}_{\substack{Generation\ of\ NH4N\ due\ to\ the\\ release\ by\ phytoplankton.\ Only\\ active\ if\ complexity\ level > 3.}} -$$

$$\underbrace{\left(a_{N:C,PHYTO} \cdot pref_{NH4N} \cdot R_{PHYTO,GROWTH}\right)}_{\substack{Loss\ of\ NH4N\ due\ to\ the\ uptake\ by\ phytoplankton.\\ Only\ active\ if\ complexity\ level > 3.}} +$$

$$\underbrace{R_{ORGN,MINER}}_{\substack{Generation\ of\ NH4N\ due\ to\ organic\\ matter\ (ORGN)\ mineralization}} - \underbrace{R_{NITR}}_{\substack{Loss\ of\ NH4N\ due\ to\\ nitrification}}$$

(Equation 22)

$$\frac{dNO3N}{dt} = \underbrace{R_{NITR}}_{\substack{Generation\ of\ NH4N \\ due\ to\ nitrification}} - \underbrace{\left((1 - pref_{NH4N}) \cdot a_{N:C,PHYTO} \cdot R_{PHYTO,GROWTH}\right)}_{\substack{Loss\ of\ NO3N\ due\ to\ the\ uptake\ by\ phytoplankton. \\ Only\ active\ if\ complexity\ level > 3.}} - \underbrace{R_{DENITR}}_{\substack{Generation\ of\ NO3N \\ due\ to\ denitrification}}$$

(Equation 23)

$$\frac{dORGP}{dt} = \underbrace{\left(f_{OP} \cdot a_{P:C,PHYTO} \cdot R_{PHYTO,DEATH}\right)}_{\substack{Generation\ of\ ORGP\ due\ to\ phytoplankton \\ death\ and\ respiration.\ Only\ active\ if \\ complexity\ level > 3.}} - \underbrace{R_{ORGP,MINER}}_{\substack{Loss\ of\ ORGP\ due\ to\ organic \\ matter\ mineralization}}$$

(Equation 24)

$$\frac{dPO4P}{dt} = \underbrace{\left((1 - f_{OP}) \cdot a_{P:C,PHYTO} \cdot R_{PHYTO,RESP}\right)}_{\substack{Generation\ of\ PO4P\ due\ to\ the \\ release\ by\ phytoplankton.\ Only \\ active\ if\ complexity\ level > 3.}} - \underbrace{a_{P:C,PHYTO} \cdot R_{PHYTO,GROWTH}}_{\substack{Loss\ of\ PO4P\ due\ to\ the\ uptake\ by \\ phytoplankton. \\ Only\ active\ if\ complexity\ level > 3.}} + \underbrace{R_{ORGP,MINER}}_{\substack{Generation\ of\ PO4P\ due\ to\ organic \\ matter\ (ORGP)\ mineralization.}}$$

(Equation 25)

$$\frac{dPHYC}{dt} = \underbrace{R_{PHYTO,GROWTH}}_{\substack{Generation\ of\ PHYC\ due\ to \\ the\ growth}} - \underbrace{R_{PHYTO,DEATH,RESP}}_{\substack{Loss\ of\ PHYC\ due\ to \\ the\ death\ and\ respiration}}$$

(Equation 26)

The process rates and their auxiliary variables were given in Table 2. The dissolved oxygen saturation ($DOXY_{SAT}$) and reaeration rate constant (k_A) formulas and calculation procedures were too long to be placed into the Table 2 and were therefore given in Appendix. Water Quality Model 1 does not distinguish between the dissolved and particulate parts of state variables. Instead, it allows the user to associate each state variable on each box with a settling velocity time series. In case of salinity and dissolved oxygen; if a non-zero settling velocity occurs, the effect of the settling will still be set back to zero as a failsafe. All of the other state variables

Table 2

Process Rates and Auxiliary Variables of Water Quality Kinetics Sub Model 1

Process Rate	Description	Equation and Auxiliary Variables
$R_{CBOD,MINER}$	Mineralization of CBOD	$k_{CBOD,MINER,20} \cdot \theta_{CBOD,MINER}^{(TEMP-20)} \cdot CBOD \cdot \frac{DOXY}{DOXY + k_{HS,MINER,DOXY}}$
R_{REAR}	Atmospheric reaeration	$k_A \cdot (DOXY_{SAT} - DOXY)$
$R_{ORGN,MINER}$	Mineralization of ORGN	$k_{ORGN,MINER,20} \cdot \theta_{ORGN,MINER}^{(TEMP-20)} \cdot ORGN$
R_{NITR}	Nitrification	$k_{NITR,20} \cdot \theta_{NITR}^{(TEMP-20)} \cdot NH4N \cdot \frac{DOXY}{DOXY + k_{HS,NITR,DOXY}}$
R_{DENIT}	Denitrification	$k_{DENITR,20} \cdot \theta_{DENITR}^{(TEMP-20)} \cdot NO3N \cdot \frac{K_{HS,DENITR,DOXY}}{DOXY + K_{HS,DENITR,DOXY}}$
$R_{ORGP,MINER}$	Mineralization of ORGP	$k_{ORGP,MINER,20} \cdot \theta_{ORGP,MINER}^{(TEMP-20)} \cdot ORGP$
$R_{PHYTO,GROWTH}$	Phytoplankton growth	$k_{PHYTO,GROW,20} \cdot \theta_{PHYTO,GROW}^{(TEMP-20)} \cdot lim_{LIGHT} \cdot lim_{NUT} \cdot PHYC$ Light limitation factor $lim_{LIGHT} = \frac{2.718 \cdot f_{DAY}}{k_E \cdot H} \cdot \left(exp\left(-\frac{I_A}{I_S} \cdot exp(-1 \cdot k_E \cdot H) \right) - exp\left(-\frac{I_A}{I_S} \right) \right)$ Light extinction coefficient $k_E = k_{B,E} + (8.8 \cdot 10^{-3} \cdot CHLA) + \left(5.4 \cdot 10^{-2} \cdot CHLA^{2/3}\right)$ Chlorophyll-A $a_{CHLA:C,PHYTO}$·PHYC·1000 Nutrient limitation factor $lim_{NUT} = min\left(\frac{NH4N + NO3N}{k_{HS,N} + NH4N + NO3N}, \frac{PO4P}{k_{HS,P} + PO4P} \right)$
$R_{PHYTO,DEATH}$	Phytoplankton death	$k_{PHYTO,DEATH,20} \cdot \theta_{PHYTO,DEATH}^{(TEMP-20)} \cdot PHYC$
$R_{PHYTO,RESP}$	Phytoplankton death	$k_{PHYTO,RESP,20} \cdot \theta_{PHYTO,RESP}^{(TEMP-20)} \cdot PHYC$

Table 3

Derived Variables of Water Quality Kinetics Sub Model 1

Derived Variable No	Derived Variable	Representation in Model	Unit	Derivation
1	Conductivity	COND	µS/cm	UNESCO (1983) is used reversely*
2	Dissolved inorganic nitrogen	DIN	g/m^3	NH4N + NO3N
3	Total Organic Nitrogen	TON	g/m^3	For complexity levels 2 and 3 ORGN For complexity level 4 ORGN + (PHYC · $a_{N:C,PHYTO}$)
4	Total Kjeldahl Nitrogen	TKN	g/m^3	NH4N + TON
5	Total Nitrogen	TN	g/m^3	DIN + TON
6	Total Organic Phosphorus	TOP	g/m^3	For complexity level 3 ORGP For complexity level 4 ORGP + (PHYC · $a_{P:C,PHYTO}$)
7	Total Phosphorus	TP	g/m^3	PO4P + TOP
8	Chlorophyll-a	CHLA	µg/L	For complexity level 4 PHYC · $a_{CHLA:C,PHYTO}$ · 1000
9	Ultimate CBOD	CBODU	g/m^3	For complexity levels 1, 2, 3 CBOD For complexity level 4 CBOD + (PHYC · $a_{O2:C,PHYTO}$)
10	5 days Biochemical Oxygen Demand	BOD5	g/m^3	If the bottle BOD decay rate constant is available CBODU · (1 - exp(-$k_{d,bott}$ ·5)) otherwise CBODU · (1 - exp(-k_{dc} ·5))

***** The original method is for the calculation of salinity based on conductivity. Future versions may include other options.

were allowed to settle assuming that the related decision was a user initiative. As discussed previously, the water quality kinetics sub model 1 could derive additional variables listed in Table 3 using the state variables and output them.

Water Quality Sub Model 2

Water quality kinetics sub model 2 is a detailed and aquatic science oriented model where building a more realistic model was intended, at the cost of simplicity for scientific studies where a higher complexity and a more detailed representation of the aquatic ecosystem could be desired. The main aim of the water quality kinetics sub model 2 is the analysis of dynamics of eutrophication, an important problem of many developed and developing countries. Unlike the water quality kinetic sub model 1, this kinetics sub model does not have any complexity level and must be fully used without any simplifications. It includes 14 state variables (Table 4).

Table 4

State Variables and Complexity Levels of Water Quality Kinetics Sub Model 2

State Variable No	State Variable	Representation in the Model
1	Phytoplankton Carbon	PHYC
2	Detrital Particulate Organic carbon	FPOC
3	Detrital Particulate Organic Nitrogen	FPON
4	Detrital Particulate Organic Phosphorus	FPOP
5	Dissolved Organic Carbon	DOC
6	Dissolved Organic Nitrogen	DON
7	Dissolved Organic Phosphorus	DOP
8	Ammonium Nitrogen	NH4N
9	Nitrate Nitrogen	NO3N
10	Soluble Reactive Phosphorus	SRP
11	Particulate Inorganic Phosphorus	PIP
12	Dissolved Oxygen	DOXY
13	Inorganic Suspended Solids	ISS
14	Salinity	SALT

The interactions among the state variables were illustrated in Figure 6. The kinetic rates of model state variables were given in the Equations (27-38). Salinity is considered to be conservative and total suspended solids undergo settling that is handled during the solution of the main transport equation only.

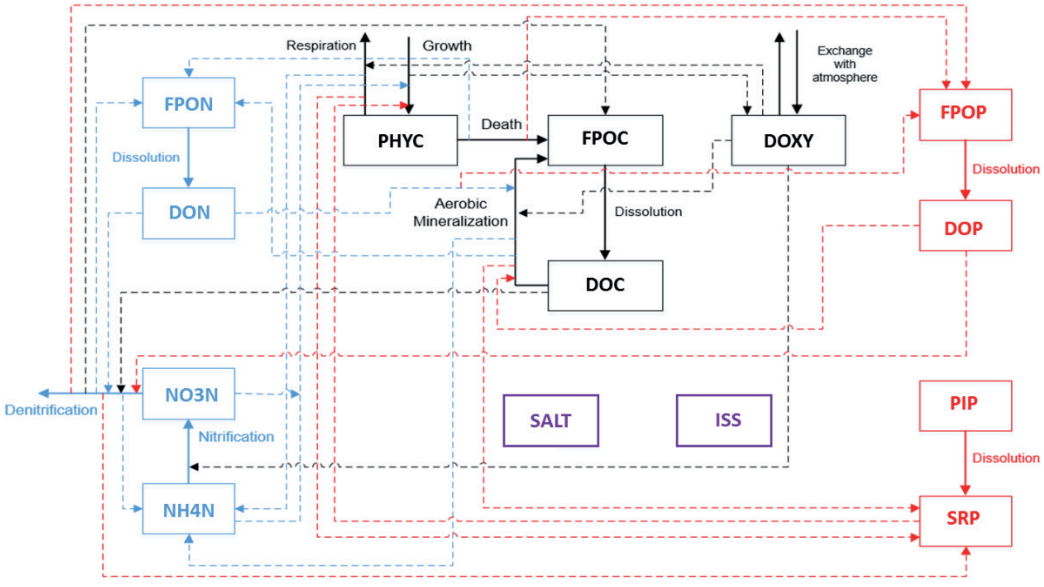
Water Quality Sub Model 2 has a state variable that was not common in water quality models, namely the particulate inorganic phosphorus. This state variable represents the phosphorus that is in inorganic form, however not readily available as soluble reactive phosphorus. It is incorporated to simulate the delayed effects of adsorbed or mineral incorporated phosphorus after dissolution to SRP. Its sources are

- Attached to eroded soil/sediments, especially during wet season. It is known that the erosion rates in Turkey are relatively high
- Resuspension of suspended sediments in stormy weather

As Water Quality Sub Model 2 was further developed, these physical processes would also be realistically incorporated.

Figure 6

Water Quality Model 2 State Variable Kinetic Interactions



Colour codes: Black: Carbon and oxygen related state variables, Blue: Nitrogen related state variables, Red: Phosphorus related state variables, Violet: Other state variables.

$$\frac{dPHYC}{dt} = \underbrace{R_{PHYTO,GROWTH}}_{\text{Generation of PHYC due to the growth}} - \underbrace{R_{PHYTO,RESP}}_{\text{Loss of PHYC due to the respiration}} - \underbrace{R_{PHYTO,DEATH}}_{\text{Loss of PHYC due to the death}}$$

(Equation 27)

$$\frac{dFPOC}{dt} = \underbrace{R_{PHYTO,DEATH}}_{\text{Generation of FPOC due to the growth of phytoplankton}} + \underbrace{Y_{AERHET} \cdot R_{DOC,MINER}}_{\text{Generation of FPOC due to the gain of the aerobic heteretroph bacteria biomass because of the consumption of DOC as carbon source during organic matter mineralization}} + \underbrace{a_{C:N,DENITR} \cdot Y_{DENITR} \cdot R_{DENITR}}_{\text{Generation of FPOC due to the gain of the denitrifying bacteria biomass because of the consumption of DOC as carbon source during denitrification}} - \underbrace{R_{FPOC,DISS}}_{\text{Loss of FPOC due to the dissolution of particulate organic matter}}$$

(Equation 28)

$$\frac{dFPON}{dt} = \underbrace{a_{N:C,PHYTO} \cdot R_{PHYTO,DEATH}}_{\text{Generation of FPON due to the growth of phytoplankton}} + \underbrace{Y_{AERHET} \cdot R_{DON,MINER}}_{\text{Generation of FPON due to the gain of the aerobic heteretroph bacteria biomass because of the consumption of DON as nitrogen source during organic matter mineralization}} + \underbrace{a_{C:N,DENITR} \cdot Y_{DENITR} \cdot R_{DENITR} \cdot \frac{DON}{DOC}}_{\text{Generation of FPOC due to the gain of the denitrifying bacteria biomass because of the consumption of DOC as carbon source during denitrification}} - \underbrace{R_{FPON,DISS}}_{\text{Loss of FPON due to the dissolution of particulate organic matter}}$$

(Equation 29)

$$\frac{dFPOP}{dt} = \underbrace{a_{P:C,PHYTO} \cdot R_{PHYTO,DEATH}}_{\substack{\text{Generation of FPON due to the growth of phytoplankton}}} + \underbrace{Y_{AERHET} \cdot R_{DOP,MINER}}_{\substack{\text{Generation of FPOP due to the gain of the aerobic heteretroph bacteria biomass because of the consumption of DOP as nitrogen source during organic matter mineralization}}} +$$

$$\underbrace{a_{C:N,DENITR} \cdot Y_{DENITR} \cdot R_{DENITR} \cdot \frac{DOP}{DOC}}_{\substack{\text{Generation of FPOC due to the gain of the denitrifying bacteria biomass because of the consumption of DOC as carbon source during denitrification}}} - \underbrace{R_{FPOP,DISS}}_{\substack{\text{Loss of FPOP due to the dissolution of particulate organic matter}}}$$

(Equation 30)

$$\frac{dDOC}{dt} = \underbrace{R_{FPOC,DISS}}_{\substack{\text{Generation of DOC due to the dissolution of FPOC}}} - \underbrace{R_{DOC,MINER}}_{\substack{\text{Loss of DOC due to the organic matter mineralization by the aerobic heterotrophic bacteria}}} - \underbrace{a_{C:N,DENITR} \cdot R_{DENITR}}_{\substack{\text{Loss of DOC due to the organic matter mineralization by the denitrifying bacteria}}}$$

(Equation 31)

$$\frac{dDON}{dt} = \underbrace{R_{FPON,DISS}}_{\substack{\text{Generation of DON due to the dissolution of particulate FPON}}} - \underbrace{R_{DON,MINER}}_{\substack{\text{Loss of DON due to the organic matter mineralization by the aerobic heterotrophic bacteria}}} - \underbrace{a_{C:N,DENITR} \cdot R_{DENITR} \cdot \frac{DON}{DOC}}_{\substack{\text{Loss of DON due to the organic matter mineralization by the denitrifying bacteria}}}$$

(Equation 32)

$$\frac{dDOP}{dt} = \underbrace{R_{FPOP,DISS}}_{\substack{\text{Generation of DOP due to the dissolution of particulate FPOP}}} - \underbrace{R_{DOP,MINER}}_{\substack{\text{Loss of DOP due to the organic matter mineralization by the aerobic heterotrophic bacteria}}} - \underbrace{a_{C:N,DENITR} \cdot R_{DENITR} \cdot \frac{DOP}{DOC}}_{\substack{\text{Loss of DOP due to the organic matter mineralization by the denitrifying bacteria}}}$$

(Equation 33)

$$\frac{dNH4N}{dt} = \underbrace{a_{N:C,PHYTO} \cdot R_{PHYTO,RESP}}_{\substack{\text{Generation of NH4N due to} \\ \text{the respiration of} \\ \text{phytoplankton}}} - \underbrace{a_{N:C,PHYTO} \cdot pref_{NH4N} \cdot R_{PHYTO,GROWTH}}_{\substack{\text{Loss of NH4N due to} \\ \text{the growth of} \\ \text{phytoplankton}}} - \underbrace{R_{NITR}}_{\substack{\text{Loss of NH4N due to} \\ \text{nitrification}}} +$$

$$\underbrace{(1 - Y_{AERHET}) \cdot R_{DON,MINER}}_{\substack{\text{Generation of NH4N due to the} \\ \text{internal respiration of the} \\ \text{aerobic heteretroph} \\ \text{bacteria biomass because} \\ \text{of the consumption of DON as} \\ \text{nitrogen source during} \\ \text{organic matter mineralization}}} + \underbrace{a_{C:N,DENITR} \cdot (1 - Y_{DENITR}) \cdot R_{DENITR} \cdot \frac{DON}{DOC}}_{\substack{\text{Generation of NH4N due to the} \\ \text{internal respiration of the denitrifying} \\ \text{bacteria biomass because} \\ \text{of the consumption of DOC as} \\ \text{nitrogen source during} \\ \text{denitrification}}}$$

(Equation 34)

$$\frac{dNO3N}{dt} = \underbrace{R_{NITR}}_{\substack{\text{Generation of NO3N} \\ \text{due to nitrification}}} - \underbrace{a_{N:C,PHYTO} \cdot (1 - pref_{NH4N}) \cdot R_{PHYTO,GROWTH}}_{\text{Loss of NH4N due to the respiration of phytoplankton}} - \underbrace{R_{DENITR}}_{\substack{\text{Loss of NO3N due to} \\ \text{denitrification}}}$$

(Equation 35)

$$\frac{dSRP}{dt} = \underbrace{a_{N:C,PHYTO} \cdot R_{PHYTO,RESP}}_{\substack{\text{Generation of PO4P due to} \\ \text{the respiration of} \\ \text{phytoplankton}}} - \underbrace{a_{P:C,PHYTO} \cdot R_{PHYTO,GROWTH}}_{\substack{\text{Loss of PO4P due to} \\ \text{the growth of} \\ \text{phytoplankton}}} + \underbrace{R_{PIP,DISS}}_{\substack{\text{Generat.on of PO4P due to} \\ \text{the dissolution of PIP}}} +$$

$$\underbrace{(1 - Y_{AERHET}) \cdot R_{DON,MINER}}_{\substack{\text{Generation of PO4P due to the} \\ \text{internal respiration of the} \\ \text{aerobic heteretroph} \\ \text{bacteria biomass because} \\ \text{of the consumption of DOP as} \\ \text{phosphorus source during} \\ \text{organic matter mineralization}}} + \underbrace{a_{C:N,DENITR} \cdot (1 - Y_{DENITR}) \cdot R_{DENITR} \cdot \frac{DOP}{DOC}}_{\substack{\text{Generation of PO4P due to the} \\ \text{internal respiration of the denitrifying} \\ \text{bacteria biomass because} \\ \text{of the consumption of DOP as} \\ \text{phosphorus source during} \\ \text{denitrification}}}$$

(Equation 36)

$$\frac{dPIP}{dt} = - \underbrace{R_{PIP,DISS}}_{\substack{\text{Loss of PIP due to} \\ \text{the dissolution}}}$$

(Equation 37)

$$\frac{dDOXY}{dt} = \underbrace{R_{REAR}}_{\substack{Gain\ of\ DOXY \\ due\ to\ atmospheric \\ reaeration}} - \underbrace{R_{CBOD,MINER}}_{\substack{Loss\ of\ DOXY\ due\ to \\ aerobic\ mineralization \\ of\ organic\ matter}} - \underbrace{a_{O2:C,PHYTO} \cdot R_{PHYTO,RESP}}_{\substack{Loss\ of\ DOXY\ due\ to\ the \\ respiration\ \ of\ phtoplankton}} +$$

$$\underbrace{a_{O2:C,PHYTO} \cdot R_{PHYTO,GROWTH}}_{\substack{Generation\ of\ DOXY\ due\ to \\ primary\ production}} - \underbrace{\frac{64}{14} \cdot R_{NITR}}_{\substack{Loss\ of\ DOXY\ due\ to \\ nitrificaiton}}$$

(Equation 38)

The process rates and their auxiliary variables are given in Table 5. The dissolved oxygen saturation ($DOXY_{SAT}$) and reaeration rate constant (k_A) formula and calculation procedures are too long to be placed into Table 5 and are therefore given in Appendix.

Unlike the Water Quality Model 1, Water Quality Model 2 includes state variables that are intended to be of dissolved or particulate form. However, all the state variables, no matter dissolved or particulate are associated to with a settling velocity time series, assuming that the related decision is a user initiative. There is no fail-safe as in Water Quality Model 1. Moreover, Water Quality Model 2 is designed to consider the bacterial loop by assuming the non-algal organic carbon, nitrogen and phosphorus as detritus, the non-living organic matter plus the bacteria associated to them. Hence, the nutrient and organic matter feedback loops are more detailed than the Water Quality Model 1. Additional variables listed in Table 6 can be derived using the state variables in Water Quality Model 2.

Table 5

Process Rates and Auxiliary Variables of Water Quality Kinetics Sub Model 2

Process Rate	Description	Equation and Auxiliary Variables
$R_{DOC,MINER}$	Mineralization of DOC	$k_{DOC,MINER,20} \cdot \theta_{DOC,MINER}^{(TEMP-20)} \cdot DOC \cdot min\left((1 - lim_{O2,DENITR}), \frac{DOC}{DOC + k_{HS,DOC,MINER}}\right)$
R_{REAR}	Atmospheric reaeration	$k_A \cdot (DOXY_{SAT} - DOXY)$
$R_{ORGN,MINER}$	Mineralization of DON	$k_{DON,MINER,20} \cdot \theta_{DON,MINER}^{(TEMP-20)} \cdot DON \cdot min\left((1 - lim_{O2,DENITR}), \frac{DON}{DON + k_{HS,DON,MINER}}\right)$
R_{NITR}	Nitrification	$k_{NITR,20} \cdot \theta_{NITR}^{(TEMP-20)} \cdot NH4N \cdot \frac{NH4N}{NH4N + k_{HS,NITR,NH4N}} \cdot \frac{DOXY}{DOXY + k_{HS,NITR,DOXY}}$
R_{DENIT}	Denitrification	$k_{DENITR,20} \cdot \theta_{DENITR}^{(TEMP-20)} \cdot NO3N \cdot min\left(lim_{NO3N,DENITR}, min\left(lim_{O2,DENITR}, lim_{DOC,DENITR}\right)\right)$ Nitrate Limitation Factor $lim_{NO3N,DENITR} = \frac{NO3N}{NO3N + k_{HS,DENITR,NO3N}}$ Dissolved Oxygen Limitation (Inhibition) Factor $lim_{O2,DENITR} = \frac{k_{HS,DENITR,DOXY}}{DOXY + k_{HS,DENITR,DOXY}}$ Dissolved Organic Carbon Limitation Factor $lim_{DOC,DENITR} = \frac{DOC}{DOC + k_{HS,DENITR,DOC}}$
$R_{ORGP,MINER}$	Mineralization of DOP	$k_{DOP,MINER,20} \cdot \theta_{DOP,MINER}^{(TEMP-20)} \cdot DOP \cdot min\left((1 - lim_{O2,DENITR}), \frac{DOP}{DOP + k_{HS,MINER,DOP}}\right)$

Table 5

(Continued)

Process Rate	Description	Equation and Auxiliary Variables
$R_{PHYTO,GROWTH}$	Phytoplankton growth	$k_{PHYTO,GROW,20} \cdot \theta_{PHYTO,GROW}^{(TEMP-20)} \cdot min(lim_{LIGHT}, lim_{NUT}) \cdot PHYC$ Light limitation factor $lim_{LIGHT} = \frac{2.718 \cdot \mathrm{f_{DAY}}}{\mathrm{k_E \cdot H}} \cdot \left(exp\left(-\frac{I_A}{I_S} \cdot exp(-1 \cdot k_E \cdot H) \right) - exp\left(-\frac{I_A}{I_S} \right) \right)$ Light extinction coefficient $\mathrm{k_E = k_{E,W} + (5.2 \cdot 10^{-2} \cdot ISS) + (1.74 \cdot 10^{-1} \cdot DVSS) + (8.8 \cdot 10^{-3} \cdot CHLA) + \left(5.4 \cdot 10^{-2} \cdot CHLA^{2/3}\right)}$ Chlorophyll-a $CHLA = a_{CHLA:C,PHYTO} \cdot$PHYC$\cdot 1000$ Detrital Volatile Suspended Solids $DVSS = a_{VSS:C,FPOC} \cdot$FPOC Nutrient limitation factor $lim_{NUT} = min\left(\frac{[NH4N] + [NO3N]}{k_{HS,N} + [NH4N] + [NO3N]}, \frac{[SRP]}{k_{HS,P} + [SRP]} \right)$
$R_{PHYTO,DEATH}$	Phytoplankton death	$k_{PHYTO,DEATH,20} \cdot \theta_{PHYTO,DEATH}^{(TEMP-20)} \cdot PHYC$
$R_{PHYTO,RESP}$	Phytoplankton respiration	$k_{PHYTO,RESP,20} \cdot \theta_{PHYTO,RESP}^{(TEMP-20)} \cdot PHYC$
$R_{FPOC,DISS}$	Dissolution of non-algal particulate organic carbon	$k_{FPOC,DISS,20} \cdot \theta_{FPOC,DISS}^{(TEMP-20)} \cdot FPOC \cdot \frac{FPOC}{FPOC + k_{HS,DISS,FPOC}}$

Table 5

(Continued)

Process Rate	Description	Equation and Auxiliary Variables
$R_{FPON,DISS}$	Dissolution of non-algal particulate organic nitrogen	$k_{FPON,DISS,20} \cdot \theta_{FPON,DISS}^{(TEMP-20)} \cdot FPON \cdot \frac{FPON}{FPON + k_{HS,DISS,FPON}}$
$R_{FPOP,DISS}$	Dissolution of non-algal particulate organic phosphorus	$k_{FPOP,DISS,20} \cdot \theta_{FPOP,DISS}^{(TEMP-20)} \cdot FPOP \cdot \frac{FPOP}{FPOP + k_{HS,DISS,FPOP}}$
$R_{PIP,DISS}$	Dissolution of non-algal particulate inorganic phosphorus	$k_{PIP,DISS,20} \cdot \theta_{PIP,DISS}^{(TEMP-20)} \cdot PIP \cdot \frac{PIP}{PIP + k_{HS,DISS,PIP}}$

Water Quality Sub Model 3

Water quality kinetics sub model 3 is a generic water quality model considering the decay of multiple and unlimited number of pollutants. Calculations can be made using the desired order kinetics. Interactions of all pollutants with each other and with the by-products formed are not considered. Differential equation for generic pollutants is provided in Equation 39.

$$\frac{dC}{dt} = -k_{20} \cdot \theta_{20}^{(T-20)} \cdot C^n$$

(Equation 39)

where,

C : Generic pollutant concentration [g/m^3]

T : Temperature [°C]

θ : Arrhenius temperature correction factor [-]

k_{20} : Loss rate at 20°C [1/day]

n : Reaction order [-]

Table 6

Derived Variables of Water Quality Kinetics Sub Model 2

Derived Variable No	Derived Variable	Representation in Model	Unit	Derivation
1	Conductivity	COND	µS/cm	UNESCO (1983) is used reversely*
2	Dissolved Inorganic Nitrogen	DIN	g/m^3	NH4N + NO3N
3	Total Organic Nitrogen	TON	g/m^3	FPON + DON + (PHYC · N:C ratio)
4	Total Kjeldahl Nitrogen	TKN	g/m^3	NH4N + TON
5	Total Nitrogen	TN	g/m^3	DIN + TON
6	Total Organic Phosphorus	TOP	g/m^3	FPOP + DOP + (PHYC · P:C ratio)
7	Total Phosphorus	TP	g/m^3	SRP + PIP + TOP
8	Chlorophyll-a	CHLA	µg/L	CHLA
9	Ultimate Carbonaceous BOD	CBODU	g/m^3	FPOC + (DOC · O_2:C ratio) + (PHYC · O_2:C ratio)
10	5 day Biochemical Oxygen Demand	BOD5	g/m^3	If the bottle BOD decay rate constant is available CBODU· (1 - exp(-$K_{d,bott}$ ·5)) otherwise CBODU · (1 - exp(-K_{dc} ·5))
11	Biochemical Oxygen Demand for Dissolved Organic Carbon	DCBOD	g/m^3	DOC · O_2:C ratio
12	Biochemical Oxygen Demand for Particulate Organic Carbon	PCBOD	g/m^3	(PHYC · O_2:C ratio) + (DOC · O_2:C ratio)
13	Carbonaceous Biochemical Oxygen Demand (Carbonaceous BOD representing non-living organic matter)	CBOD	g/m^3	(FPOC + DOC) · (O_2:C_{DOC} ratio)
14	Suspended Solids	TSS	g/m^3	(PHYC · (PHYC:VSS coefficient)) + (FPOC · (FPOC:VSS coefficient)) + ISS
15	Volatile Suspended Solids	VSS	g/m^3	(PHYC · (PHYC:VSS coefficient)) + (FPOC · (FPOC:VSS coefficient))
16	Phosphate Phosphorus	PO4P	g/m^3	SRP + PIP

***** The original method is for the calculation of salinity based on conductivity. Future versions may include other options.

Software Development

Programming Language

Since the transport equation is solved using a matrix method, a matrix-oriented programming language was considered as a logical choice. MATLAB (MATrix LABoratory) was chosen for the following reasons:

- It is a high-level language, which is popular and used by many scientists and engineers. A high-level programming language such as MATLAB, Python, R and Julia provides automatic services for the programmer including automatic initialization of variables, preventing memory leaks and automatic garbage collection once the life cycle of a program object is over. High level programming languages usually run on an interpreter sub system and therefore ease the software development process. On the other hand, programmers that choose lower level programming languages (such as Fortran, C, C++, Pascal) must deal with most of these jobs that would have been provided by high level programming languages themselves. The advantage of lower level programming languages is faster code that needs less memory to execute since no interpreter is involved, however at a cost of high and complex software development time and a more complex debugging process. Most high-level language-based environments make use of precompiled libraries (called packages, plugins, etc.) and just in time compilers that precompile the code lines into a virtual machine code and call that machine code when the relevant code section is repeatedly called (such as a time loop in a water quality model) without losing time for interpretation.

- MATLAB code is easy to read and understand. With a few lines of code, it is possible to solve many programming tasks that would result in tens of lines of code using other popular programming languages (such as Fortran, C, C++) in water quality modelling arena.

- MATLAB is an interpreted language; however, it is not as slow as the traditional interpreted programming languages. With a smart way of programming, code that would create a comparable performance to compiled languages can be developed. Software development using an interpreted programming language is more productive than using a compiled programming language, because of easier and faster debugging during the development stage. After the development stage, code could easily be compiled and distributed with MATLAB runtime.

- MATLAB has access to many standard and commonly used file formats (such as spreadsheet files).

- MATLAB has standard library functions that ease many common programming tasks. Development of such utility functions in other programming languages would have taken months of work.

Because MATLAB is a proprietary commercial software and not everybody may obtain a legal copy; Octave (Eaton et.al, 2021) that is highly compatible with MATLAB was considered for parallel development. Most of the water quality code is designed to run in both environments identically. Some issues that would be not compatible in both interpreters are separately written. Therefore, the water quality includes routines that check the interpreter from which it was called so that the water quality simulator is aware of its environments and use different alternatives for specific tasks, which should be conducted differently in MATLAB and Octave.

Input/Output Organization

Since most of the model, inputs are tabular; spreadsheet workbooks are used for input. Spreadsheets provide a comfortable environment for creating model inputs. The model requires xlsx files that are native to Microsoft Excel. For the users, which cannot obtain a legal copy of Microsoft Excel several free spreadsheet software that can also read and write xlsx files (such as Libre Office Calc) exist. Another alternative to assemble model input data sets is to develop a graphical user interface, either a general one for the individual user or a specific one for institutional users and/or institutes with more focused tasks. The model outputs are generated as comma separated value (csv) files for state and derived variables. The model generates three basic outputs:

- Daily outputs for each box

- Diurnal outputs for user specified dates where output is given for each time step in that day

- Spatially and temporally averaged monthly results, which are averaged over one or several box groups prescribed by the user

Modules of the Code

The water quality simulation code consists of the following modules

- The pre-processor and its utilities that assemble the model data structures using the model input datasets.
- The geometry module that conducts the geometrical computations at each time step considering the water budget and the possibly irregular shape of this box.
- The advection-diffusion-reaction module that solves the main transport equation and conducts book-keeping for each box and state variable at each time step
- The water quality kinetic sub model codes that calculate the reaction rates and interact with the advection-diffusion-reaction module

Results

The result of this study is a water quality simulation system that could be applied for a wide range of applications. The model can be used under MATLAB and Octave interpreters and can be distributed as an executable as well.

Under MATLAB, the model can be executed at a satisfying performance, a typical simulation with 30-40 model boxes takes around one minute on a standard pc based laptop. Under Octave, the performance is less satisfactory, 5 to 10 times slower, since Octave is not equipped with a JIT (Just In Time) compiler like MATLAB. However, since Octave is a completely free software, the water quality code can be run or experimented with for free from the software environment point of view. This makes the legal use of the model in low income countries possible.

The water quality simulation software developed in this study has many options to compensate if some of the model inputs are missing. Moreover, it contains three water quality kinetics sub models and can therefore address a wide range of problems in different type of aquatic ecosystems.

Water quality kinetics sub model 1 can be run under four different complexity levels. It can be used for both addressing basic water quality problems and more advanced studies such as planning the program of measures against more

complicated water quality and ecology problems such as eutrophication. As the model complexity increases, the data requirements will increase as well. It is also possible to start from complexity level 1 and increase the complexity level as more data become available. Another approach is that any user can start from complexity level 1 and can progress slowly watching out for his or her user mistake and progress into the higher complexity levels once the complexity level being worked on is proven to be user mistake free.

Water quality kinetics sub model 2 is tailored for more complex problems and is research oriented. It is designed to be more realistic than conventional water quality models and is heavily focusing on the investigation of the eutrophication dynamics. Unlike the water quality kinetics sub model 1, it does not have complexity levels. It is structured to be easily expandable for further development in academic studies, so that it could be considered as the "complexity level 1" template of more advanced eutrophication models that would be upcoming for both generally advanced studies or ecosystem specific studies. Future enhancements may include inorganic carbon-alkalinity-pH modelling, simulation of multiple phytoplankton groups, benthic algae and organisms that are on the higher level of the aquatic foodweb (zooplankton, fish, etc.).

Water quality kinetics sub model 3 is intended for initial studies related to a wide range of pollutants except the dissolved gasses, nutrients and semi-natural pollutants such as (organic carbon, BOD and COD). It will be more useful for screening approach in cases where multiple pollutants usually of type synthetic organics, toxics such as pesticides, and hazardous materials in aquatic environment are of concern. Some of those pollutants are of course more complex, so that a generic model would not be suitable to simulate their fate in the aquatic environment thoroughly. However, in watershed management studies especially related to water framework directive related studies, where a need to simulate the behaviour of priority and specific pollutants may arise. In such studies, many pollutants are considered first, but not all of them will be important enough to be modelled. To decide which pollutant should be modelled first, a screening approach simulating all of the potential pollutants is necessary. Then the water quality simulation software developed in this study can be extended with additional subprograms that would include all of the relevant details of case study specific pollutants. Another application of the water quality sub model 3 would be the simulation of several bacterial and viral pathogens in waterbodies since it can simulate the degradation process of any generic pollutant assuming temperature dependence and any order of reaction.

Discussion and Suggestion for Future Work

A software for water quality modelling simulation was developed in Turkey with the collaboration of multiple institutions (universities, state agencies and techno-parks) based on 5 criteria aiming the end product to be compatible and can be integrated with the water quality modelling needs in Turkey.

Considering the Criteria 1 and 5; the model code should be developed in a way that the transport scheme should be general for all water quality variables and several water quality kinetic codes should exist to: (i) serve as templates and (ii) be ready to allow saleable and general applications of the model. In other words, a decoupled model development strategy with a transport code and several water quality codes that should easily plugged into the transport code is encouraged.

Considering Criterion 2, the models state variables or derived variables should be included in the standard variables in water quality analysis. For example, the most of the water quality models use ultimate carbonaceous BOD as state variable, but the most of the laboratories measure BOD_5. Since BOD is used for dissolved oxygen dynamics as a state variable, the model should be able to produce BOD_5 as result. Phytoplankton carbon is another example. Using phytoplankton carbon is more convenient than Chlorophyll-a as a model state variable. However, most of the laboratories have experts to measure Chlorophyll-a, and to measure phytoplankton carbon is very tedious and needs experts that can identify different phytoplankton species, count them and convert each of the species to phytoplankton carbon. However, it is worth to note that some of the already available models such as AQUATOX (Park & Clough, 2018), CE-QUAL-W2 (Wells, 2021) and WASP (United States Environmental Protection Agency, 2020) contain similar derived variables.

Considering the Criterion 3, a box model is the best option for spatial discretization and the transport scheme. The spatial resolution can be easily varied using a box model as well. Each box can represent a waterbody or just a computational element according to the needs that arise in any study.

Criteria 4 and 5 necessitate a readable code written in a high-level language that is easy to study and is supported with standard functions that keeps the programmer away from common programming tasks. The experts that would study and modify the source code can then concentrate on model development and not on the less productive tasks such as developing subroutines that read some data from a

spreadsheet file, where the binary format of the spreadsheet file should be parsed to retrieve the data.

The result of this study is the successful implementation of a water quality box model on a high-level programming language styled as an easy-to-read computer code with acceptable performance. The computer code developed is easily extendible and can be run on a computer environment with free software if desired. Its inputs can be generated by using popular spreadsheet applications (Microsoft Excel and Libre Office Calc). Details are given in the results section.

This is the first time for Turkey, that a water quality simulation software was developed at such a level of collaboration and was delivered to the Minister of Agriculture and Forestry of the Republic of Turkey. It was already integrated into the HIDROTURK modelling platform-water quality and ecology module, which is under continuous development and consists of the box model described in this paper (a general transport sub-model, three water quality kinetics sub-models as components), a water ecology module based on Product Unit Neural Networks (PUNN), several utilities for assisting model input generation and a GIS based graphical user interface developed in Python. All of these components of HIDROTURK, including the box model core described in this paper are under continuous development. Additional water quality model cores (such as the one described in this paper) as well as new utilities may be added into the HIDROTURK water quality and ecology module.

To develop a universally accepted and industry style water quality model takes decades and therefore the product of this study should be further developed. This stage of development could be considered as a working prototype and should be further tested for Quality Control and Quality Assurance (QC/QA).

The software was implemented on the high-level programming language - MATLAB, an easy to read and understand coding style- and was also run under Octave, the free software environment. As it was delivered to the Minister of Agriculture and Forestry, it could be released after the QC/QA in several forms; open source that can run both under Octave and MATLAB or as an executable that would run seamlessly without installing any integrated development environment. The software could also be integrated to other water resources management-oriented software development projects such as water allocation models.

Suggestions for the future work are:

- The model developed in this study does not contain any algorithms to calculate the flow fields and turbulent diffusion and accepts user provided time series files for these important inputs. In the future utilities that use the outputs from several hydrodynamic models can be developed. Such type of hydrodynamic linkage will help to speed up the water quality modelling process considerably. Hydrodynamic models can also provide information for the water temperature that can directly be used by the water quality model.

- The only numerical solution algorithm to solve the system of differential equations implemented in the model is the simple Euler method. In the future more advanced numerical solution schemes can be implemented, that the user can trade-off which numerical algorithm so choose.

- The modelling software developed in this study consists of a main model code only. Utilities to support steps of the modelling processes such as the model calibration, sensitivity analysis and uncertainty analysis could be further developed. To support these tools; a database of model constants which can produce probability density functions of each relevant model constant would be useful.

- Development of a suit of post processing tools that calculate several indexes such as water quality classes, eutrophication indexes or ecological processes such as primary production, respiration or nutrient mass balance information would be beneficial as well. For these purposes, the model outputs should be extended to include process-based outputs.

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Appendix A

Dissolved Oxygen Saturation for Water Quality Model 1 and Water Quality Model 2

Dissolved oxygen saturation concentration given below is a function of temperature, salinity and elevation. Here the equation given by American Public Health Association (1992) has been utilized.

$$\mathrm{DOXY_{SAT}} = \left(1 - (0{,}1148 \cdot \mathrm{ELEV})\right) \cdot \exp\left(-139.34411 + \frac{157570.1}{T_K} - \frac{66423080}{T_K^2} + \frac{12438000000}{T_K^3} - \frac{862194900000}{T_K^4} - SALT \cdot \left(0.017674 - \frac{10.754}{T_K} + \frac{2140.7}{T_K^2}\right)\right)$$

(Equation 40)

where,

T_K : Temperature in degrees Kelvin (°K)
SALT : Salinity (ppt)
ELEV : Elevation above the mean sea level (km)

Reaeration Rate Constant for Water Quality Model 1

Reaeration rate constant is a function of average water velocity, depth, wind speed and temperature. In the model, the user can define a single reaeration rate constant, define variable reaeration rate constants depending on location, or instruct the model to calculate the variable reaeration constants depending on flow (KAHYDRA subroutine) or wind (KAWIND subroutine). Bigger reaeration rate constant calculated by flow or by the wind is used by the model.

Reaeration by Hydraulics

Model calculates the reaeration rate that occurs with the effect of flow by Covar Method (Covar, 1976). This method calculates reaeration rate as a function of velocity and depth using formula by Owens (Equation 41), Churchill (Equation 42) or O'Connor Dobbins (Equation 43).

$$k_{qj}(20\,^{\circ}C) = 5{,}349_{vj}^{0{,}67} \cdot D_j^{-1.85} \quad \text{(Equation 41)}$$

$$k_{qj}(20\,^{\circ}C) = 5{,}049_{vj}^{0{,}97} \cdot D_j^{-1.67} \quad \text{(Equation 42)}$$

$$k_{qj}(20\,^{\circ}C) = 3{,}93_{vj}^{0{,}5} \cdot D_j^{-1.50} \quad \text{(Equation 43)}$$

where,

k_{qj} : flow-induced reaeration rate coefficient at 20°C [1/day]

v_j : average water velocity in model box j [m/s]

D_j : Average model box depth [m]

Owens formula is used for model boxes with a depth of less than 60 cm. For model boxes with a depth of more than 60 cm, O'Connor Dobbins or Churchill formula is chosen by taking depth and velocity into consideration. For deep and slow flowing rivers O'Connor Dobbins Formula, while relatively shallow and fast flowing rivers Churchill formula is used. Depending on model box temperature, k_{qj} (20°C) coefficient is corrected by using Equation 44.

$$k_{qj}(T) = k_{qj}(20\,^{\circ}C) \cdot \theta_a^{T-20} \quad \text{(Equation 44)}$$

where,

T : water temperature [°C]

$k_{qj}(T)$: Reaeration rate constant at model box temperature [day^{-1}]

Θ_a : Temperature correction factor for reaeration rate constant [-]

Reaeration by Wind

Wind-induced reaeration is determined by O'Connor (1983). This method calculates reaeration as a function of wind speed, air and water temperatures and depth using either Equation 45 or Equation 46 or Equation 47.

$$k_{wj} = \frac{86400}{100\,D_j} \cdot \left(\frac{D_{OW}}{v_W}\right)^{2/3} \cdot \frac{\kappa^{1/3}}{\Gamma} \cdot \sqrt{\frac{\rho_a}{\rho_W} \cdot C_d} \cdot 100 \cdot W$$

(Equation 45)

$$k_{wj} = \frac{86400}{100\,D_j} \cdot \left[\frac{1}{\left(\frac{D_{OW}}{v_W}\right)^{2/3} \cdot \frac{\kappa^{1/3}}{\Gamma} \cdot \sqrt{\frac{\rho_a}{\rho_W} \cdot C_d} \cdot 100 \cdot W} + \frac{1}{\sqrt{\frac{D_{OW}}{\kappa\, z_0} \cdot \frac{\rho_a v_a}{\rho_W v_W} \cdot \sqrt{C_d} \cdot 100 \cdot W}}\right]^{-1}$$

(Equation 46)

$$k_{wj} = \frac{86400}{100 \cdot D_j} \cdot \sqrt{\frac{D_{OW}}{\kappa\, z_e} \cdot \frac{\rho_a v_a}{\rho_W v_W} \cdot \sqrt{C_d} \cdot 100 \cdot W}$$

(Equation 47)

where,

k_{wj} : wind-induced reaeration rate coefficient [1/day]

W : time-varying wind speed at 10 m above surface [m/s]

T_a : air temperature [°C]

T : water temperature [°C]

ρ_a : density of air as a function of T_a [g/cm^3]

ρ_w : density of water [1.0 g/cm^3]

v_a : viscosity of air as a function of T_a [cm^2/s]

v_W : viscosity of water as a function of T [cm^2/s]

D_{OW} : diffusivity of oxygen in water as a function of T [cm^2/s]

κ : von Karman's coefficient, 0.4

v_t : transitional shear velocity, set to 9, 10, and 10 for small, medium and large scale [cm/s]

v_c : critical shear velocity, set to 22, 11, and 11 for small, medium and large scales [cm/s]

z_e : equivalent roughness, set to 0.25, 0.35, and 0.35 for small, medium and large scales [cm]

z_0 : effective roughness as a function of, z_e, Γ, C_d, v_t, v_a, and W [cm]

λ : inverse of Reynold's number, set to 10, 3, and 3 for small, medium and large scales

Γ : nondimensional coefficient, set to 10, 6.5, and 5 for small, medium and large scales [-]

Γ_u : nondimensional coefficient as function of, Γ, v_c, C_d, and W [-]

C_d : drag coefficient as a function of z_e, Γ, v_a, κ, v_t ve W [-]

The model uses Equation 45 for wind speeds of up to 6 m/s, where interfacial conditions are smooth and viscous forces dominate momentum transfer. Equation 46 is used by the model for wind speed over 20 m/s, where interfacial conditions are rough and momentum transfer is dominated by turbulent eddies. Equation 47 is used for wind speeds between 6 and 20 m/s, and represents a transition zone in which the diffusional sublayer decays and the roughness height increases.

Reaeration Rate Constant for Water Quality Model 2

Reaeration coefficient k_A is defined to the module by the user. If this value is negative, it is estimated by the model, through a subroutine that calculate reaeration rate.

If $k_A < 0$,

$$k_A = k_1/H \qquad \text{(Equation 48)}$$

where

k_A: reaeration rate coefficient [1/day]

k_1: dissolved oxygen interfacial transfer coefficient [m/day]

Reaeration Options for River Type Segment

Option 1 (O'Connor & Dobbins, 1958):

$$k_1 = 3.93 \cdot \frac{U^{0.5}}{H^{1.5}} \cdot H \qquad \text{(Equation 49)}$$

Option 2 (Churchill et al., 1962):

$$k_1 = 5.026 \cdot \frac{U}{H^{1.67}} \cdot H \qquad \text{(Equation 50)}$$

Option 3 (Owens et al., 1964):

$$k_1 = 5.32 \cdot \frac{U^{0.67}}{H^{1.85}} \cdot H \qquad \text{(Equation 51)}$$

Option 4 (Langbein & Drum, 1967):

$$k_1 = 5.13 \cdot \frac{U}{H^{1.33}} \cdot H \qquad \text{(Equation 52)}$$

Units given in Equation 49-Equation 52 are as follows: ka (d^{-1}), U(mps), H(m)

Reaeration Options for Lake/Reservoir Type Segment

Option 1 (Broecker et al., 1978):

$$k_1 = 0.864 \cdot U_{W,10} \qquad \text{(Equation 53)}$$

Option 2 (Banks, 1975; Banks & Herera, 1977):

$$k_1 = \left(0.728 \cdot \sqrt{U_{W,10}}\right) - \left(0.317 \cdot U_{W,10}\right) + \left(0.0372 \cdot U_{W,10}^2\right) \qquad \text{(Equation 54)}$$

Option 3 (Wanninkhof et al., 1991):

$$k_1 = 0.864 \cdot U_{W,10}^{1.64} \quad \text{(Equation 55)}$$

Reaeration Options for Estuary Type Segment

Homann & Fitzpatrick, 1982

$$k_1 = 5.32 \cdot \frac{U^{0,5}}{H^{1,5}} \cdot H + 0.728 \cdot U^{0,5} - 0.317 \cdot U + 0.0372 \cdot U^2 \quad \text{(Equation 56)}$$

If $k_a > 0$,

$$k_A = k_A/H \quad \text{(Equation 57)}$$

where,

$U_{W,10}$: wind speed at 10 m above water surface (m/s)

k_A : Reaeration rate constant (1/day)

H : Depth (m)

Appendix B
Kinetic and Stoichiometric Constants for Water Quality Kinetics Sub Model 1

Appendix B
Model Constants That Can Be Spatially Variable

Model constant	Unit	Relevant State Variable	Description
$k_{NITR,20}$	1/day	NH4N	Nitrification rate at 20°C
θ_{NITR}	-	NH4N	Arrhenius temperature correction factor for nitrification rate constant
$k_{HS,NITR,DOXY}$	mg O_2/L	NH4N	Monod half saturation concentration of dissolved oxygen for nitrification
$k_{DENITR,20}$	1/day	NO3N	Denitrification rate at 20°C
θ_{DENITR}	-	NO3N	Arrhenius temperature correction factor for denitrification rate constant
$K_{HS,DENITR,DOXY}$	mg O_2/L	NO3N	Reversed Monod half saturation concentration of dissolved oxygen for denitrification
$k_{PHYTO,GROW,20}$	1/day	PHYC	Phytoplankton growth rate constant at 20°C
$\theta_{PHYTO,GROW}$	-	PHYC	Arrhenius temperature correction factor for phytoplankton growth rate constant
$k_{HS,N}$	mg N/L	PHYC	Monod half saturation concentration for phytoplankton nitrogen uptake
$k_{HS,P}$	mg P/L	PHYC	Monod half saturation concentration for phytoplankton phosphorus uptake
$k_{PHYTO,DEATH,20}$	1/day	PHYC	Phytoplankton death rate constant at 20°C
$\theta_{PHYTO,DEATH}$	-	PHYC	Arrhenius temperature correction factor for phytoplankton death rate constant
$k_{PHYT,RESP,20}$	1/day	PHYC	Phytoplankton respiration rate constant at 20°C
$\theta_{PHYTO,RESP}$	-	PHYC	Arrhenius temperature correction factor for phytoplankton respiration rate constant
$k_{HS,AMM,PREF,NH4N}$	mg N/L	PHYC	Monod half saturation concentration for ammonia preference of phytoplankton
$k_{CBOD,MINER,20}$	1/day	CBOD	Carbonaceous BOD deoxygenation rate constant at 20°C
$\theta_{CBOD,MINER}$	-	CBOD	Arrhenius temperature correction factor for CBOD deoxygenation rate constant
$k_{HS,MINER,DOXY}$	mg O_2/L	CBOD	O_2 half saturation concentration for CBOD mineralization
k_A	1/day	DOXY	Reaeration rate at 20°C If equal to zero ⇨calculated by model
$k_{ORGN,MINER,20}$	1/day	ORGN	Organic nitrogen mineralization rate at 20°C
$\theta_{ORGN,MINER}$	-	ORGN	Arrhenius temperature correction factor for mineralization rate constant for organic nitrogen
$k_{ORGP,MINER,20}$	1/day	ORGP	Organic phosphorus mineralization rate at 20°C
$\theta_{ORGP,MINER}$	-	ORGP	Arrhenius temperature correction factor for mineralization rate constant for organic phosphorus
$k_{d,bott}$	1/day	*	Bottle BOD decay rate constant

* This constant is related with derived parameter BOD_5.

Appendix C
Kinetic and Stoichiometric Constants for Water Quality Kinetics Sub Model 2

Table C2

Model Constants That Can Be Spatially Variable

Model constant	Unit	Relevant State Variable	Description
$k_{PHYTO,GROW,20}$	1/day	Phytoplankton Carbon	Phytoplankton growth rate constant at 20°C (1/day)
$\theta_{PHYTO,GROW}$	-	Phytoplankton Carbon	Arrhenius temperature correction factor for phytoplankton growth
$k_{PHYTO,RESP,20}$	1/day	Phytoplankton Carbon	Phytoplankton respiration rate constant at 20°C
$\theta_{PHYTO,RESP}$	-	Phytoplankton Carbon	Arrhenius temperature correction factor for phytoplankton respiration
$k_{PHYTO,DEATH,20}$	1/day	Phytoplankton Carbon	Phytoplankton death rate constant at 20°C
$\theta_{PHYTO,DEATH}$	-	Phytoplankton Carbon	Arrhenius temperature correction factor for phytoplankton death
$k_{HS,AMM,PREF,NH4N}$	-	Phytoplankton Carbon	Ammonia preference of phytoplankton as DIN source
$k_{HS,N}$	g N/m^3	Phytoplankton Carbon	Monod half saturation concentration for phytoplankton DIN uptake
$k_{HS,P}$	g P/m^3	Phytoplankton Carbon	Monod half saturation concentration for phytoplankton SRP uptake
I_S	Langley	Phytoplankton Carbon	Saturation light intensity
$k_{FPOC,DISS,20}$	1/day	Particulate Organic Carbon	Particulate organic carbon dissolution rate constant at 20°C
$\theta_{FPOC,DISS}$	-	Particulate Organic Carbon	Arrhenius temperature correction factor for fine particulate organic carbon dissolution
$k_{HS,FPOC,DISS,20}$	gC/m^3	Particulate Organic Carbon	Monod half saturation concentration of fine particulate organic carbon dissolution
$k_{FPON,DISS,20}$	1/day	Particulate Organic Nitrogen	Particulate organic nitrogen dissolution rate constant at 20°C
$\theta_{FPON,DISS}$	-	Particulate Organic Nitrogen	Arrhenius temperature correction factor for fine particulate organic nitrogen dissolution
$k_{HS,PON,DISS}$	g N/m^3	Particulate Organic Nitrogen	Monod half saturation concentration of fine particulate organic nitrogen dissolution
$k_{FPOP,DISS,20}$	1/day	Particulate Organic Phosphorus	Particulate organic phosphorus dissolution rate constant at 20°C

Table C2

Model Constants That Can Be Spatially Variable (continued)

Model constant	Unit	Relevant State Variable	Description
$\theta_{FPOP,DISS}$	-	Particulate Organic Phosphorus	Arrhenius temperature correction factor for fine particulate organic phosphorus dissolution
$k_{HS,POP,DISS}$	g P/m^3	Particulate Organic Phosphorus	Monod half saturation concentration of fine particulate organic phosphorus dissolution
Y_{AERHET}	g C/g C	Dissolved Organic Carbon	Bacterial biomass yield of DOC mineralization
$k_{DOC,MINER,20}$	1/day	Dissolved Organic Carbon	Dissolved organic carbon mineralization rate constant at 20°C
$\theta_{DOC,MINER}$	-	Dissolved Organic Carbon	Arrhenius temperature correction factor for dissolved organic carbon mineralization
$k_{HS,DOC,MINER}$	g C/m^3	Dissolved Organic Carbon	Monod half saturation concentration of dissolved organic carbon mineralization
$k_{DON,MINER,20}$	1/day	Dissolved Organic Nitrogen	Dissolved organic nitrogen mineralization rate constant at 20°C
$\theta_{DON,MINER}$	-	Dissolved Organic Nitrogen	Arrhenius temperature correction factor for dissolved organic nitrogen mineralization
$k_{HS,DON,MINER}$	g N/m^3	Dissolved Organic Nitrogen	Monod half saturation concentration of dissolved organic nitrogen mineralization
$k_{DOP,MINER,20}$	1/day	Dissolved Organic Phosphorus	Dissolved organic phosphorus mineralization rate constant at 20°C
$\theta_{DOP,MINER}$	-	Dissolved Organic Phosphorus	Arrhenius temperature correction factor for dissolved organic phosphorus mineralization
$k_{HS,DOP,MINER}$	g P/m^3	Dissolved Organic Phosphorus	Monod half saturation concentration of dissolved organic phosphorus mineralization
$k_{NITR,20}$	1/day	Ammonium Nitrogen	Nitrification rate constant at 20°C
θ_{NITR}	-	Ammonium Nitrogen	Arrhenius temperature correction factor for nitrification
$k_{HS,NITR,NH4N}$	g N/m^3	Ammonium Nitrogen	Monod half saturation concentration of ammonia nitrogen for nitrification
$k_{HS,NITR,DOXY}$	g O_2/m^3	Ammonium Nitrogen	Monod half saturation concentration of dissolved oxygen for nitrification

Table C2

Model Constants That Can Be Spatially Variable (continued)

Model Constant	Unit	Relevant State Variable	Description
Y_{DENITR}	g C/g N	Nitrate Nitrogen	Bacterial biomass yield of denitrification
$k_{DENITR,20}$	1/day	Nitrate Nitrogen	Denitrification rate constant at 20°C
θ_{DENITR}	-	Nitrate Nitrogen	Arrhenius temperature correction factor for denitrification
$k_{HS,DENITR,NO3N}$	g N/m^3	Nitrate Nitrogen	Monod half saturation concentration of nitrate nitrogen for denitrification
$k_{HS,DENITR,DOXY}$	g O_2/m^3	Nitrate Nitrogen	Monod half saturation concentration of dissolved oxygen for denitrification
$k_{HS,DENITR,DOC}$	g C/m^3	Nitrate Nitrogen	Monod half saturation concentration of dissolved organic carbon for denitrification
$k_{PIP,DISS,20}$	1/day	Particulate Inorganic Phosphorus	Particulate inorganic phosphorus dissolution rate constant at 20°C
$\theta_{PIP,DISS}$	-	Particulate Inorganic Phosphorus	Arrhenius temperature correction factor for particulate inorganic phosphorus dissolution rate constant
$k_{HS,PIP,DISS}$	g P/m^3	Particulate Inorganic Phosphorus	Monod half saturation concentration of particulate inorganic phosphorus dissolution
k_{ew}	1/m	Phytoplankton Carbon	Background light extinction parameter
k_A	1/day	Dissolved Oxygen	Reaeration rate constant

Table C1

Model Constants That Cannot Be Spatially Variable

Model constant	Unit	Relevant State Variable	Description
$a_{O2:C,PHYTO}$	mg O_2/mg C	PHYC	32/12 mg O_2/mg C in phytoplankton
$a_{P:C,PHYTO}$	mg P/mg C	PHYC	P:C ratio in phytoplankton
$a_{N:C,PHYTO}$	mg N/mg C	PHYC	N:C ratio in phytoplankton
$a_{CHLA:C,PHYTO}$	mg C/mg Chl-a	PHYC	Chlorophyll-a to Carbon ratio

Table C3

Model Constants That Cannot Be Spatially Variable

Model constant	Unit	Relevant State Variable	Description
$a_{CHLA:C,PHYTO}$	mg Chl-a/mg C	Phytoplankton Carbon	Stoichiometric Chlorophyll-a to phytoplankton carbon ratio
$a_{N:C,PHYTO}$	mg N/mg C	Phytoplankton Carbon	Stoichiometric nitrogen to phytoplankton carbon ratio
$a_{P:C,PHYTO}$	mg P/mg C	Phytoplankton Carbon	Stoichiometric phosphorus to phytoplankton carbon ratio
$a_{O2:C,PHYTO}$	mg O_2/mg C	Phytoplankton Carbon	Stoichiometric oxygen to phytoplankton carbon ratio
$a_{VSS:C,FPOC}$	mg C/mg C	Non-algal Particulate Organic carbon	Stoichiometric volatile suspended solids to Non-algal Particulate Organic carbon ratio
$a_{O_2:C,\,DOC}$	mg O_2/mg C	Dissolved Organic Carbon	Stoichiometric oxygen to dissolved organic carbon ratio for dissolved organic carbon
$a_{C:N,DENITR}$	mg C/mg N	Nitrate Nitrogen	Stoichiometric carbon to nitrogen ratio for denitrification

Water Quality Model 1 – Expression for Ammonia Preference Factor

$$pref_{NH4N} = \frac{NH4N \cdot NO3N}{\left(k_{HS,AMM,PREF,NH4N} + NH4N\right) \cdot \left(k_{HS,AMM,PREF,NH4N} + NO3N\right)} + \frac{k_{HS,AMM,PREF,NH4N} \cdot NH4N}{(NH4N + NO3N) \cdot \left(k_{HS,AMM,PREF,NH4N} + NO3N\right)}$$

Water Quality Model 2 – Expression for Ammonia Preference Factor

$$pref_{NH4N} = \frac{NH4N}{k_{HS,AMM,PREF,NH4N} + NH4N}$$

Extended Turkish Abstract
(Genişletilmiş Türkçe Özet)

Matris Cebrine Dayanan Esnek Bir Su Kalitesi Simülatörü

Su ekosistemlerinin sürdürülebilir yönetimi için bütünleşik bir yaklaşım uygulanması gereklidir. Bu nedenle, havza esaslı yönetim, su kalitesinin iyileştirilmesi için giderek daha popüler bir araç haline gelmektedir. Su kalitesi modelleri havza yönetiminin merkezi bir parçasıdır. Su kalitesi tahminleri yapan modeller su kütlesine dışarıdan gelen etkileri değerlendirmek, sistemin işleyişini anlamak, verilerdeki boşlukları doldurmak ve senaryo analizleri yapabilmek açısından değerli araçlardır ancak hem işletme hem de yazılım geliştirme açısından genellikle karmaşık altyapıya sahiptirler. Dünyadaki ihtiyaç ve gelişmeleri takiben, bazıları ücretsiz, bazıları açık kaynak kodlu olmak üzere konvansiyonel su kirliliği ve ötrofikasyon problemini araştırmak için birçok su kalitesi kodu geliştirilmiştir. Türkiye'de besin elementi kökenli su kirliliği ve ötrofikasyon modelleme çalışmalarının sayısı ABD ve Avrupa Birliği ile karşılaştırıldığında fark edilir ölçüde azdır. Bu çalışmada Türkiye'de aşağıda listelenen kriterleri sağlayacak HİDROTÜRK modeline alt modül olarak bağımsız bir su kalitesi simülasyon kodunun geliştirilmesi hedeflenmiştir.

Kriter 1. Model, biyocoğrafik çeşitlilik ve veri kullanılabilirliği açısından Türkiye şartlarına uygun olmalıdır. Birden çok su kalitesi kinetiği alt modelinin uygulanmasını mümkün kılabilmesi için esnek bir su kalitesi modelleme çerçevesi gerektirmektedir. Model ayrıca düzensiz veriler ve eksik verilerle başa çıkabilmelidir. Ayrıca, basit alt modellerden daha karmaşık alt modellere geçiş yapılabilmelidir.

Kriter 2. Model, Türkiye'de yıllardır başarılı bir şekilde uygulanmakta olan su kalitesi konuları ile saha ve laboratuvar yöntemleri hakkındaki bilgilere dayanılarak uygulanabilir ve işletilebilir olmalıdır. Su kalitesi modellerinin basit durumlar için bile uygulanması ve işletilmesi, saha yöntemleri konusunda eğitilmiş sahada çalışan bilim insanları ekibi, eğitimli teknisyenlerle laboratuvar altyapısı ve geniş teorik bilgi ve bilgisayar becerilerine sahip modelleme uzmanları tarafından yürütülen bir ekip çalışmasını gerektirecektir.

Kriter 3. Model, akarsular, göller, rezervuarlar, haliçler ve kıyı suları gibi farklı su kütleleri için kullanılabilmelidir. Modelin taşınım şeması bu kriter dikkate alınarak tasarlanmalıdır.

Kriter 4. Model, akademisyenler ve kurumlar için genel modelleme bilgisine katkıda bulunmalıdır. Genel amaçlı su kalitesi modelleri zaten mevcut olduğundan, bu önemli bir konudur. Bununla birlikte, farklı kinetik alt modellerle spesifik uygulamalar yapmak mümkün olsa da basit değildir.

Kriter 5. Model kodu, farklı su kalitesi kinetik alt modellerini içerebilmeli ve bu nedenle incelenmesi ve anlaşılması kolay olmalıdır. Daha önce belirtildiği gibi, Türkiye'nin karmaşık biyocoğrafyası farklı su kalitesi kinetik alt modellerinin uygulanmasını gerektirmektedir. Tüm farklı su kalitesi alt modellerini yapmak için bir altyapı geliştirmek mümkün olmakla birlikte oldukça zor bir iştir. Bu nedenle, modelin genel kodunun incelenmesi ve genişletilmesi kolay olmalıdır.

Bu çalışmanın amacı, daha büyük bir hidro-ekolojik modelleme çerçevesinin ana su kalitesi simülatörünü geliştirmektir. Su kalitesi sorunları çok çeşitli olduğundan, tüm su kalitesi sorunlarına

uygulanabilecek tek bir su kalitesi kinetiği alt modelinin geliştirilmesi imkânsızdır. Bu nedenle; su kalitesi simülatörü yazılım kodu, açık kaynak felsefesini takip ederek geliştirilerek yüksek seviyede (ancak yüksek performanslı) bir programlama dilinde yazılmış ve kod okunabilirliğini artırmak için iyi bir şekilde belgelendirilmiştir. Matris cebrine dayalı olarak geliştirilen temel su kalitesi simülatör yazılımı, genel bir taşınım alt modeli, üç su kalitesi kinetiği alt modeli ve yardımcı programlardan oluşmaktadır.

Taşınım alt modelinde her bir su kütlesi tam karışımlı olduğu varsayılan kontrol hacimlerine ayrılmakta ve kontrol hacimlerinin her biri için diğer kontrol hacimleri ile veya su kütlesinin temasta olduğu coğrafi bileşenler ile su ve madde alışverişlerini dikkate alan zamana göre dinamik su kütle dengeleri kurulmaktadır. Taşınım, adveksiyon ve difüzyon denklemi ile hesaplanmaktadır. Su kütleleri öncelikle yatay yönde segmentlere ayrılmakta, her segment ise düşeyde kutulara ayrılmaktadır. Segmentler birbirleriyle ve sınır koşullarıyla arayüz alanları üzerinden madde alışverişi yapmaktadır. Her kütle dengesinin taşınım dışında tam karışımlı reaktör içindeki madde dönüşümlerini temsil eden kinetik bileşeni de bulunmaktadır. Bu yaklaşım "Kutu Modeli" olarak bilinmektedir. Bu yaklaşımın üstünlüğü kutuların herhangi bir şekil ve büyüklük kısıtı olmaksızın tanımlanabilmelerinin mümkün olmasıdır. Kutuların dizilimlerine göre tek, iki veya üç boyutlu modellerinin oluşturulması mümkündür. Böylece aynı yaklaşımla akarsular (seri olarak dizilmiş tam karışımlı reaktörler olarak), sığ göller (yan yana dizilmiş tam karışımlı reaktörler olarak) ve derin göl ve baraj gölleri (kısmen yan yana, kısmen alt alta dizilmiş tam karışımlı reaktörler olarak) modellenebilmektedir.

Genel su kalitesi kinetiği alt modeli verilerin veya sistem ile ilgili bilgilerin kısıtlı olduğu durumlarda konvansiyonel kirleticiler ve ötrofikasyon problemi için kullanılmak üzere tasarlanmıştır. 10 adet durum değişkeni (Tuzluluk, Toplam Katı Madde, Karbonlu BOİ, Çözünmüş Oksijen, Canlı Olmayan Organik Azot, Amonyum Azotu, Nitrat Azotu, Canlı Olmayan Organik Fosfor, Fosfat Fosforu, Fitoplankton Karbonu) modellenebilmektedir. Model ayrıca 10 adet türetilmiş değişkeni (İletkenlik, Çözünmüş İnorganik Azot, Toplam Organik Azot, Toplam Kjeldahl Azotu, Toplam Azot, Toplam Organik Fosfor, Toplam Fosfor, Klorofil-a, Nihai Karbonlu BOİ, 5 Günlük Biyokimyasal Oksijen İhtiyacı) için sonuç vermektedir. Durum değişkenleri ve türetilmiş değişkenler model tarafından her zaman adımında ve her kutuda hesaplanmaktadır. Model karmaşıklık seviyeleri (1. Seviye, 2. Seviye, 3. Seviye, 4. Seviye) kullanıcı tarafından seçilebilmektedir. Seçilen model karmaşıklığı seviyesine göre modellenen durum değişkeni sayısı farklılık göstermektedir.

Detaylı yönetim uygulamaları için geliştirilen ileri su kalitesi kinetiği alt modelinde 14 adet durum değişkeni (Fitoplankton Karbonu, Partikül Haldeki Organik Karbon, Partikül Haldeki Organik Azot, Partikül Haldeki Organik Fosfor, Çözünmüş Organik Karbon, Çözünmüş Organik Azot, Çözünmüş Organik Fosfor, Amonyum Azotu, Nitrat Azotu, Çözünmüş Reaktif Fosfor, Partikül Haldeki İnorganik Fosfor, Çözünmüş Oksijen, İnorganik Askıda Katı Madde, Tuzluluk) mevcut olup bu değişkenlerin tamamı modellenmektedir. Model ayrıca 16 adet türetilmiş değişkeni [İletkenlik, Çözünmüş İnorganik Azot, Toplam Organik Azot, Toplam Kjeldahl Azotu, Toplam Azot, Toplam Organik Fosfor, Toplam Fosfor, Klorofil-a, Nihai Karbonlu BOİ, 5 Günlük Biyokimyasal Oksijen İhtiyacı, Çözünmüş Organik Karbon Esaslı Biyokimyasal Oksijen İhtiyacı, Partiküler Organik Karbon Esaslı Biyokimyasal Oksijen İhtiyacı, Karbonlu Biyokimyasal Oksijen İhtiyacı (Cansız organik maddeye karşılık gelen karbonlu BOİ), Askıda Katı Madde, Uçucu Askıda Katı Madde, Fosfat Fosforu] için sonuç vermektedir.

Genel kirletici kinetiği alt modelinde istenilen sayıda genel kirletici için istenilen mertebe kinetiği kullanılarak hesaplama yapılabilmektedir. Bütün kirleticilerin birbirleri ile ve oluşan yan ürünler ile etkileşimleri dikkate alınmamaktadır.

Model yazılım, okunması ve anlaşılması kolay bir kodlama stili kullanılarak üst düzey programlama dili MATLAB ile yapılmıştır. Ayrıca Octave ücretsiz yazılım ortamında da çalıştırılabilmektedir.

Sonuç olarak, Türkiye'de çok sayıda enstitünün (üniversiteler, devlet kurumları ve teknoparklar) işbirliği ile bir su kalitesi modelleme simülasyon yazılımı geliştirilmiştir. Türkiye için ilk kez, böyle bir işbirliği düzeyinde bir su kalitesi simülasyon yazılımı geliştirilmiş ve TC Tarım ve Orman Bakanlığı'na teslim edilmiştir. Dünyaca kabul gören ve endüstri tarzı bir su kalitesi modeli geliştirmek on yıllar almaktadır ve bu nedenle bu çalışmanın ürünü daha da geliştirilmeli, Kalite Güvence (QA) & Kalite Kontrol (QC) testlerinden geçirilmelidir.