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Automatic Calibration of Water Quality and Hydrodynamic Model (CE-QUAL-W2)

by

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Abstract

One of the most important purposes of surface water resource management is to develop predictive models to assist in identifying and evaluating operational and structural measures for improving water quality. To better understand the effects of external and internal nutrient and organic loading and the effects of reservoir operation, a model is often developed, calibrated, and used for sensitivity and management simulations. The importance of modeling and simulation in the scientific community has drawn interest towards methods for automated calibration. This study addresses using an automatic technique to calibrate the water quality model CEQUAL-W2 (Cole and Wells, 2013). CE-QUAL-W2 is a two-dimensional (2D) longitudinal/vertical hydrodynamic and water quality model for surface water bodies, modeling eutrophication processes such as temperature-nutrient-algae-dissolved oxygen-organic matter and sediment relationships. The numerical method used for calibration in this study is the particle swarm optimization method developed by Kennedy and Eberhart (1995) and inspired by the paradigm of birds flocking. The objective of this calibration procedure is to choose model parameters and coefficients affecting temperature, chlorophyll a, dissolved oxygen, and nutrients (such as NH_4, NO_3, and PO_4). A case study is presented for the Karkheh Reservoir in Iran with a capacity of more than 5 billion cubic meters that is the largest dam in Iran with both agricultural and drinking water usages. This algorithm is shown to perform very well for determining model parameters for the reservoir water quality and hydrodynamic model. Implications of the use of this procedure for other water quality models are also shown.

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1. Introduction

Water quality models are increasingly developed to achieve water quality goals and to evaluate the impacts of climate, land use, and land on the quantity and quality of water resources. Calibration of these models is a critical step in the overall model development before using them in research and/or real-world applications.

During the last 2 decades, the incorporation of monitoring programs and water quality modeling has provided useful tools for water quality management in impounding reservoirs (Hay et al.,1998; Isazadeh et al., 2005; Sullivan and Round, 2005; Afshar and Saadatpour, 2008; Diogo et al., 2008). Most water quality models are characterized by complex functional relationships and large number of parameters to achieve a system that closely resembles the actual system being represented by the model. Manual trial and error calibration is time consuming and depends on the modeler's experience, skill, and knowledge of the model's processes and dynamics. While overcoming the shortcomings of manual trial and error calibration, automatic calibration of complex hydrosystem models requires a tremendous amount of computation (Mahinthakumar G. and Sayeed M. 2005; Chung S.W., and Oh J.K. 2006; Kuo J.T., Wang Y.Y. and Lung W.S. 2006). In fact, both hydrodynamic and water quality behavior of a water body simulated with a representative model may be affected by a set of calibration parameters which are not necessarily independent of each other. This makes automatic calibration of such models more challenging. Calibration of complex river –reservoir water quality models is an excellent example where the model must be calibrated for both hydrodynamic and water quality behavior. In such cases, one may define multiple calibration objectives to account for both hydrodynamic and water quality behavior of the model. In such cases multiple objective optimizations may improve model calibration but further increase the computational requirements and cost. One of the most common multi-objective optimization methods involve transforming multiple objectives into a single function, by the weighted sum principle where the objectives are multiplied with user-defined weights and added together to form a single function (Deb K. 2001). In recent years different versions of evolutionary and/or metaheuristic algorithms have been successfully used for various hydrosystems. (Genetic Algorithm (GA), Chang et al., 2005; ant colony optimization algorithm (ACO), Jalali et al., 2007; honey bees mating optimization (HBMO), Bozorg Haddad et al., 2006; particle swarm optimization (PSO), Fallah-Mehdipour et al., 2011).

In spite of broad investigations about automatic calibration of CE-QUAL-W2 model, still finding an automatic optimization approach to calibrate model parameters with reasonable performance is a real challenge (Baker and Dycus, 2004; Nielsen, 2005; Kuo et al., 2006; Chaves and Kojiri, 2007; Gelda and Effler, 2007; Liu et al., 2008; Shourian et al., 2008; Karamouz et al., 2009; Etemad shahidi et al., 2009; and Afshar et al., 2011). The aim of the present study is to show the result of coupling of the particle swarm optimization (PSO) method to the CE-QUAL-W2 model for automatic calibration of temperature, chlorophyll a, dissolved oxygen, and nutrients of a water body.

2. Calibration

It is important to consider the possible reactions of the water body before taking any action and making any management decisions. Surface waters are the complex environmental systems and understanding and predicting their behavior is difficult. During decades, scientists have tried to develop mathematical models to predict the response of water bodies to pollution loads originating from human activities. These models are able to quantitatively describe the physical, chemical and biological behavior of the water bodies and include a collection of mathematical relationships that contain many parameters (e.g., reaction rate coefficients, biological and chemical constants) that are specific to the system modeled. The modeler should decide about the value of these parameters through the calibration phase giving the near optimum model parameters possible for a successful modeling practice. Water quality and hydraulics models generally require a relatively large number of parameters to define, and since prior information on parameter values is limited, these are commonly defined by fitting the model to observed data.

Water quality variables are often highly correlated (Van Griensven et al., 2002). Many model parameters affect more than a single state variable and when this is the case, it is more appropriate to estimate the parameter for all affected state variables simultaneously (Little and Williams, 1992). For example, BOD decay rate affects both BOD and DO values within the system. If parameter estimation is conducted using both DO and BOD data, the estimates will be more accurate than the estimates based only on the DO data (Mulligan and Brown, 1998). Moreover, when all the output variables are used simultaneously during the calibration process, all the available information will be used. In addition, the risk of error accumulation at the end step will be reduced (Van Griensven et al., 2002). However, incorporating all the output variables simultaneously to the calibration process will increase the computational complexity substantially. For such intricate systems, exercising typical nonlinear techniques for the solution may be problematic. Moreover, in these multi-dimensional complex systems, the setback of converging to local optima is prominent.

Calibration methods include two major categories:

- Manual calibration
- Automatic calibration

In the manual method, the modeler adjusts the model parameters by running the model for different parameter values several times until achieving a reasonable fitness between the observations and the predictions. This can be time consuming work. The method is subjective since the success of a manual calibration essentially depends on the experience of the modelers and their knowledge of the basic approaches and interactions in the model. The modelers are left unsure whether the calibration result is the best that can be achieved or not. Different methods of automatic calibration were developed to increase the probability of improvement of these weaknesses.

Automatic calibration methods which are computer-aided optimization techniques increases the efficiency of the modeling process by using objective, statistically valid methods and increase the reliability of the calibration outcome. By this way, the bias introduced by judgment of the modeler is minimized. Moreover, the time allocated for the process can be considerably decreased.

Bowles and Grenney (1978) applied sequential extended Kalman filters as a technique for calibration and water quality modeling of a river. They used the method for a real river system. In their study, they clearly showed the calibration ability of the filter procedure. Coefficients in the model were estimated at the same time as the state variables.

The sum-of-least-squares approach as an objective function was employed in the most of the model calibration studies using optimization (Yih and Davidson, 1975; Wood et al., 1990; Little and Williams, 1992; Mulligan and Brown, 1998; Van Griensven and Bauwens, 2001). Minimizing the error between the observed and simulated state variables is the general objective in all of these studies, although they applied different methods to find the best solution for the objective function such as Kalman filters, Nelder mead algorithm, etc.

Wood et al. (1990) developed a system to use in the calibration process and a stream-quality simulation model. The author linked a biochemical oxygen demand (BOD) –

dissolved oxygen model, graphics software, and a code to perform the model calibration to an expert system shell. The objective function was an average absolute-value deviation of the calculated values from the measured ones in the calibration process. The pattern search technique was applied in calibration to determine the search direction that would cause a lower error. He has calibrated four parameters for river model in his research. The calibration process was applied on each reaches separately and sequentially instead of consideration of whole system to simplify the procedure.

Today, water quality models are developed in a highly advanced and complex way. They can simulate a high variety of water quality constituents, and require a high number of input parameters. For the calibration of these models, using new, global optimization techniques may give better results compared to the traditional methods. These new techniques are more robust to messy problems such as discontinuities and difficult-to-evaluate or nonexistent derivatives (Little and Williams, 1992). Most of them use statistical, probabilistic or heuristic algorithms that rarely trapped at the local optima (Cooper et al., 1997; Goldberg, 1989).

For example, Mulligan and Brown (1998) used genetic algorithms to calibrate the steady-state Streeter-Phelps model. They compared genetic algorithms performance with a more traditional optimization technique, the Marquardt algorithm, and found GA results is superior. Although there exist quite a number of studies for implementing objective methods in water quality model calibration, application of such methods in practice has gained importance recently. Recent developments in the global search techniques and advancements in the computer technology will promote their application.

3. Particle Swarm Optimization

One of the population-based evolutionary algorithms that has shown great potential in various optimization problems of water resources management (Izquierdo, J., 2008) is Particle Swarm Optimization. The PSO algorithm was introduced by Kennedy and Eberhart (1995) and is based on the simulation of the social behavior of migrating birds trying to reach a destination. Since PSO requires low memory and CPU speed, it is computed inexpensively and is implemented easily.

The computer simulations of various interpretations of the movement of organisms in a bird flock or fish school have been created by a number of scientists. Firstly, Reynolds C. W. (1987) and Heppner and Grenander (1990) presented simulations of bird flocking. Reynolds was interested in the aesthetics of bird flocking choreography, and Heppner, a zoologist, has worked in discovering the primary principal that showed how a large numbers of birds can flock synchronously, can change direction suddenly, can separate and reform a group. Both of these scientists had understood that local processes, such as those modeled by cellular automata, are basically the unpredictable group dynamics of bird social behavior. Both models were based on modification of distance between birds flying together. The flocking behavior of birds was considered as a function of birds' efforts to maintain an optimum distance between themselves and their neighbors. (Kennedy and Eberhart, 1995)

Wilson (1975), a sociobiologist, has written, in reference to fish schooling, In theory at least, individual members of the school can profit from the discoveries and previous experience of all other members of the school during the search for food. This advantage can become decisive, outweighing the disadvantages of competition for food items, whenever the resource is unpredictably distributed in patches. This idea was behind the particle swarm optimization.

In PSO, each bird is a potential solution and is called a particle. Second, there is social-psychological tendency among individuals with communication and information exchange in the population to emulate the success of other individuals. The position of each particle is changed based on individual intelligence and the intelligence of its neighbors to coordinate their movement towards the best position. At the first swarm, the position and velocity of particles have been determined randomly and then an objective function of each particle is then evaluated to find the optimal solution by iteration.

Particle swarm optimization and the genetic algorithm are similar in that the system is initialized with a population of random solutions. They are not the same because in PSO for each potential solution is also assigned a randomized velocity, and the potential solutions, called particles, are then “flown” through hyperspace. In PSO, velocity is in the unit of [L] not [L/T]. So, velocity, in this case, is just a direction that defines the direction of movement to each particle in search space. This term helps increase the time efficiency of procedure by preventing of particles to move toward positions that are far from optimum solution. Each particle memorizes track of its coordinates in hyperspace which are known as the best solution (fitness) it has achieved so far. (The value of that fitness is also stored.) This value is called pbest. Another “best” value is also tracked. Each particle also keeps the overall best value, and its location obtained thus far by any particle in the population; this is called gbest. Particles in the case of water quality are the vector of all calibrated parameters. PSO tries to find the best particle which is the near optimum solution and defines optimum parameters to CE-QUAL-W2 model.

Algorithm below explains all steps of original PSO which used in this study. (Poli et. al. 2007)

“1: Initialize a population array of particles with random positions and velocities on D dimensions in the search space.

2: loop

3: For each particle, evaluate the desired optimization fitness function in D variables.

4: Compare particle’s fitness evaluation with its pbest_i. If current value is better than pbest_i ,then set pbest_i equal to the current value, and $\vec{p}_i$ equal to the current location $\vec{x}_i$ in D-dimensional space.

5: Identify the particle in the neighborhood with the best success so far, and assign its index to the variable g.

6: Change the velocity and position of the particle according to the following equation

$$\vec{v}_i \leftarrow \vec{v}_i + \vec{U}(0,\varphi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0,\varphi_2) \otimes (\vec{p}_g - \vec{x}_i) \qquad (1)$$

$$\vec{x}_i \leftarrow \vec{x}_i + \vec{v}_i$$

7: If a criterion is met (usually a sufficiently good fitness or a maximum number of iterations), exit loop.

8: end loop

Where:

– $\vec{U}$ (0,φ_i) represents a vector of random numbers uniformly distributed in [0,φ_i] which is randomly generated at each iteration and for each particle.

– ⊗ is component-wise multiplication.

– In the original version of PSO, each component of $\vec{v}_i$ is kept within the range [−Vmax, +Vmax]”

3.1. Parameters

There are a small number of parameters that need to be fixed in the PSO algorithm. The size of the population is one parameter that should be set. The size of the population is dependent on the basis of the dimensionality and perceived difficulty of a problem. The common values are in the range 20–50. There are other parameters including acceleration coefficients, inertia weight, and constriction coefficients which I will discuss below.

3.1.1. Acceleration coefficients

The other parameters φ_1 and φ_2 in equation (1) which are often called acceleration coefficients shows the magnitude of the random forces in the direction of personal best $\vec{p}_i$ and global best $\vec{p}_g$. The behavior of a PSO changes radically with the value of φ_1 and φ_2. Poli et. al. (2007) interpreted the components $\vec{U}$ (0,φ_1) ⊗ ($\vec{p}_i - \vec{x}_i$) and $\vec{U}$ (0,φ_2) ⊗ ($\vec{p}_g - \vec{x}_i$). In (1) as attractive forces produced by springs of random stiffness and they interpreted the motion of a particle as the integration of Newton’s second law. In this interpretation, $\varphi_1/2$ and $\varphi_2/2$ represent the mean stiffness of the springs pulling a particle. When φ_1 and φ_2 are modified, the PSO get more or less “responsive” and unstable if particle speeds are increased without control. The common value of φ_1 and φ_2 is 2.0. But it is better to control their values to protect search from harmful bias and to balance system between exploration and exploitation. The idea behind these parameters was to bound velocities and to keep $\vec{v}_i$ within the range [−Vmax, +Vmax]. If acceleration coefficients set the large-scale steps in the system, exploratory search is represented.

3.1.2. Inertia weight

Shi and Eberhart (1998b) presented inertia weight parameter to better control the scope of the search, reduce the importance of Vmax, and to eliminate it altogether. So updated equations were proposed:

$$\vec{v}_i \leftarrow w\vec{v}_i + \vec{U}(0,\varphi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0,\varphi_2) \otimes (\vec{p}_g - \vec{x}_i), \tag{2}$$

$$\vec{x}_i \leftarrow \vec{x}_i + \vec{v}_i$$

Where, ω is the inertia weight. Poli et al. (2007) mentioned if $\vec{U}(0,\varphi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0,\varphi_2) \otimes (\vec{p}_g - \vec{x}_i)$ is interpreted as the external force, $\vec{f}_i$, acting on a particle, then the change in a particle's velocity (i.e., the particle's acceleration) can be written as $\Delta\vec{v}_i = \vec{f}_i - (1 - \omega)\,\vec{v}_i$. The constant 1 − ω uses as a friction coefficient, and so ω might be considered as the fluidity of the medium in which a particle moves. Because of this effect, researchers set ω to some relatively high value (e.g., 0.9) which corresponds to a system where particles move in a low viscosity medium and perform extensive exploration, and gradually reducing ω to a much lower value (e.g., 0.4), where the system would be more dissipative and exploitative and would be better at homing into local optima. (Poli et al. 2007)

Eberhart and Shi (2000) used other methods to adjust the inertia weight. They applied a fuzzy system which improved significantly PSO performance. Moreover, Eberhart and Shi (2001) used an inertia weight with a random component, rather than time-decreasing.

Zheng et al. (2003) also reported that with increasing inertia weight, better results were obtained. Finally, appropriate choice of ω and of the acceleration coefficients, φ_1 and φ_2, make PSO more stable.

3.1.3. Constriction coefficients

It is realized that using some forms of damping is required (e.g., Vmax) to help algorithm stay stable within running. Clerc and Kennedy (2002) noted a strategy for the placement of "constriction coefficients" which controlled the convergence of the particle to prevent explosion, ensure convergence, and eliminate the arbitrary Vmax parameter. One of the simplest methods of incorporating of the constriction coefficient based on Clerc and Kennedy (2002) research is:

$$\vec{v}_i \leftarrow \chi(\vec{v}_i + \vec{U}(0,\varphi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0,\varphi_2) \otimes (\vec{p}_g - \vec{x}_i)), \tag{3}$$

$$\vec{x}_i \leftarrow \vec{x}_i + \vec{v}_i$$

Where $\phi_1 + \phi_2 = \Phi \geq 4$ and

$$\chi = \frac{2}{\Phi - 2 + \sqrt{\Phi^2 - 4\Phi}} \tag{4}$$

If Clerc's constriction method is applied, $\varphi_1 = \varphi_2 = 4.1$, and the constant multiplier χ is 0.7298. So the previous velocity is multiplied by 0.7298 and each of the two $(\vec{p} - \vec{x})$ terms being multiplied by a random number limited by $0.7298 \times 2.05 \approx 1.49618$.

In this method without using any V_{max}, the constricted particles will converge. Eberhart and Shi (2000) also noted that it is better to limit V_{max} to X_{max} , the dynamic range of each variable on each dimension, in conjunction with equations (3) and (4) resulting a particle swarm optimization algorithm with no problem-specific parameters. In comparison of equation 2 with 3, we can say they are equivalent to a PSO with inertia. They can be transformed into one another via the mapping ω ↔ χ and $\varphi_i \leftrightarrow \chi\varphi_i$. So, the optimal settings suggested by Clerc correspond to $\omega = 0.7298$ and $\varphi_1 = \varphi_2 = 1.49618$ for a PSO with inertia.

In a D-dimensional space, where D is the number of variables involved in the problem, the i^{th} particle is $Xi = (xi_1 \dots xi_D)$, and the velocity of that particle is $Vi = (vi_1 \dots vi_D)$. The best position of the i-th particle reached in a previous cycle is $Pi = (pi_1 \dots pi_D)$, and the best particle in the whole swarm is $Pg = (pg_1 \dots pg_D)$. The velocity and the position of the particle i in the iteration of $n+1^{th}$ are governed by

$$V_i^{n+1} = w.V_i^n + c_1 r_1^n (P_i^n - X_i^n) + c_2 r_2^n (P_g^n - X_i^n) \tag{5}$$

$$X_i^{n+1} = X_i^n + V_i^{n+1} \tag{6}$$

Here, c_1 and c_2 are learning factors (usually positive constant numbers); r represents a random number between 0 and 1; w is a factor of inertia that is a balance between velocity history and the new velocity. In this study, the optimal settings suggested by Clerc and Kennedy (2002) correspond to $w = 0.7298$ and $c_1 = c_2 = 1.496$. In the first generation PSO randomly creates particles, so v is zero in the initial loop.

Each particle has a position which includes D component which is 17 in this study and the velocity which is direction of that particle in search space. So, each particle defines 17 parameters of CE-QUAL-W2 and each particle includes velocity (direction) that helps to find next direction which is led next generation of particles.

4. The CE-QUAL-W2 Model

CE-QUAL-W2 (Cole and Wells, 2013) is a two-dimensional, longitudinal/vertical, hydrodynamic and water quality model for rivers, estuaries, lakes, reservoirs and river basin systems. Some of the model capabilities are hydrodynamic modeling, water quality, long term simulations, head boundary conditions, multiple branches, multiple water bodies, variable grid spacing, coupled water quality with hydrodynamics, auto stepping, restart provision, layer/segment addition and subtraction, multiple inflows and outflows, ice cover calculations, selective withdrawal calculations, and time-varying boundary conditions. The governing equations are laterally averaged which may be inappropriate just for large water bodies exhibiting significant lateral variations in water quality. The CE-QUAL-W2 model uses information such as geometric data, initial conditions, boundary conditions, hydraulic parameters, kinetic parameters, and calibration data and includes a graphical pre- and postprocessor for plotting/ visualization. The required data is hourly meteorological data such as air temperature, dew point temperature (or relative humidity), wind speed and direction, solar radiation and cloud cover, bathymetric x-y-z data of the reservoir, flow rates (Q) and temperatures (T), chlorophyll a, dissolved oxygen, and nutrients (such as NH_4, NO_3, and PO_4) for all inflows, flow rates and locations of outflows from the system, including the dam outlet, irrigation and other water withdrawals, outlet structure details for the power house and spillways, including rating curves for the spillways, and water surface elevation data.

4.1. Algae

Algae are a very diverse group of organisms categorized from diatoms to multicellular and can be broken down into greens, and cyanobacteria (blue-greens). CE-QUAL-W2 includes the capability to specify the kinetic rate parameters that define the characteristics of each algal group regarding given kinds of algal groups.

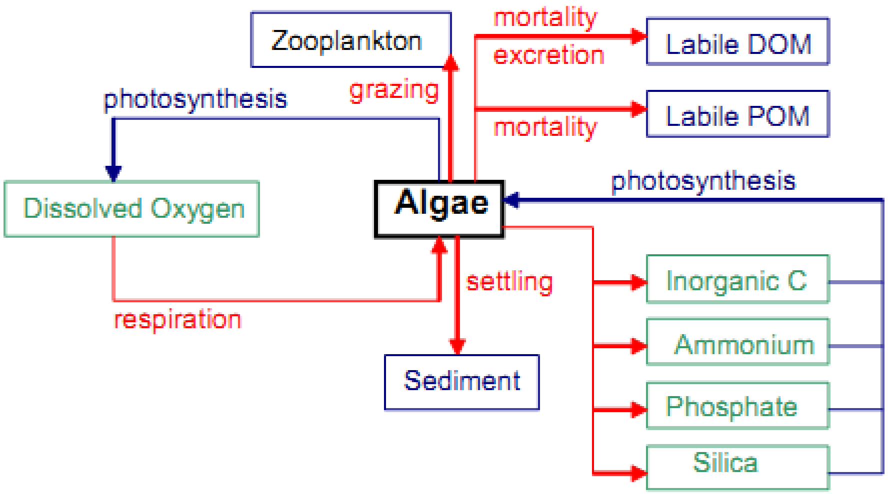


Figure 1. Internal flux between algae and other compartments, (Cole and Wells, 2013)

Algal biomass in the system is affected by Algal growth (AG), mortality (AM), and settling (AS), Algal half-saturation for phosphorus limited growth, (AHSP) g m^{-3}, Algal half-saturation for nitrogen limited growth, (AHSN) g m^{-3}, Light saturation intensity at maximum photosynthetic rate, (ASAT) W m^{-2} as fig 1 represented. Moreover maximum growth rate is strongly affected by temperature, light, and nutrient availability. [AG] in the CE-QUAL-W2 is not the net production rates. It is the maximum gross production rate that is not corrected for respiration, mortality, excretion, or sinking.

Chlorophyll a (chl a) is most commonly considered as an index for algal biomass. Multiplying chla by the given algae ratio (as g m-3 or mg/l dry weight OM)/chl a (as μg chlorophyll a/L) convert simply chl a to algal biomass. The ratio between algal biomass and chlorophyll a [ACHLA] is a function of the makeup of the algal population and algal species. [ACHLA] is also changed over time for a given algal species. This value is noted by regressing particulate organic matter with chl a in some previous studies. Based on EPA (1985) reports about percentages of chlorophyll a compared to dry weight algae biomass, it would be concluded that [ACHLA] is ranging from 0.01 to 0.40 for blue-green algae and total phytoplankton.

4.2. Ammonium

Ammonium is used by algae during photosynthesis to form proteins. Nitrogen is commonly the limiting nutrient for algal growth with high phosphorus loadings or in estuaries. Internal flux between ammonium and other compartments is presented in Fig 2. by Cole and Wells, 2013.

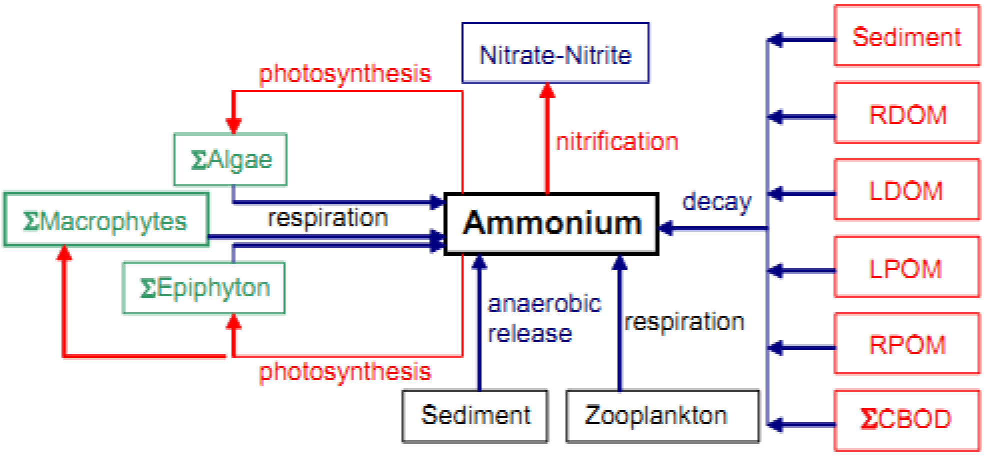


Figure 2. Internal flux between ammonium and other compartments, (Cole and Wells, 2013)

The rate that nitrification occurs in the system represented by NH4DK [day^{-1}] that is the rate which ammonium is oxidized to nitrate-nitrite. Cole and Wells, 2013 noted when there is anoxia, the rate of ammonia release is approximately the (SOD rate)*(NH4R) in units of g NH4-N/m^2/day or if divided by the layer height in m in units of g NH4-N/m^3/day. These rates are modified by the temperature multiplier for SOD. Beutel (2006) showed that release rates of ammonia-N ranging from less than 5 to more than 15 mg NH4-N/m^2/day between oligotrophic to hypereutrophic lakes, respectively.

4.3. Nitrate-Nitrite

Nitrate and nitrite were considered both together in CE-QUAL-W2. As Fig. 3 has presented, during nitrification, ammonium converts to nitrate and nitrite is an intermediate production of this process. Algae and epiphyton use nitrate as a source of nitrogen during photosynthesis. As mentioned previously, nitrogen may be the limiting nutrient for algae in systems with high phosphorus loadings or in estuaries.

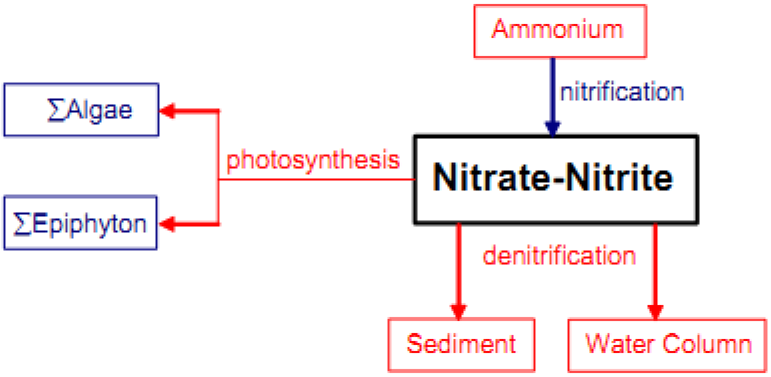


Figure 3. Internal flux between nitrate + nitrite and other compartments (Cole and Wells, 2013)

Denitrification rate in the water column and from the water column to the sediments (NO3S), m day^{-1} is analogous to a settling velocity and represents how fast nitrate is diffused into the sediments where it undergoes denitrification (Fig 3). Nitrate decay rate

(NO3DK), day^{-1} represents how fast ammonium decays to nitrite and nitrate and have ranged from 0.05-0.15 day^{-1}.

4.4. Phosphorus

Phosphorus is also an important nutrient for phytoplankton growth. In many fresh water system, phosphorus is the nutrient limiting the production of phytoplankton biomass is phosphorus (Schindler, 1971; Schindler et al., 1973; Vollenweider, 1968, 1976). Macrophytes are also taking P from the sediments or from the water column.

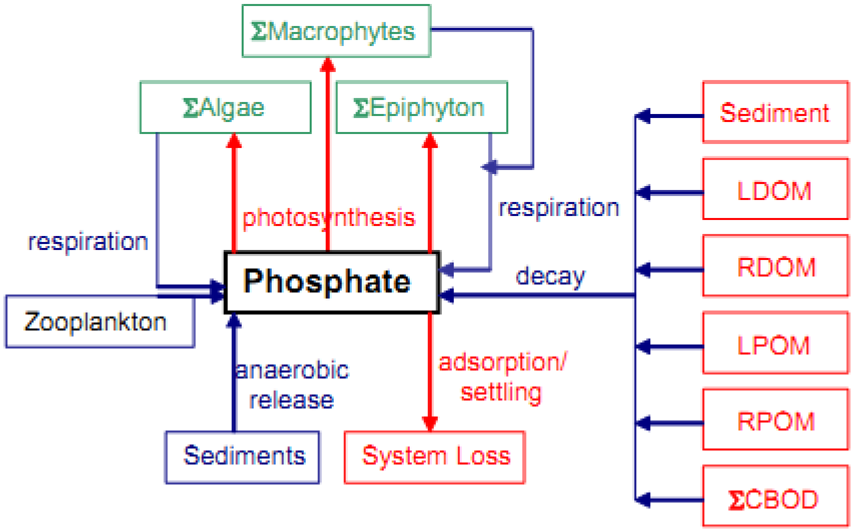


Figure 4. Internal flux between phosphorus and other compartments, (Cole and Wells, 2013)

In CE-QUAL-W2, the sediment release rate of phosphorous under anaerobic conditions (PO4R) is noted as a fraction of the sediment oxygen demand. So, the PO4 release rate under anaerobic conditions is [PO4R]×[SOD] in units of g/m^2/day modified by the temperature multiplier for SOD. So, PO4R is a function of the SOD rate and site-specific. Cole and Wells, 2013 compared PO4R reported by different researchers. Based on that comparison, Sen et al. (2004) determined an average anaerobic P release rate of 0.57 mg/m^2/day for Beaver Lake, Arkansas. Auer et al. (1993) found rates in a hypereutrophic lake from 9-21 mg/m^2/day (mean 13 mg/m^2/day). Kim et al. (2004) found rates in the summer between 20-24 ^{o}C up to 16 mg/m^2/day.

Spears et al. (2007) showed that for a large shallow lake recovering from high nutrient that the maximum P release was 12 mg/m^2 /day. James et al. (1995) found that P release rates for Lake Pepin, an impoundment on the upper Mississippi River, were between 3.8 and 15 mg/m^2/day.

4.5. Dissolved Oxygen

Oxygen is one of the most important limiting factor in aquatic ecosystems. Dissolved oxygen can provide broad information about the system state. It is essential for aquatic life, controls many chemical reactions through oxidation, and is a surrogate variable indicating the general health of aquatic systems.

CE-QUAL-W2 is capable to model both aerobic and anaerobic processes. The modeling of anaerobic processes is an important step in the water quality modeling of reservoir because simulations of that can be used to identify possibilities for both metalimnetic and hypolimnetic oxygen depletion and its impact on various water control management alternatives.

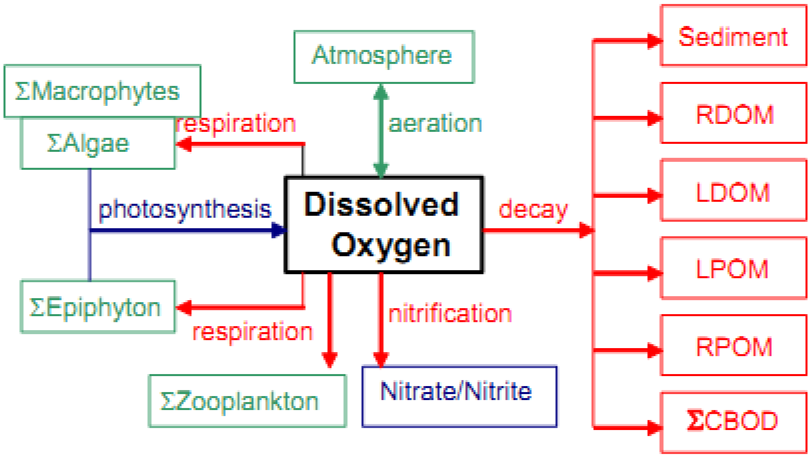


Figure 5. Internal flux between dissolved oxygen and other compartments, (Cole and Wells, 2013)

4.6. Sediments

In CE-QUAL-W2 contribution of organic sediment to nutrients and dissolved oxygen demand are simulated using two methods. The first method uses zero-order and constant sediment oxygen demand and anoxic release rates for phosphorus, ammonium, inorganic carbon, and iron (Fig 6). This method is commonly used to model sediment demands and nutrient release rates. This model requires a separate sediment compartment rather than sediment concentrations. The overall formulation is not variable over time but the decay rate is a function of temperature. So, when effects of different nutrient loadings on dissolved oxygen is evaluating in a waterbody, results should be interpreted cautiously. Sediment oxygen demand value is commonly between 0.1 to 1.0 gO2 m^{-2} day^{-1}.

According to Cole and Wells (2013), the second method uses a sediment compartment to accumulate organic sediments and allow their decay. So, 1st-order decay affects nutrient releases and oxygen demand (Fig 7). Effects of organic sediments upon water quality can be simulated by either of these methods, or a combination. SEDK is a parameter that specifies the 1^{st} order sediment decay rate value.

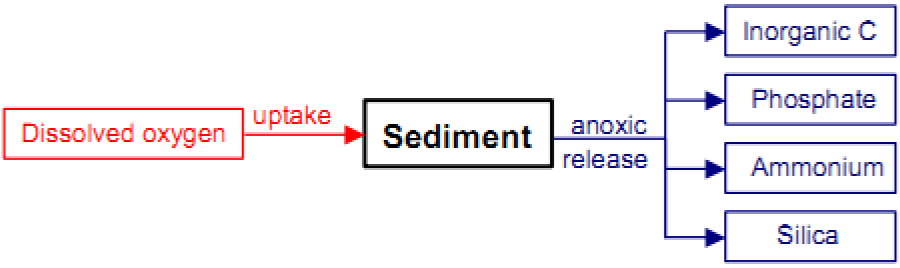


Figure 6. Internal flux between 0-order sediment compartment and other compartments (Cole and Wells, 2013)

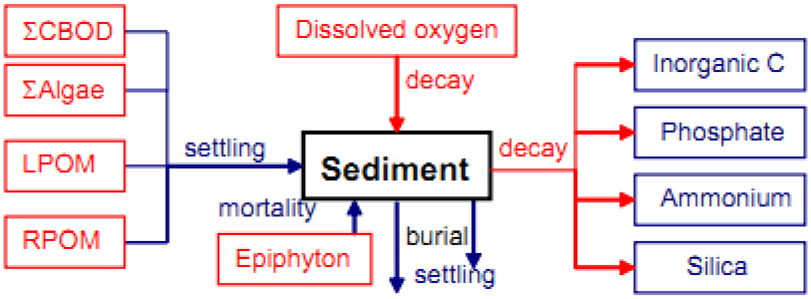


Figure 7. Internal flux between 1st-order sediment compartment and other compartments (Cole and Wells, 2013)

Based on a literature survey and screening process, the most important parameters which significantly affect reservoir's temperature profile were identified and selected as decision variables in the optimization routine. The extinction coefficient for pure water (EXH2O) that is attenuation rate due to water, and the fraction of solar radiation absorbed in the surface layer (BETA) which both control distribution of solar radiation in the water column and also wind sheltering coefficients (WSC) affect thermal stratification on reservoirs. Gas exchange is also affected by the wind sheltering coefficient [WSC]. EXH2O and BETA affect directly temperature that affects hydrodynamics but WSC directly affects hydrodynamics that affect heat and constituent transport. Cole and Wells, (2013) mentioned that the wind sheltering coefficient is approximately from 0.5-0.9 for mountainous and/or dense vegetative canopy and 1.0 for open terrain. In a very few cases, the wind-sheltering coefficient (WSC) has been increased above 1.0 to account for funneling effects on systems with steep banks.

Realizing the complex relationships between model parameters (BETA and EXH2O), it is assumed that the model parameters are independent of each others. For implicit and partial consideration of this dependency, the bounds on the model parameters are defined based on measured Secchi Disk Depth in IWPC (Iran Water and Power Company 2006) Karkheh reservoir Monitoring Program and reference values considering water turbidity. There are some other variables that also affect evaporation process (one of the phrases of surface heat exchange). These parameters are AFW, BFW, and CFW. These last parameters affect water surface elevation (water budget), too. The evaporation formulation via a user defined evaporation wind speed formula is shown in Eq. 7, (Cole TM, Wells SA 2013).

$$F(w_z) = afw + bfw \times W_z^{cfw} \tag{7}$$

$F(w_z)$; wind speed function, afw, bfw, cfw are the empirical coefficients, and W_z is the wind speed measure at 2 m above the ground.

5. The Karkheh Reservoir

The Karkheh Reservoir (Fig. 8) is located on the Karkheh River in the southeast region of Iran and has the following characteristics: a maximum of depth of 117 m, 162 km^2 surface area, 5×10^9 m^3 capacity, and 64 km length.

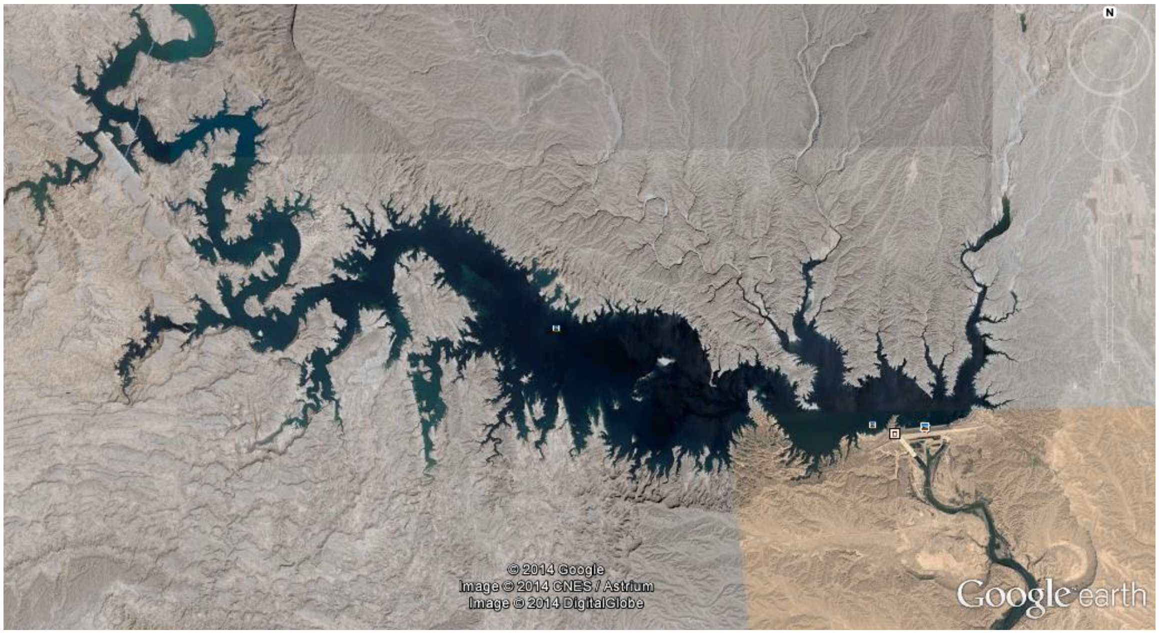


Figure 8. Karkheh Reservoir map from Google Earth

This reservoir supplies municipal drinking water and irrigation water for 350,000 ha of irrigable agriculture. Water in the Karkheh Basin is used for domestic purposes, agricultural production and limited industrial activity. The basin is third basin in surface water use and fourth basin in groundwater use in Iran (Ahmad and Giordano 2010). The Karkheh Basin is noted as the most productive basin in Iran that includes 9% of Iran’s total irrigated area and produce around 11% of country’s total wheat supply.

The Karkheh Dam on the Karkhe River is a multi-purpose dam in the northwestern Province of Khuzestan in Iran, close to the city of Andimeshk. It is designed to produce 520 MW of hydroelectric power, prevent downstream floods and provide irrigation water to 350,000 ha in the Khuzestan Plains in the lower Karkheh region. The dam has been operated since 2002 and accumulated dam outflow was measured at 2.8 Billion cubic meters in November 2002 and October 2003. The maximum storage capacity of dam is about 4.7 BCM.

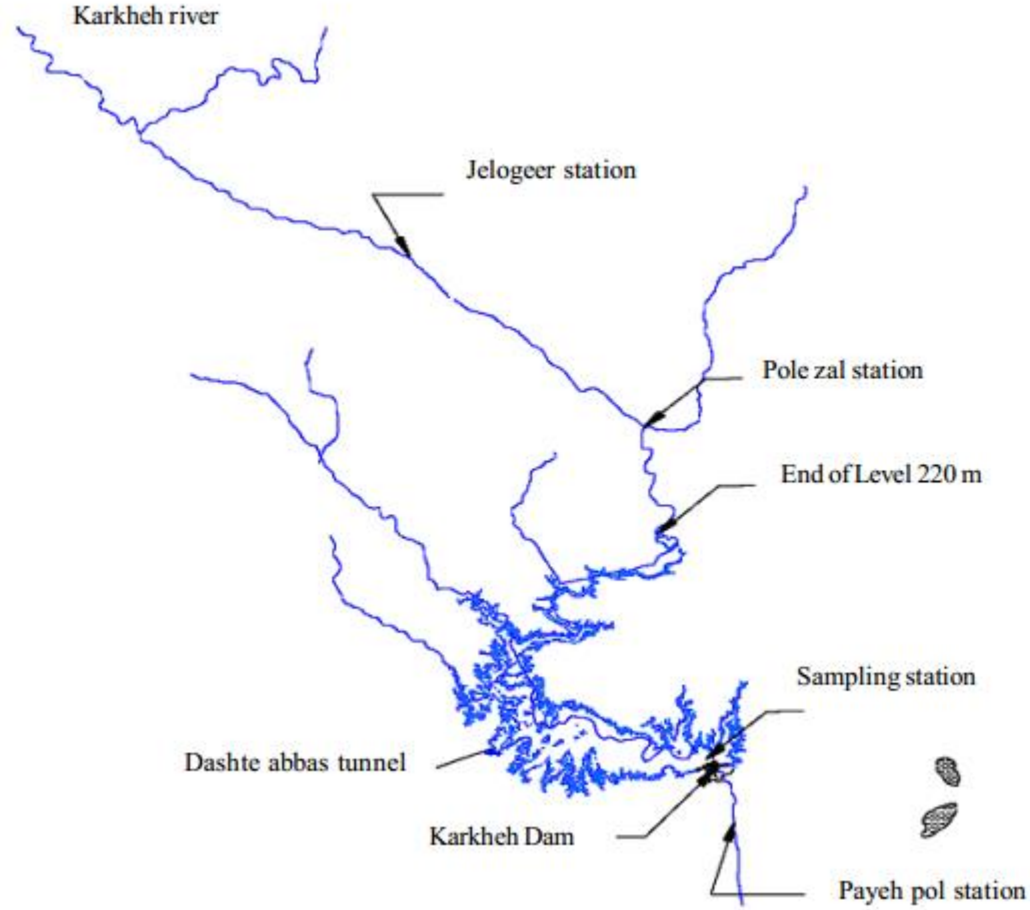


Figure 9.Karkheh River watershed, dam and sampling station

Figure 10. Photo of outlets (http://www.geosig.com)

Table 1.The Karkheh reservoir CE-QUAL-W2 model characteristics

Number of waterbodies	Number of branches	Number of segments	Segment length	Width of segments	Number of layers	Layer thickness
1	1	64	1000 m	26-2673 m	55	2 m

6. The Karkheh CE-QUAL-W2 Model

The Karkheh reservoir CE-QUAL-W2 model has 64 longitudinal segments and 55 vertical layers as shown in Figure 11, 12, and 13 and table 1. The Karkheh model includes inflows and outflows such as Karkheh River, the spillway, water supply withdrawals (Dashtabbas tunnel), and the dam outlet (hydropower and agricultural outlet) (Fig. 9 and 10). Hourly meteorological data and hydrological data were obtained from the Karkheh Meteorology Station included air temperature, dew point temperature, wind speed and direction and cloud cover. The residence time during the simulation period is 117 days which shows the simulation is highly dependent on initial condition. Therefore, accurate inflow temperatures and constituent concentrations were crucial for accurate simulations of temperature and water quality in Karkheh Reservoir.

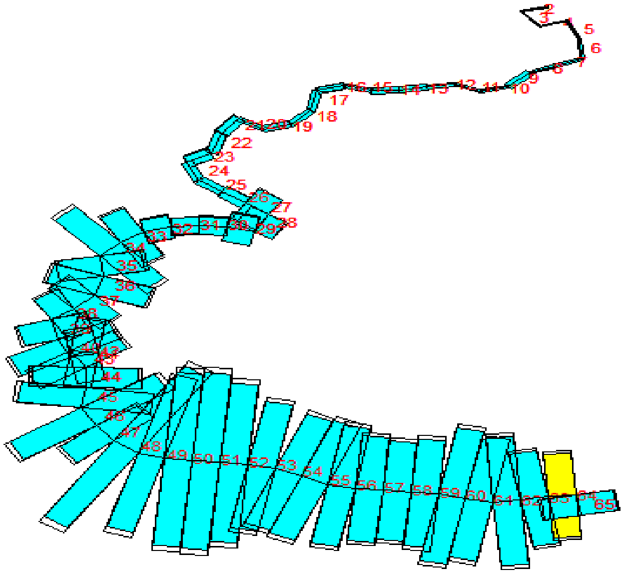


Figure 11. Model configuration plan-view

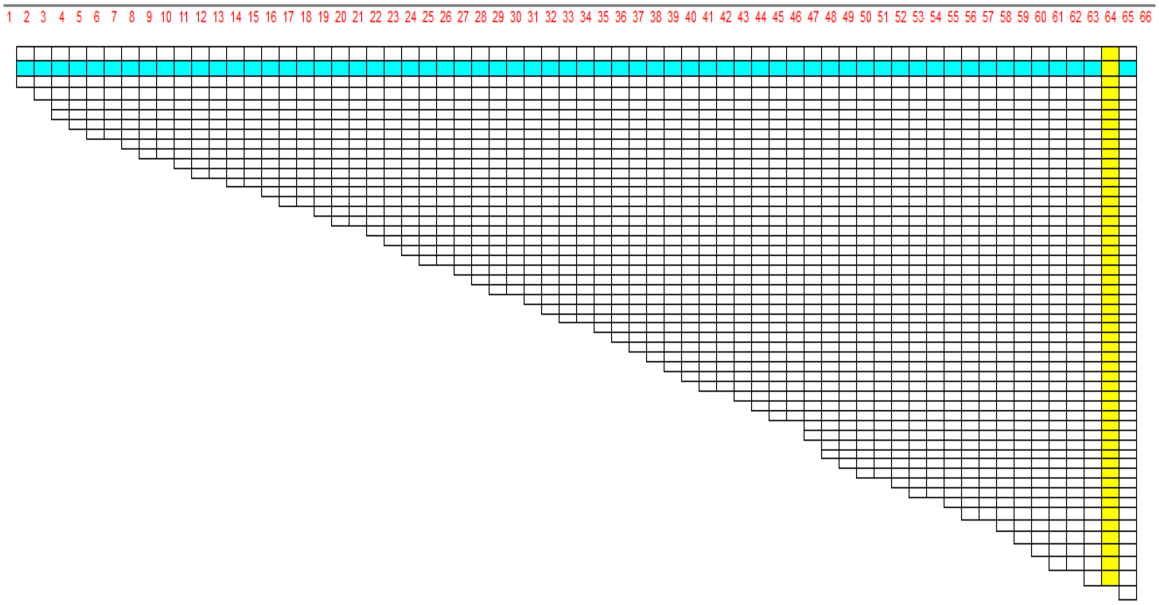


Figure 12. Model configuration side-view

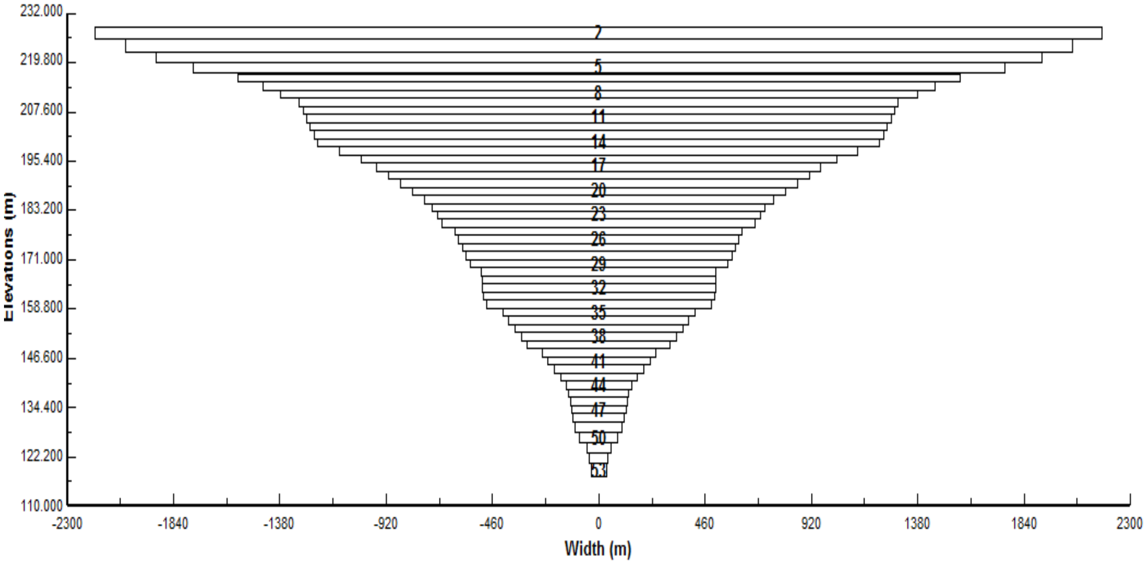


Figure 13.Vertical model segment

6.1. Outlet Structures

Spillway is located in segment 65 and elevation of weir crest is 220 m. The general equation for calculating flow over a weir takes the following form:

$$Q = \alpha_1 \Delta H^{\beta_1} \tag{8}$$

Where:

α_1 = empirical parameter = 10

β_1 = empirical parameter = 1.5

Δh = Zu-Zsp, m

Z_u = upstream head, m

Z_{sp} = the spillway crest elevation, m

And for submerged conditions:

$$Q = \alpha_2 \Delta H^{\beta_2} \tag{9}$$

Where

α_2 = empirical parameter = 20

β_2 = empirical parameter = 1

the spillway is at the down-stream end of the segment 65 (Fig. 14). In this case the water surface elevations are computed based on the right hand side of segment 65. This water surface elevation is estimated based on the slope of the water surface at 65 and 64. Also, momentum from the outflow is preserved as in a downstream structure withdrawal and inflows/outflows for the downstream spillway is set to place the inflows into a layer with similar density.

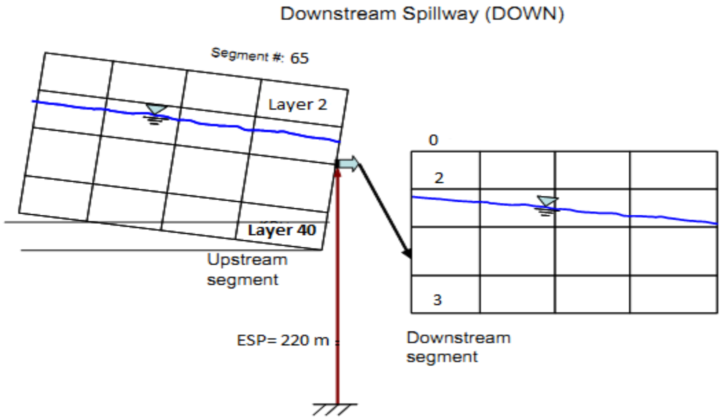
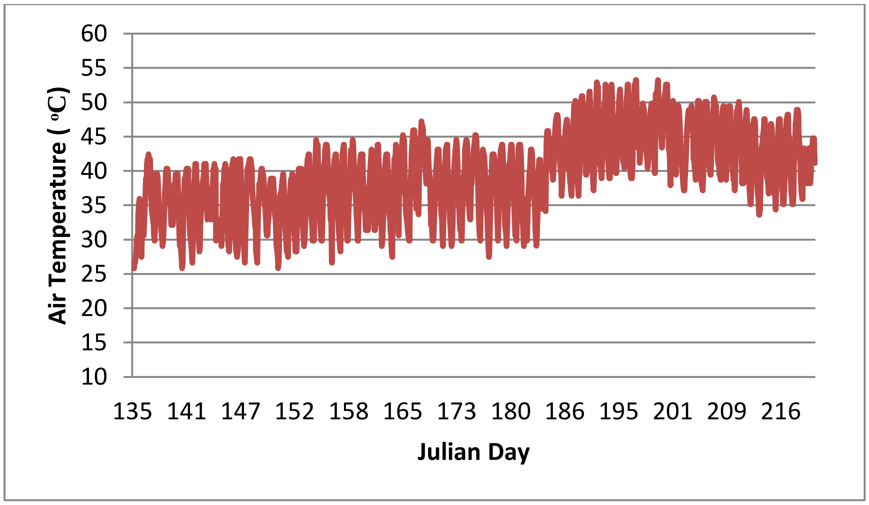


Figure 14.The layout of spillways set as a downstream (Cole and Wells, 2013)

Moreover, withdrawal will occur between layer 24 and 26 at the segment 45 in elevation of 177.5 m. Two structures have been located in to handle selective withdrawal between layer 30 and 35 through first one and between layer 18 and 27 through the second structure.

6.2. Air Temperature

Air temperature data collected at Karkheh Reservoir over the full model period is shown in Figure 15.



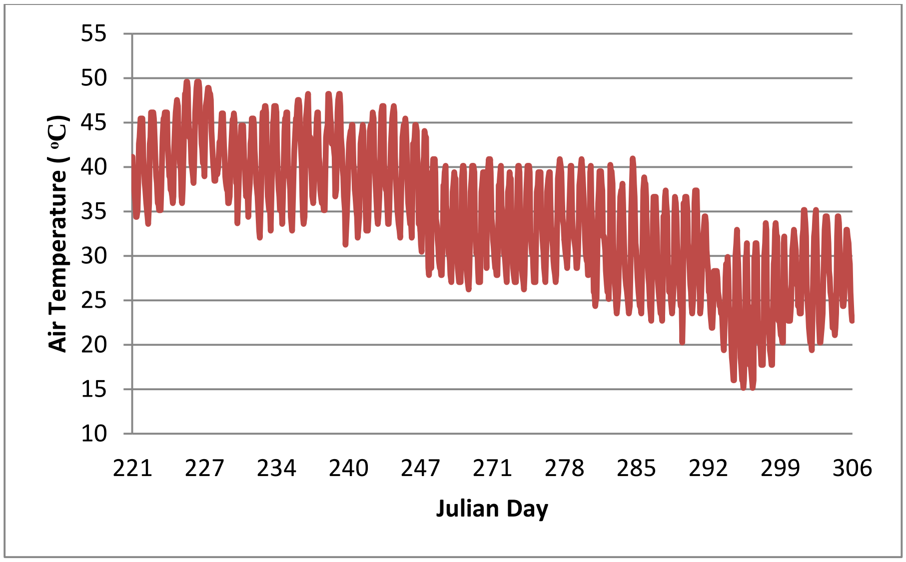
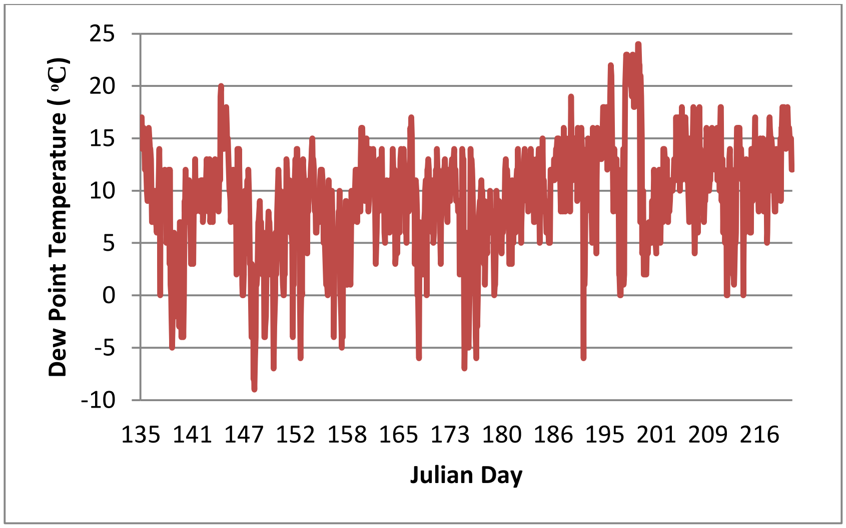


Figure 15. Karkheh Reservoir air temperature (Iran Water and Power Company)

Figure 16 shows the dew-point temperature at Karkheh Reservoir calculated using relative humidity data from Karkheh Meteorology Station. Dew-point temperature is calculated using the relationship between temperature and RH as shown in Equation 10 (Singh (1992) Elementary Hydrology):

$$RH = \left[\frac{112-0.1T+T_d}{112+0.9T}\right]^8 \tag{10}$$



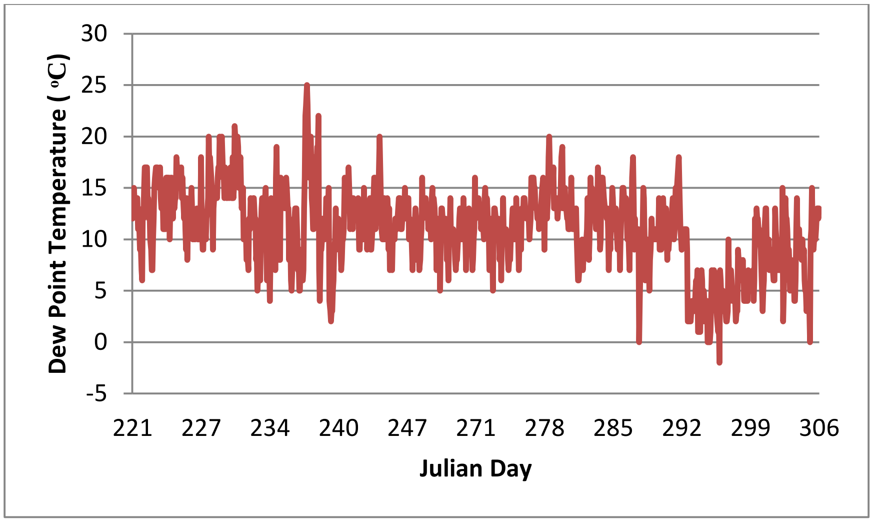
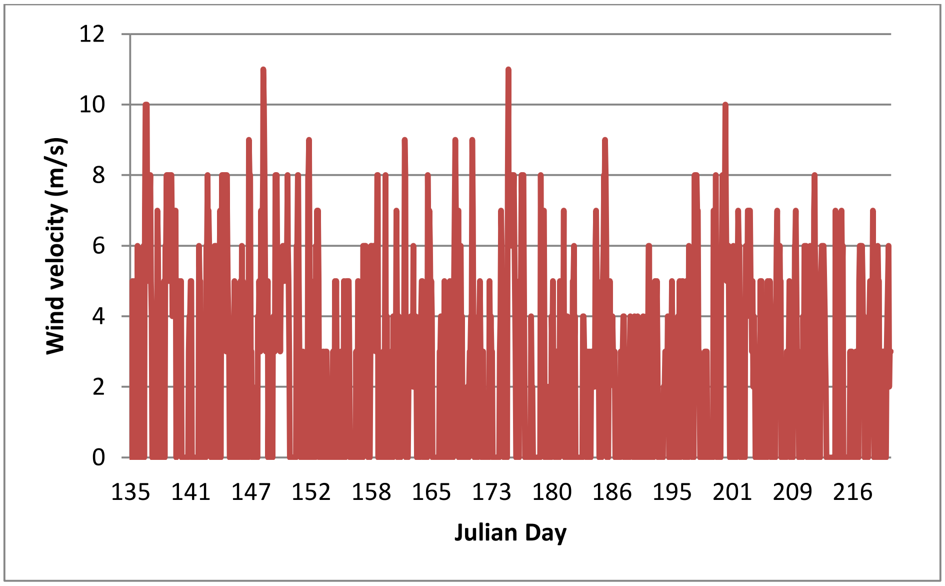


Figure 16. Karkheh Reservoir Dew Point Temperature (Iran Water and Power Company)

6.3. Wind

Figure 17 shows the wind velocity measured at Karkheh Reservoir sampling station over the full model period.



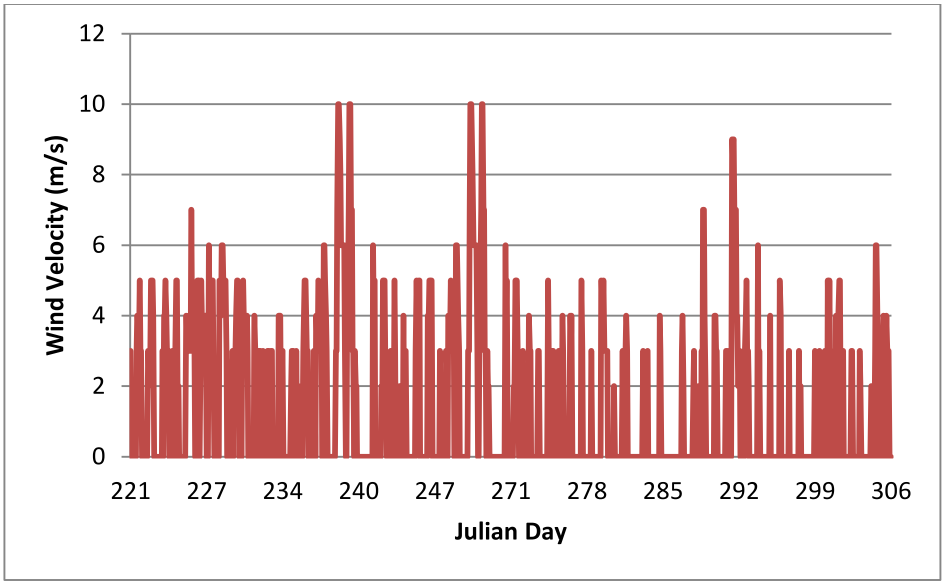


Figure 17.Karkheh Reservoir Wind Velocity (Iran Water and Power Company)

6.4. Initial Condition Data

The initial condition includes the initial temperature and concentration of chlorophyll a, dissolved oxygen, and nutrients (such as NH_4, NO_3, and PO_4). A grid-wide vertical profile was specified in the vertical profile input file.

6.5. Boundary Condition Data

Model Inflow

The Karkheh River is the third largest river in Iran (in terms of water yield), after the Karun and Dez Rivers which reaches to The Karkheh Reservoir. Fig. 18 presents the inflow rate of Karkheh River to Karkheh Reservoir.

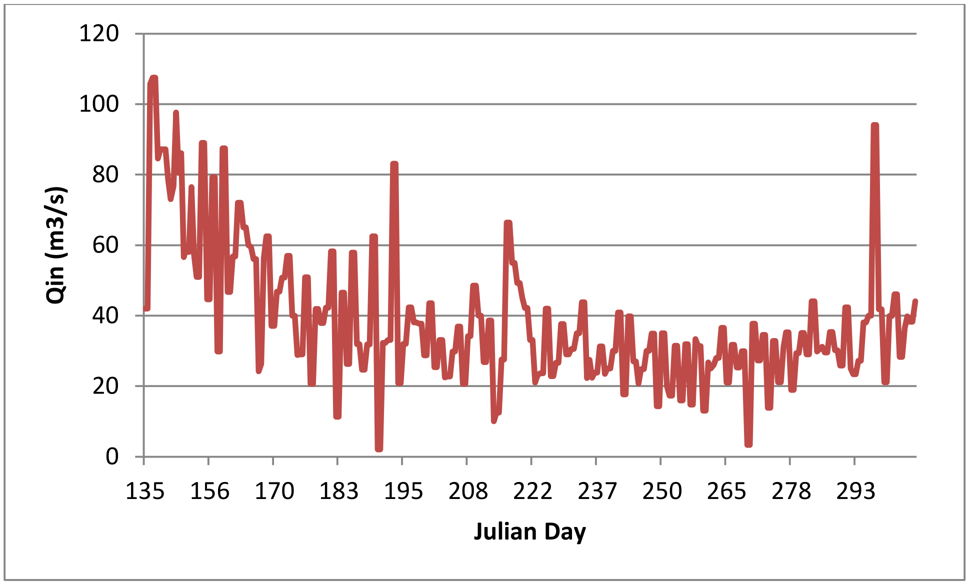
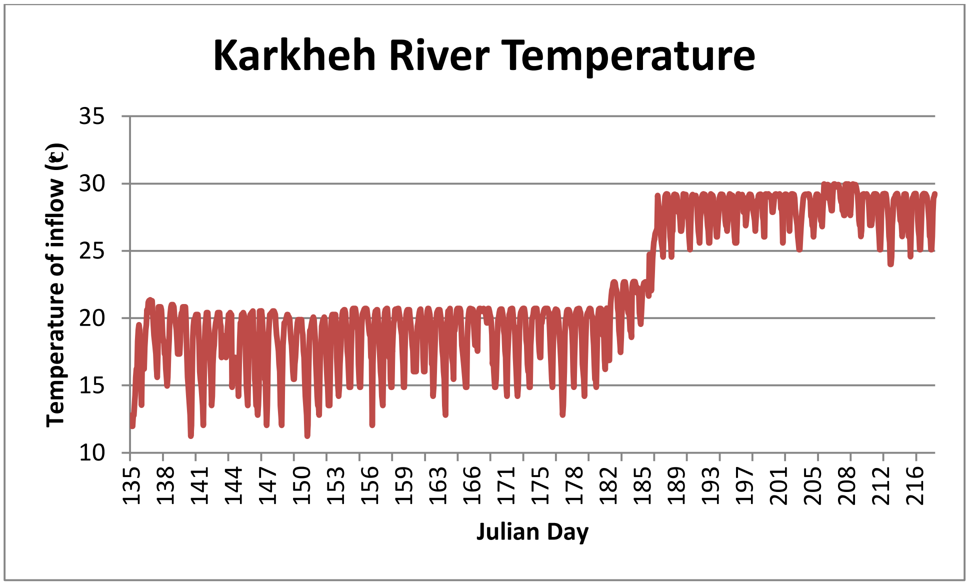


Figure 18.Karkheh River inflow to Karkheh Reservoir (Iran Water and Power Company)

Inflow Temperature

Water temperature data was available for the complete model period The Karkheh River.

Figure 19 shows a plot of recorded water temperatures on The Karkheh River.



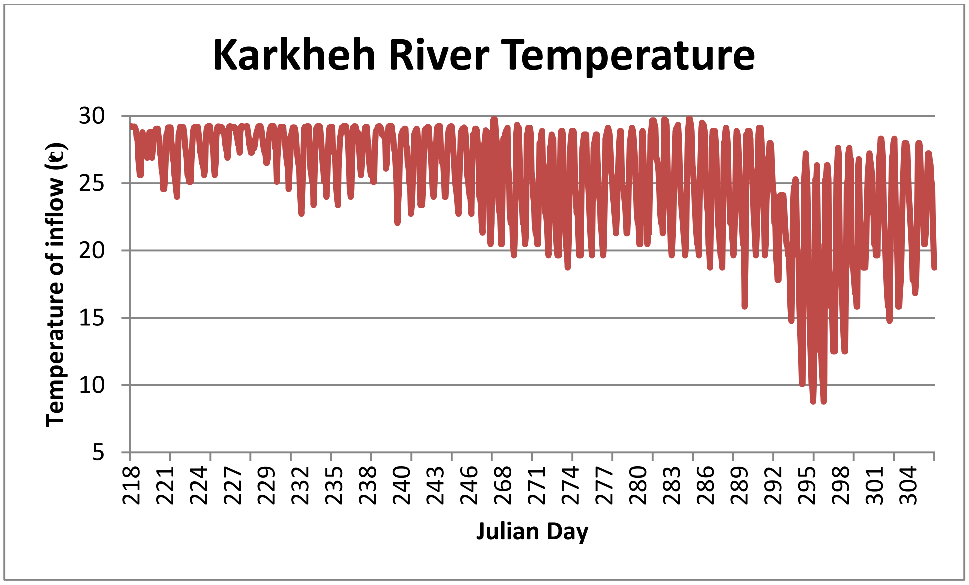


Figure 19.Karkheh River flow temperature (Iran Water and Power Company)

Model Outflow

The main outflow from The Karkheh Reservoir is released through the Dam into the Karkheh River. Figure 20 plots the stream discharge downstream from The Karkheh reservoir over the model period.

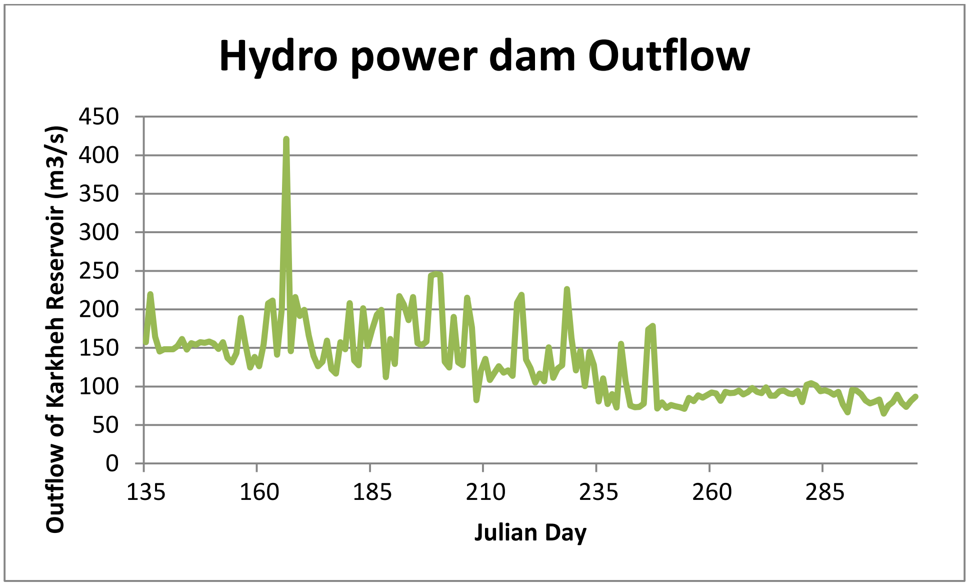


Figure 20. Karkheh Reservoir outflow (Iran Water and Power Company)

Fig. 21 shows a close match between the simulated and measured water surface elevations in Karkheh reservoirs. So model performs quite satisfactory in predicting the actual variation both in wet and dry seasons. The water surface elevation decreases gradually and reaches the lowest in the fall. The Root Mean Square Error for given period of water surface elevation is 14 cm.

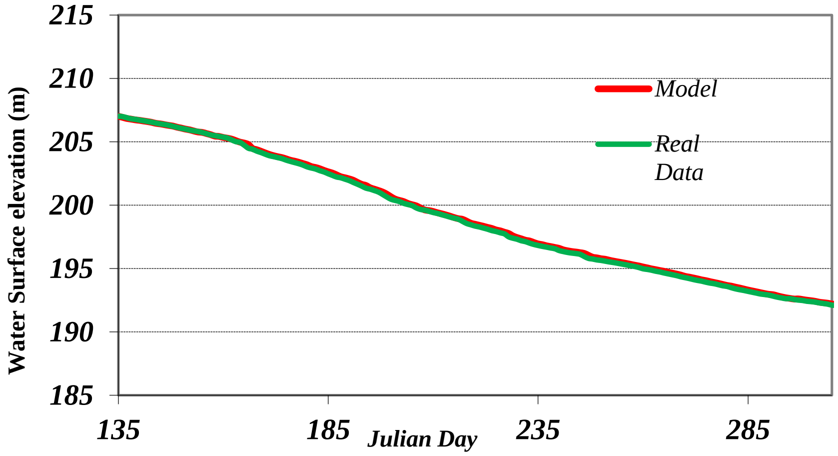


Figure 21.Water surface elevation predictions compared to observed data.

7. Automatic Calibration and Objective Function

In the proposed study, model parameters are adjusted in order to achieve satisfactory agreement between the measured field data and the model predictions for temperature (T), chlorophyll a (chl a), dissolved oxygen (DO), NH_4-N, NO_3-N, and PO_4-P concentrations in the Karkheh reservoir simultaneously. This satisfactory agreement can be expressed mathematically as:

$$\text{Minimize } F(\mathbf{X}) = f_T{}' \times w_T + f_{DO}{}' \times w_{DO} + f_{Chlr\ a}{}' \times w_{Chlr\ a} + f_{PO4}{}' \times w_{PO4} + f_{NH4}{}' \times w_{NH4} + f_{NO3}{}' \times w_{NO3} \tag{11}$$

$$w_T + w_{DO} + w_{Chlr\ a} + w_{PO4} + w_{NH4} + w_{NO3} = 1 \tag{12}$$

$$\text{Subject to} \quad \mathrm{x}_{low} < \mathrm{x} < \mathrm{x}_{up} \tag{13}$$

Where, $F(\mathrm{X})$ is an objective function for all six normalized model state variables or decision variables; w is the weight (between 0 to 1) of all decision variables profile; $\mathbf{x} = (x_1, x_2, \dots, x_D)$ is the vector of decision variables or calibration parameters, and D is the number of parameters to be calibrated which is 17 in this research; $\mathbf{x}_{low}$ and $\mathbf{x}_{UP}$ are the lower bounds and upper bounds of the parameter sets.

The main objective of the proposed modeling is to select the most appropriate calibration parameters that is a unique vector, X, which could minimize satisfactorily all objective functions simultaneously. In this study, the root mean square error (RMSE) represents the magnitude of prediction errors. In order to appropriately aggregate different errors from various variables in the formulation of an overall error function, these errors are normalized respectively to have same orders of magnitude and dimension. A general RMSE equation and normalization expression is given below applied in this research (Yongtai 2010):

$$RMSE \ = f_k(\mathrm{X}) = \sqrt[2]{\frac{\sum_{i=1}^{M} \ (c_{ik}-c^*{}_{ik})^2}{M}} \tag{14}$$

$$f_k(x)' = f_k(x)/\overline{c_k} \tag{15}$$

Where, $\mathrm{f_k}(\mathbf{x})$ represents the fitness function for each alternative combination of calibration parameters of vector X for variable k; $c^*{}_{ik}$ is the i^{th} field measurement of variable k (i = 1,…, M); c_{ik} is the simulated value corresponding to $c^*{}_{ik}$; $f_k(x)'$is the normalized dimensionless error functions; $\overline{c_k}$ is the average measurement for K$^{\mathrm{th}}$ variable; and M is the total number of measurements for variable k.

8. Model Evaluation

CE-QUAL-W2 is employed as a water quality and hydrodynamic simulation model. PSO is also run to produce a random generation of initial calibration parameters – particles and velocities in first swarm. In each iteration, model predictions of the state variables at different depths and segments are compared to field data on the monitoring day.

The overall objective function is evaluated by the summation of RMSE for each state variable. Whenever the number of iterations or a fitness criteria is satisfied, the simulation–optimization process is terminated. Otherwise, the PSO reproduces a new particle or a collection of new parameters for the CE-QUAL-W2 model based on PSO regulations and acceptable range of each parameters.

Then CE-QUAL-W2 is run with the new parameters to predict key water quality constituents and temperature. So in this approach, the simulation model (CE-QUAL-W2) is linked by the powerful optimization model (PSO) to overcome the high computational efforts in traditional calibration search techniques, while retaining the quality of the final calibration results. The flowchart in fig. 22 shows the steps in an automatic optimization-simulation process.

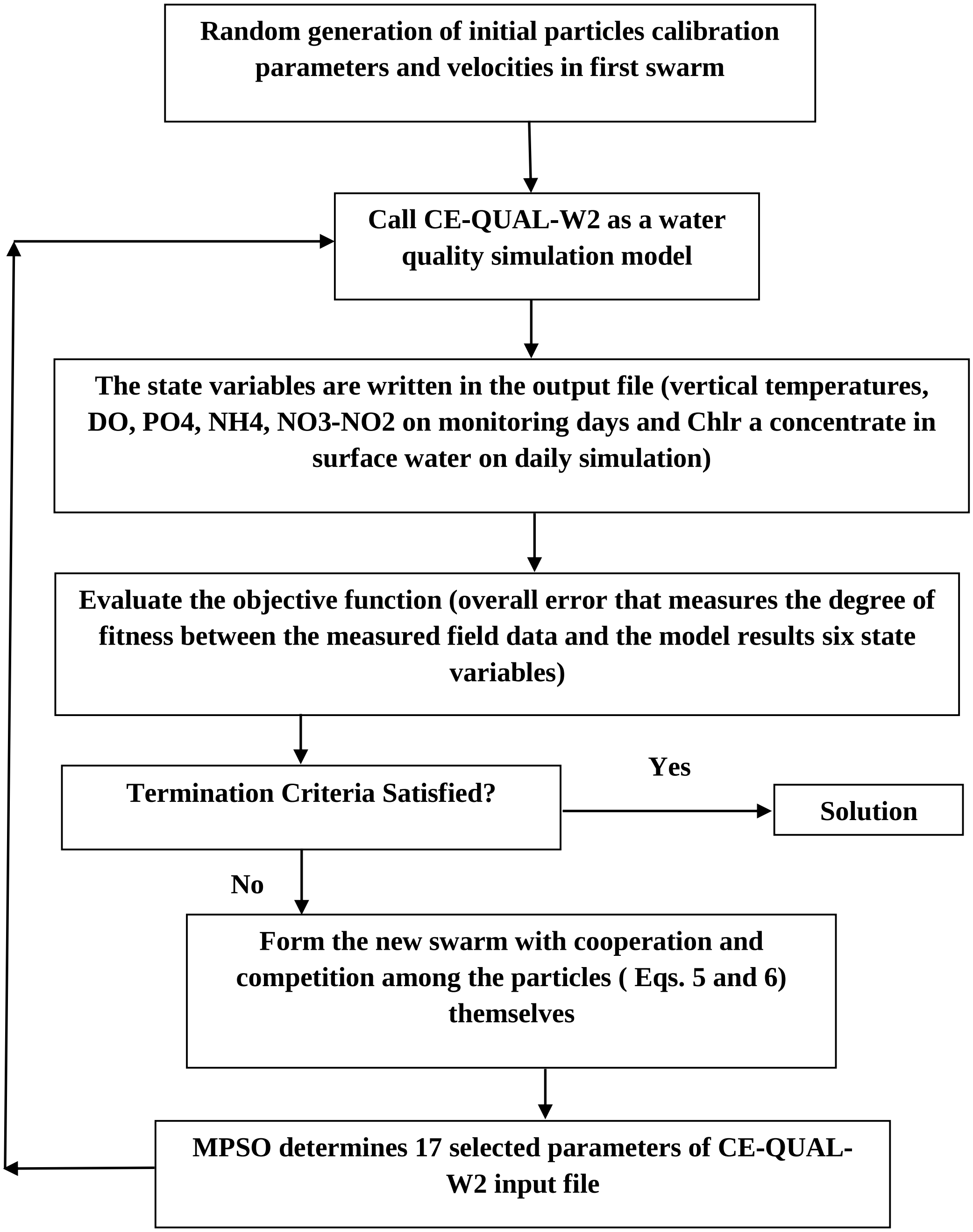


Figure 22. Flowchart of automatic calibration

The applied measured field data were compared to model predictions between May and November 2005. In the proposed study, simulator model of Karkheh reservoir with 55 layers and 64 segments runs for 114 seconds on a CORE 7 duo CPU, 8 GB RAM, 3.7 GHz computer to simulate this six month period. In this study, the 50 iterations with 30 particles is considered as a stopping criteria based on the running results of simulation-optimization procedure with different iteration values. Improvement of optimization results through different values of iteration is presented in fig. 23. The proposed simulation- optimization scheme achieves the best solution with 30 particles and 50 iterations after approximately 47 hours. The criterion for stopping would be also considered as a converging to the acceptable error. In this study, this criterion did not applied because the optimum value of objective function is not known.

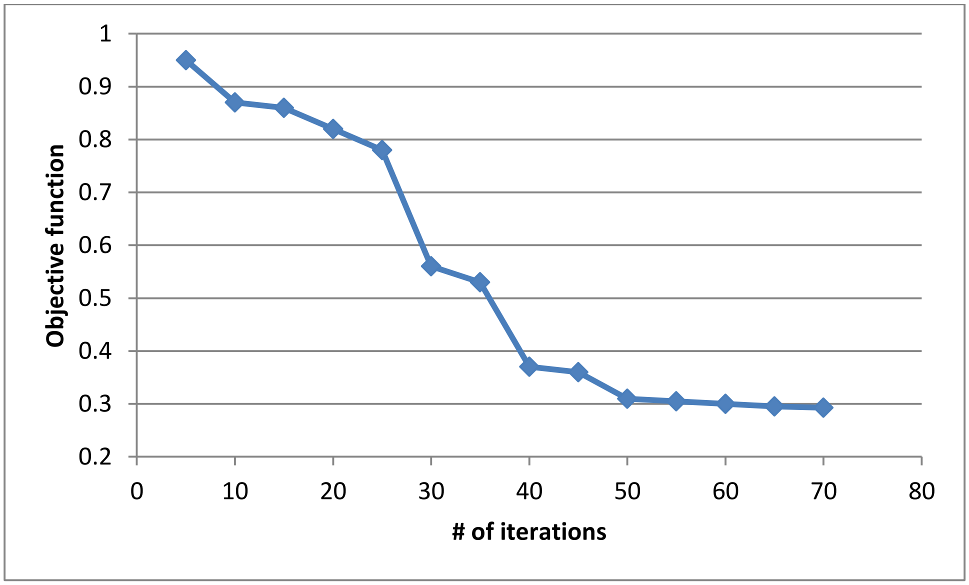


Figure 23. Improvement trend of objective function vs. increasing of calibration iteration values

9. Results and Discussion

After calibration, water surface elevation is modified by changing the value of parameters related to temperature. The objective function (RMSE) of water surface elevation simulation of model after calibration is 9 cm which shows more agreement between model simulation and measured data after calibration (fig. 24).

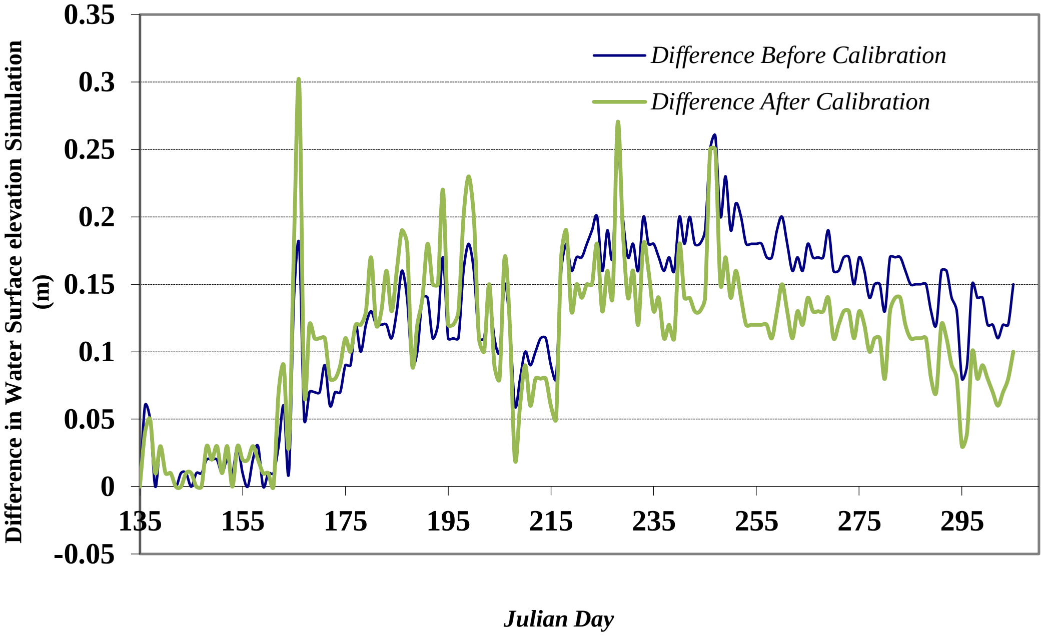


Figure 24. Difference of water surface elevation predictions after calibration compared to before calibration

Table 2 shows the resulted objective function for each month of six state variables after calibration. Final objective functions present automatic calibration lead to satisfying results for the calibration. Table 3 presents the calibrated value of parameters and their defined range in PSO.

Table 2.Resulted objective functions of five state variables

RMSE	**TEMP ©**	**PO4 (mg/l)**	**NO3(mg/l)**	**NH4(mg/l)**	**DO(mg/l)**
May15, 2005	0.37902	0.00056	0.049772	0.088183	0.163033
July 2, 2005	0.598002	0.0763	0.1533	0.15992	0.52211
July25, 2005	0.722531	0.06016	0.47508	0.117226	0.4201
Aug15, 2005	0.6069	0.01038	0.1575	0.05191	0.5354
Sep. 4, 2005	0.52078	0.02235	0.2508	0.1444	0.4992
Oct. 2, 2005	0.41308	0.1406	0.2923	0.2796	0.8244
Nov. 1, 2005	0.8267	0.037	0.1735	0.0582	0.6816
Average	**0.581002**	**0.049479**	**0.220636**	**0.128491**	**0.520835**

Samples of the observed and predicted thermal profiles at segment number 64 (near the dam) from May to November 2005 before and after calibration are presented in Fig. 25a and b. The calibrated model simulates vertical temperature profiles and the seasonal variation of temperature in the water column. It can be observed that the measured results and the simulated values after calibration match well. The difference of water temperature between the upper layers and lower layers was about 15°C.

Table 3. Calibrated value of parameters and their range

Name in CE-QUAL-W2	Description	Range	Calibrated value
EXH2O	Solar radiation extinction coefficient for pure water, m^{-1}	0.2-0.4	0.22
WSC	Wind sheltering coefficient for each segments of first and last day of calibration	0.7-1	0.8, 0.85
BFW	B coefficient in the wind speed formulation	0.45-0.7	0.53
AG	Maximum algal growth rate day^{-1}	0.1-4	1.15
AM	Maximum algal mortality rate day^{-1}	0.01-0.95	0.035
AS	Algal settling rate m. day^{-1}	0-7	0.045
AHSN	Algal half-saturation for nitrogen limited growth, g m^3	0.001-0.05	0.026
AHSP	Algal half-saturation for phosphorus limited growth, g m^{-3}	0.001-1	0.01
ASAT	Light saturation intensity at maximum photosynthetic rate $w.m^{-2}$	10-100	85
ACHL	Ratio between algal biomass and chlorophyll a	0-1	0.122
SED	Sediment decay rate	0.1-1	0.43
FSOD	Fraction of the zero-order SOD (sediment oxygen demand) rate used;	0.01-2	0.655
PO4R	Sediment release rate of phosphorus under anaerobic conditions;	0.001-0.03	0.02
NH4R	The sediment release rate of ammonium under anaerobic conditions, specified as a fraction of SOD;	0.001-0.4	0.01
NH4DK	Ammonium decay rate, day^{-1};	0.001-0.8	0.265
NO3DK	Nitrate decay rate, day^{-1};	0.05-0.15	0.078
NO3S	Denitrification rate from sediments, $mday^{-1}$;	0.01-2	0.015

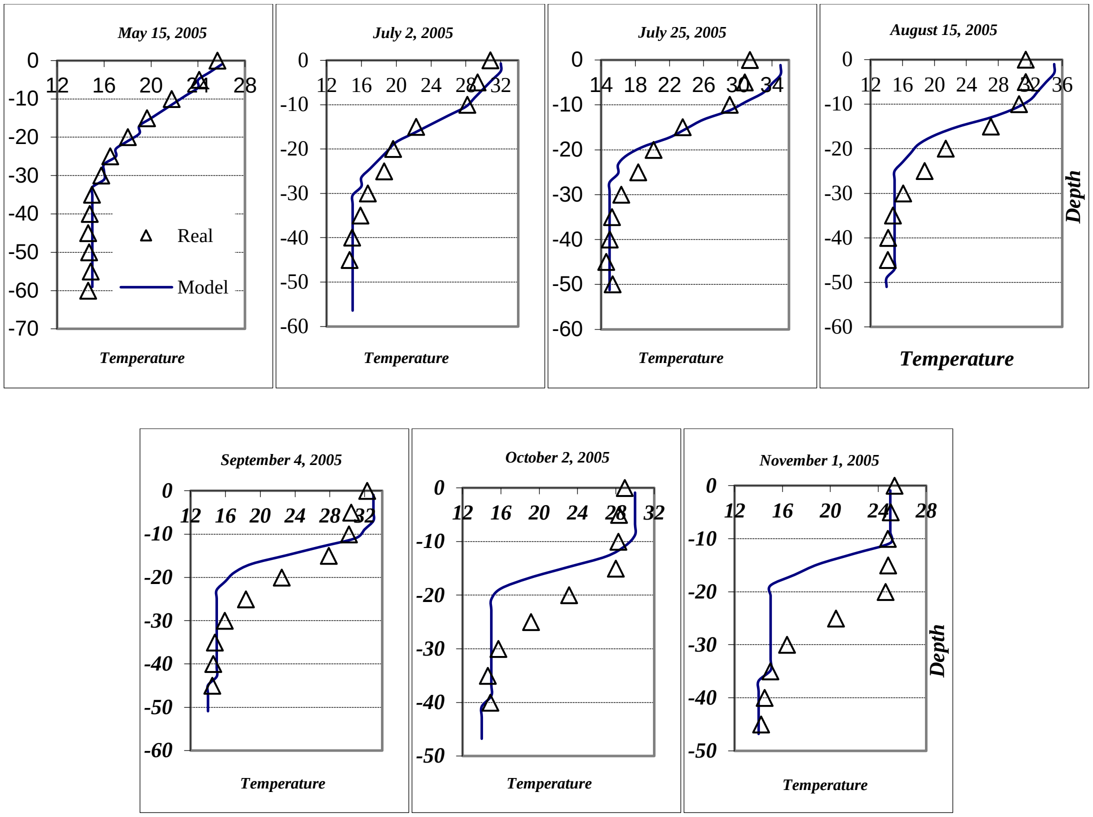
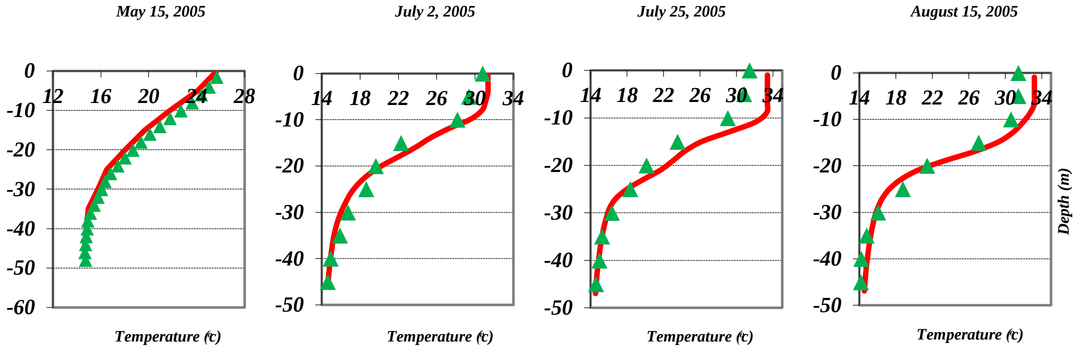


Figure 25 a. Temperature profiles compared to model predictions near the reservoir dam (Before Calibration)



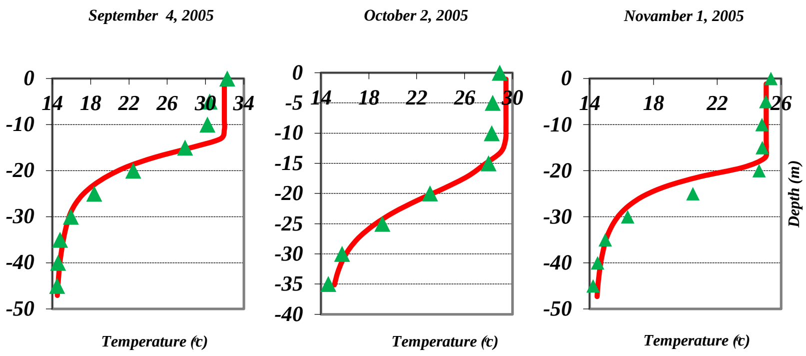


Figure 25 b. Temperature profiles compared to model predictions near the reservoir dam (After Calibration)

Figs. 26a and b show simulated and measured chlorophyll a before and after calibration at the surface. Chlorophyll a concentration approaches a peak during summer and then declines. Results after calibration show the reasonable agreement between measured and simulated after calibration. The Root Mean Square Error during given period of Chlorophyll a concentration in surface is 0.2311 μg/L. Figure 27a and b present the snapshots of DO profiles at model segment 64 (near the dam). The seasonal variation of DO in the reservoir after calibration is well simulated and the model results match the DO data well. The algae photosynthesis process affects oxygen concentration in the system: higher concentration of algae in the system higher DO concentration in the water body. Since light penetration to the lower layer is limited, chlorophyll a oxygen production and DO concentration is reduced by increasing depth.

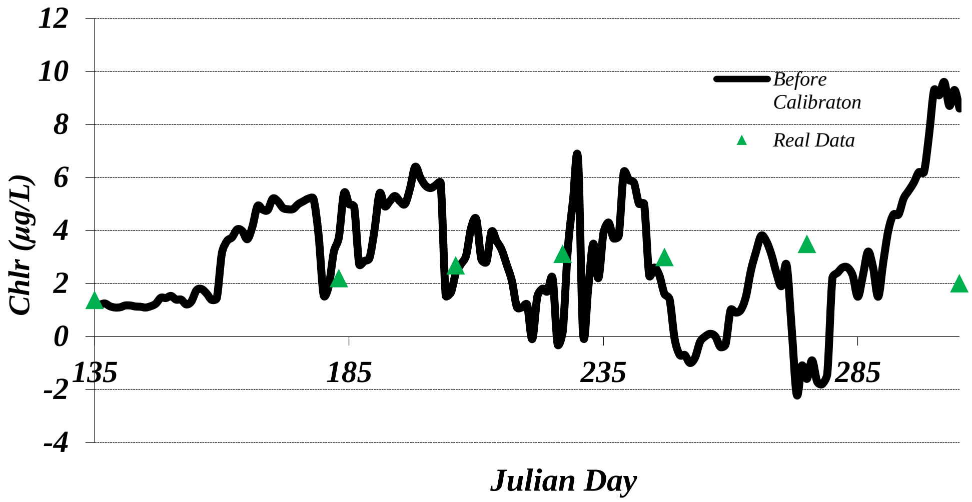


Figure 26 a. Comparing Chlr a simulation with observed data before calibration

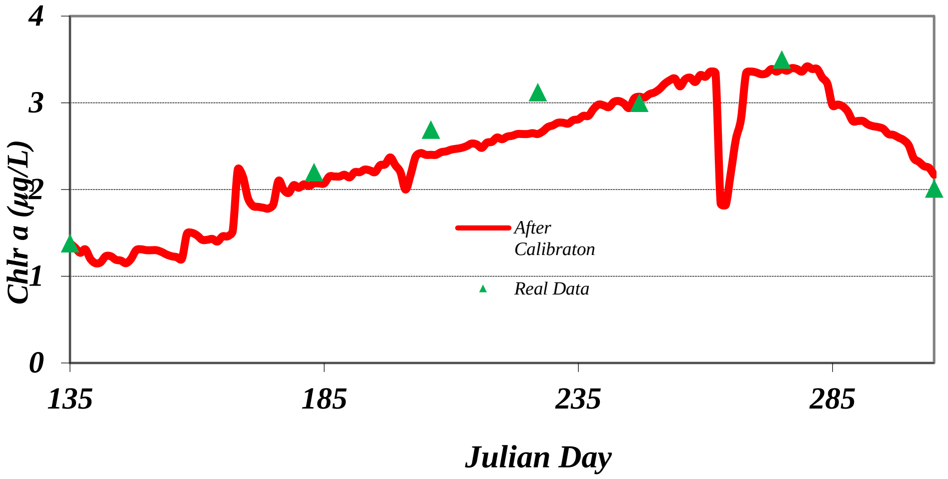


Figure 26 b. Comparing Chlr a simulation with observed data after calibration

The water quality results about NH_4, PO_4, and NO_3 compared with field data at segment 64 (at dam site) are presented in Fig. 28 to 30, respectively. Dissolved orthophosphorus, ammonia, and nitrite/nitrate concentrations measured in the field are also well matched by the model results after calibration.

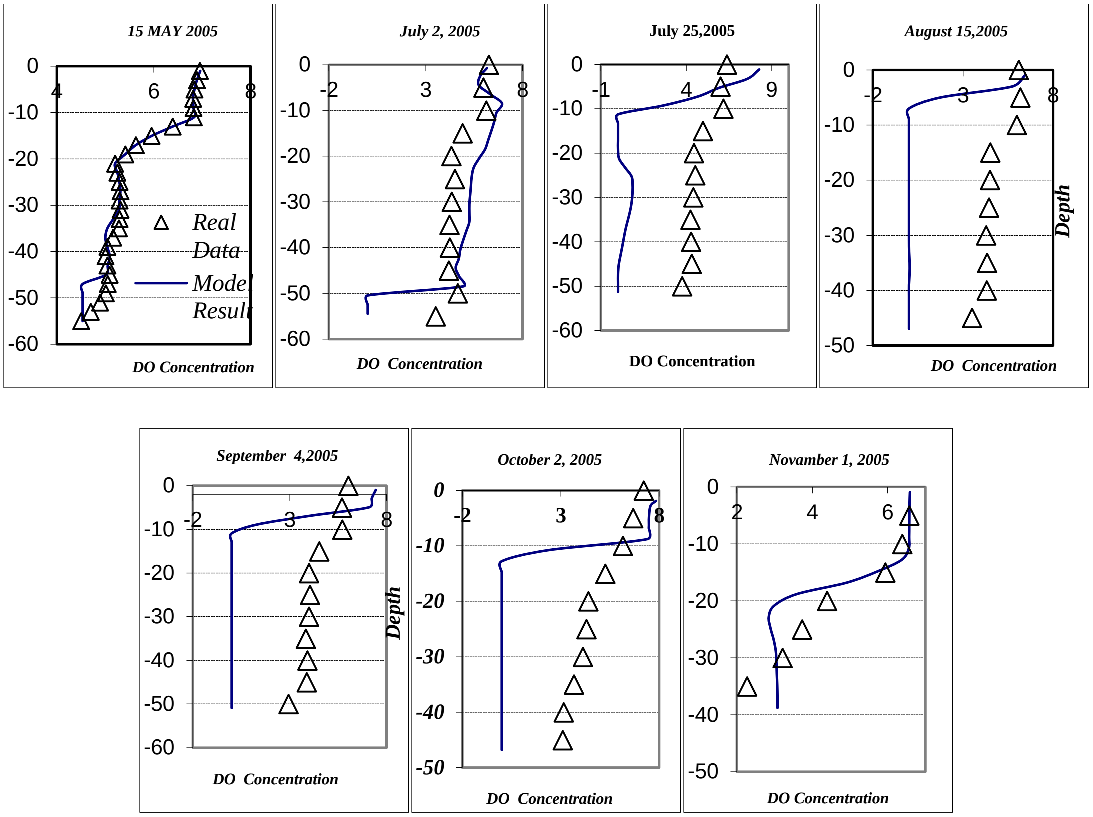
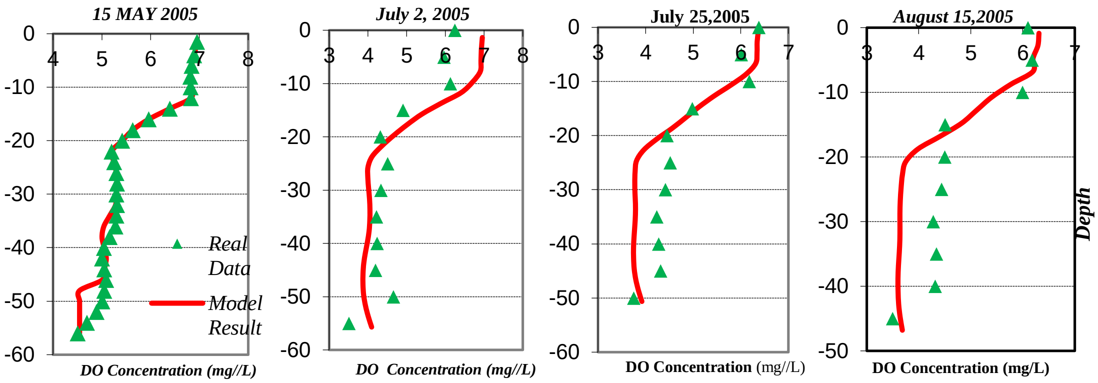


Figure 27 a. Comparing DO simulation with observed data before calibration



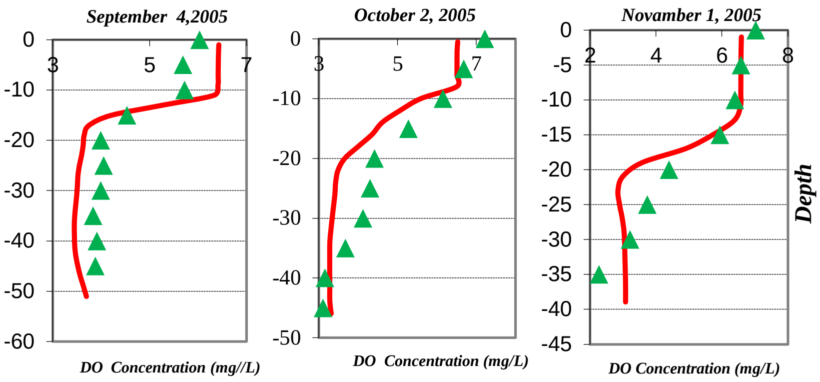


Figure 27 b. Comparing DO simulation with observed data after calibration

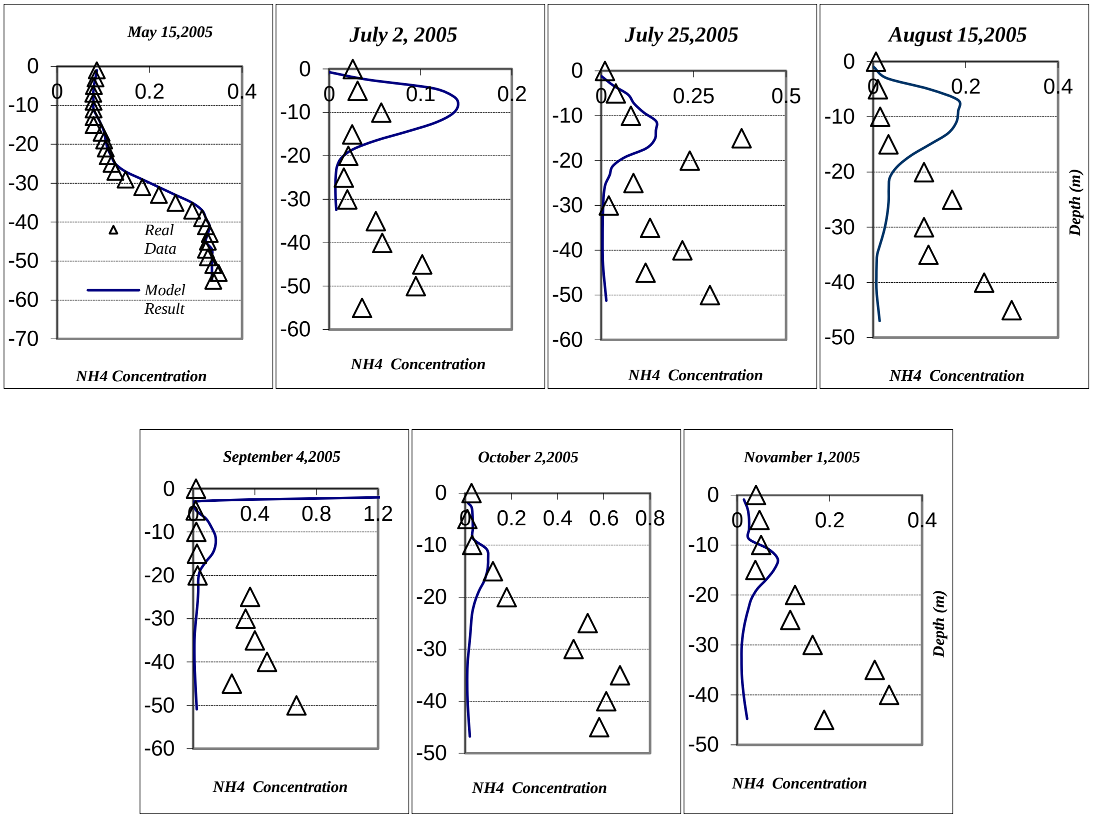


Figure 28 a. Comparing NH4 simulation with observed data before calibration

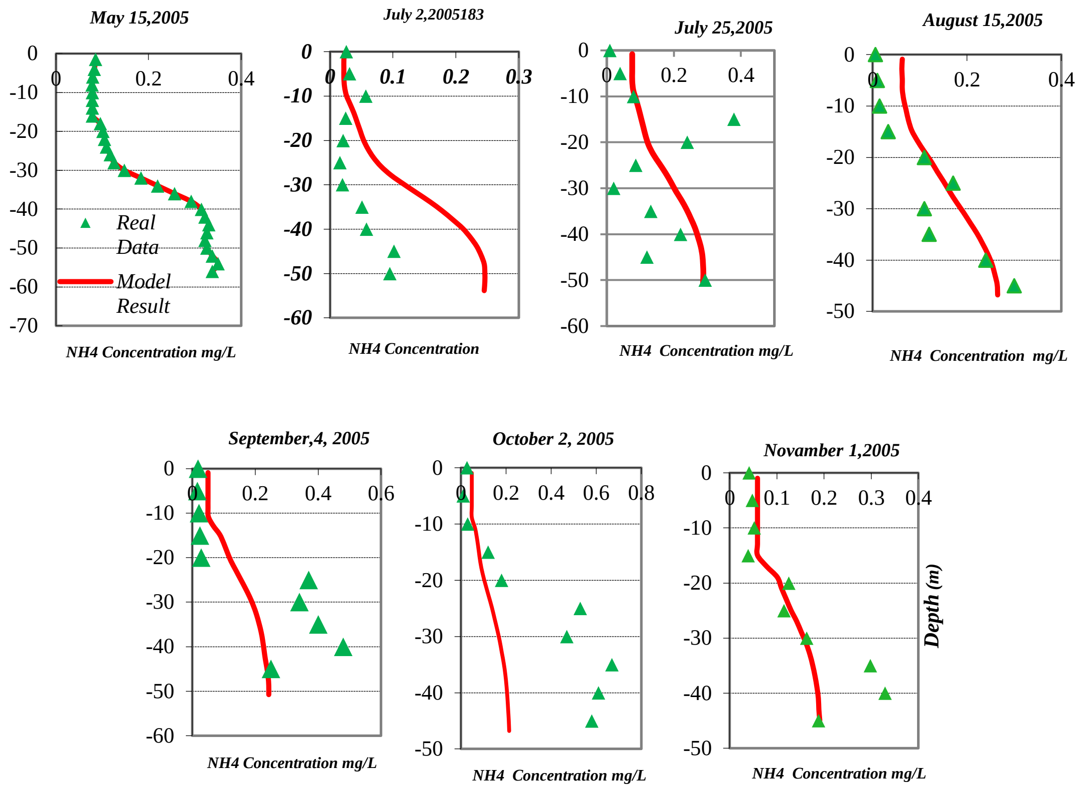
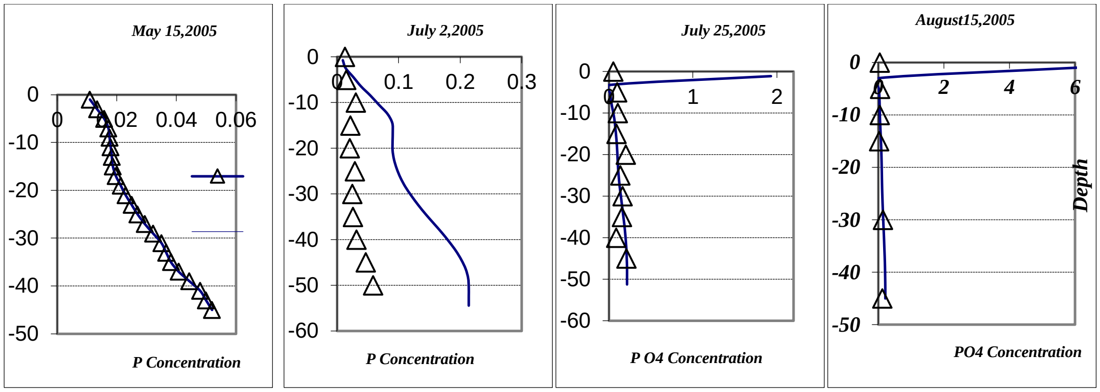


Figure 28 b. Comparing NH4 simulation with observed data after calibration



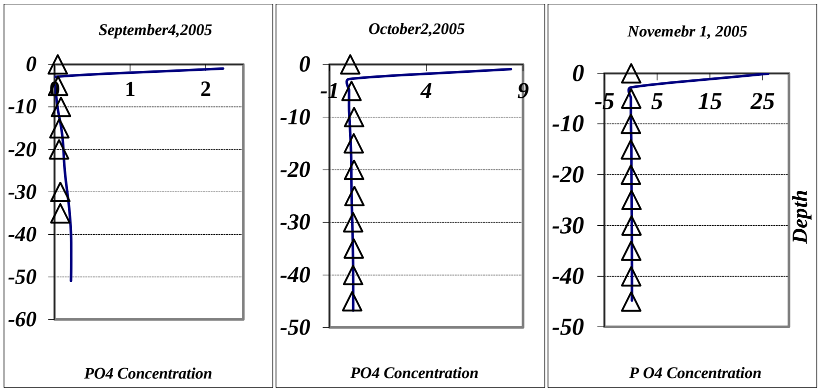


Figure 29 a. Comparing PO4 simulation with observed data before calibration

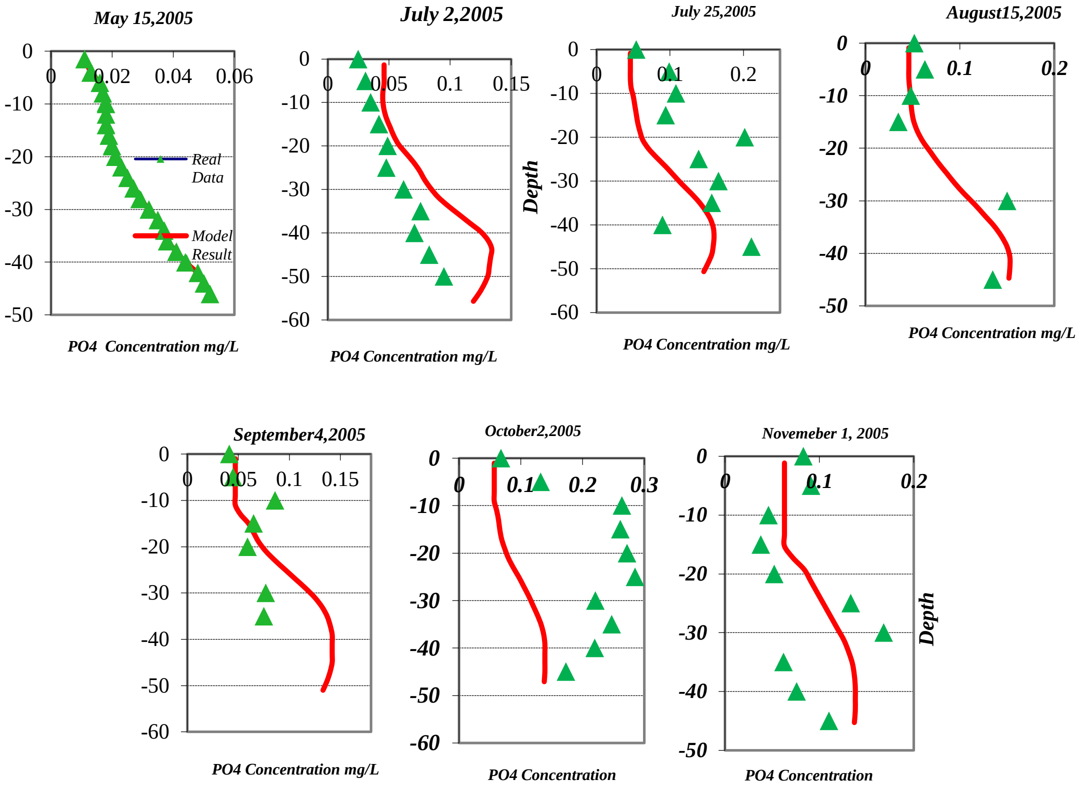


Figure 29 b. Comparing PO4 simulation with observed data after calibration

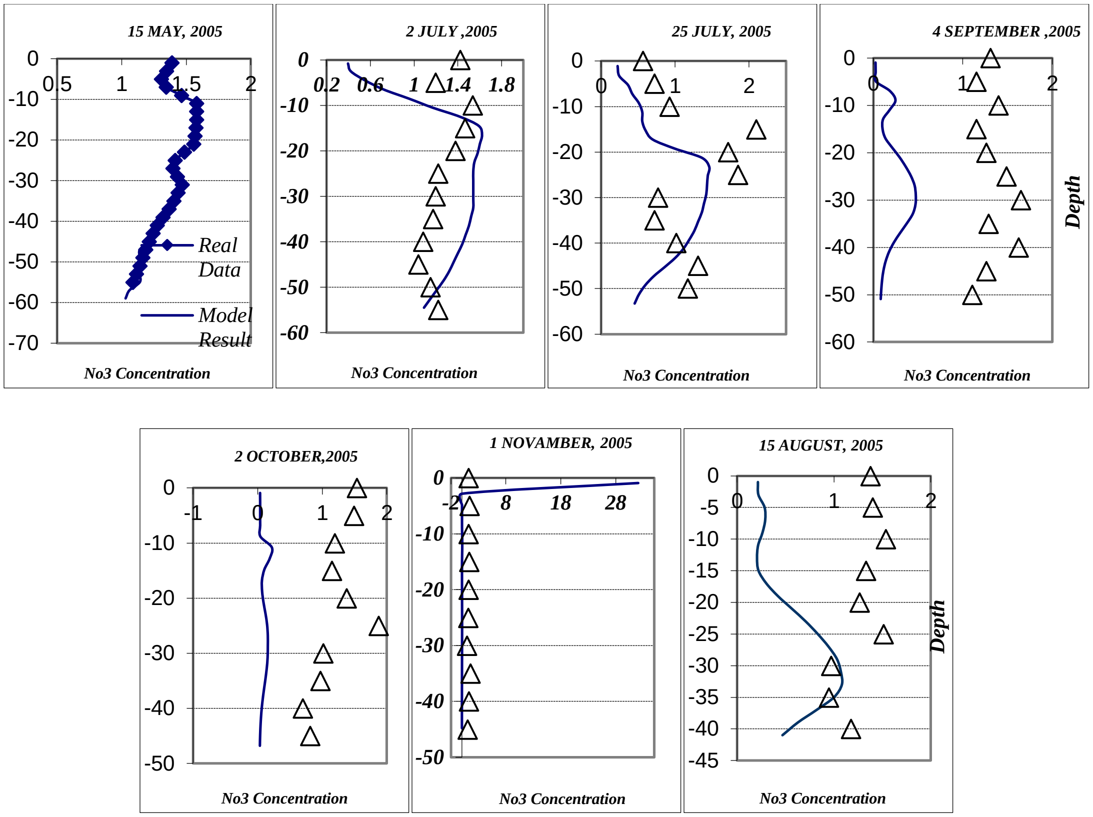
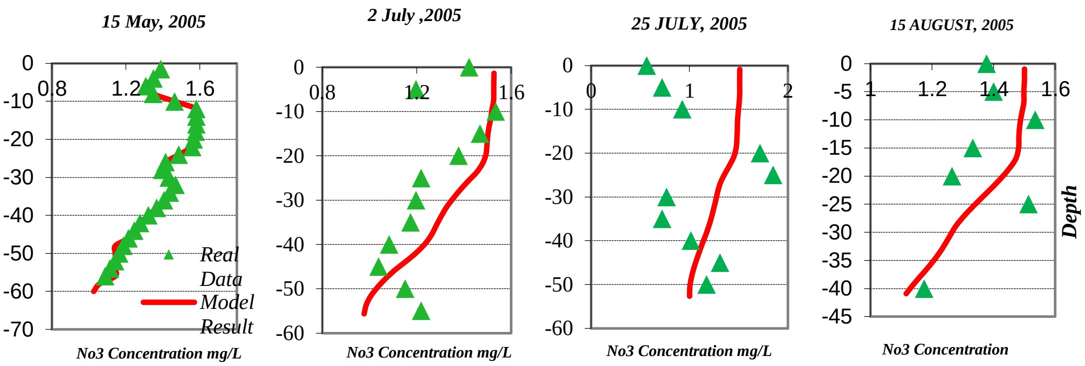


Figure 30 a. Comparing NO3-NO2 simulation with observed data before calibration



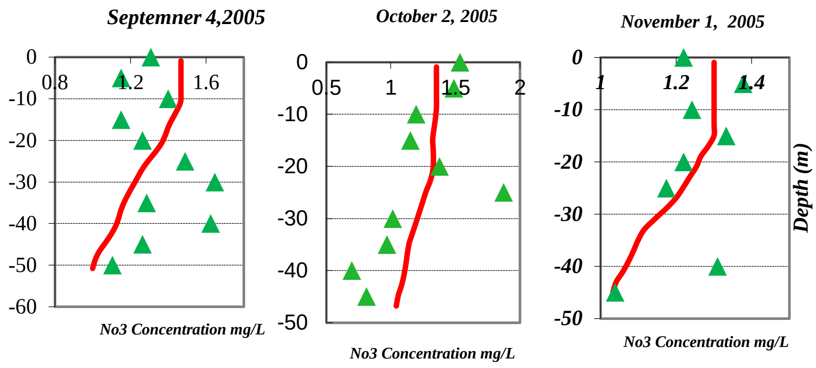


Figure 30 b. Comparing NO3-NO2 simulation with observed data after calibration

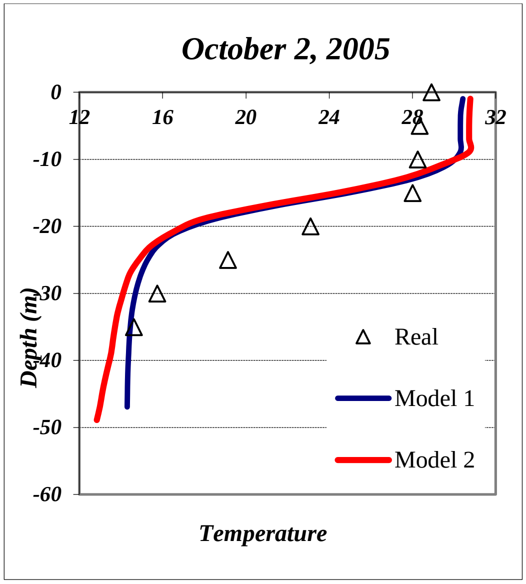
9.1. Various weighting factor

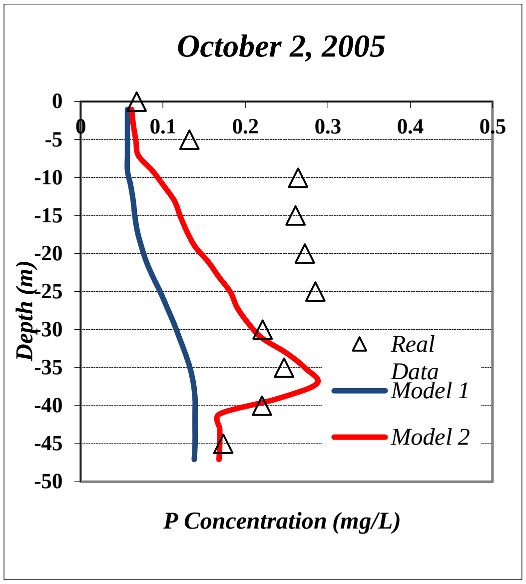
To explore the effect of weighting factors and also to improve the objective function related to ammonium and phosphate, the higher weighting factor is assigned to ammonium and phosphate than others. Table 4 shows the results of dimensionless average of objective function of six state variables for seven months with two different weighting factors. The objective function corresponded to ammonium and phosphate reduced by around 25% and the objective function of others increased by around 15% which is not that much significant. The new combination of weighting factors has led to more appropriate agreement between model and field data.

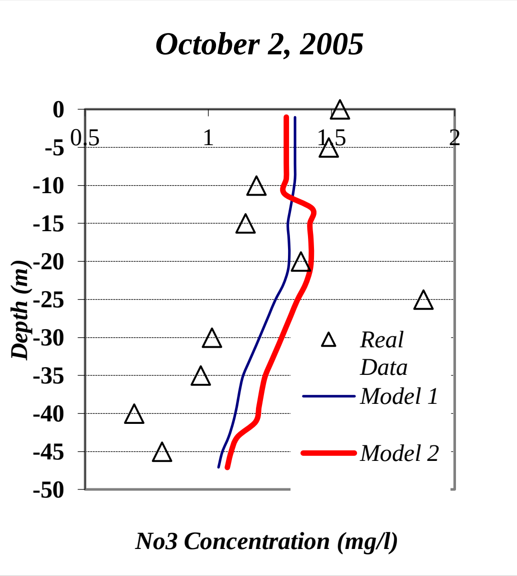
Table 4. The objective function and corresponded weighting factors

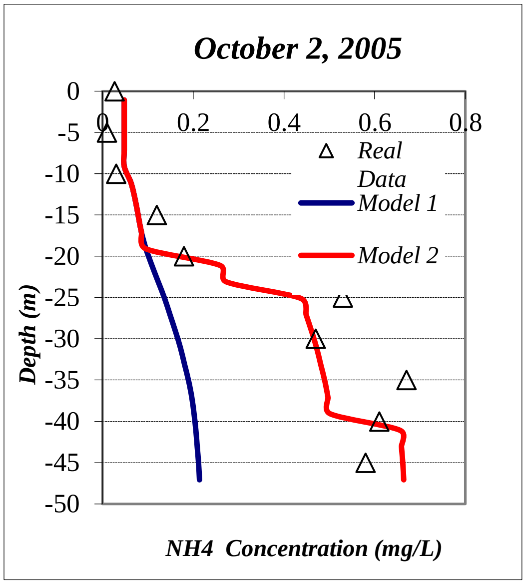
Weight/ RMSE	**TEMP**	**PO4**	**NO3**	**NH4**	**DO**	**Chlr a**
Weight	1/6	1/6	1/6	1/6	1/6	1/6
Model 1 RMSE	0.088	0.65	0.19	0.73	0.12	0.03
Weight	1/12	1/3	1/12	1/3	1/12	1/12
Model 2 RMSE	0.101	0.48	0.209	0.55	0.136	0.035

The vertical profile of temperature, Phosphate, Ammonium, Nitrite/ Nitrate, Dissolved oxygen and also chl a vs. time for one day of simulation are presented in fig. 31. Based on figure below, it is clear that model 2 has predicted phosphate and ammonium with higher agreement with field data. So, we can set weighting factor of each state variable based on the importance degree of that state variable to receive better result about that one.


October 2, 2005


October 2, 2005


October 2, 2005


October 2, 2005

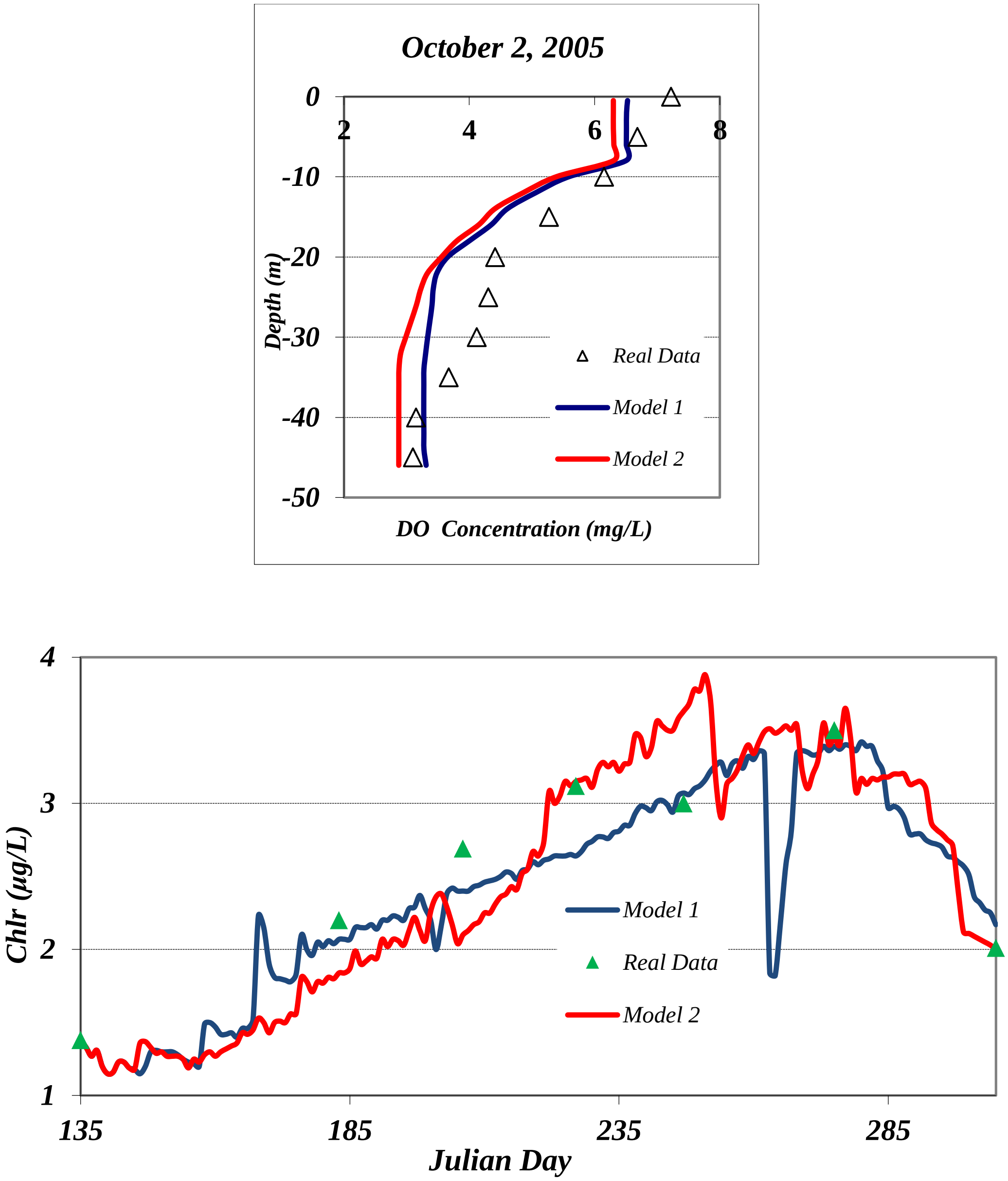


Figure 31. Comparing all state variables profile of model 1 and 2

10. Summary and Conclusions

The two-dimensional hydrodynamic and water quality model, CE-QUAL-W2, (Cole and Wells, 2013) was configured for the Karkheh Reservoir in Iran. The model was calibrated with an automatic multi-objective particle swarm optimization algorithm using field data from May to November 2005. The resulted overall dimensionless objective function was 0.3 in this study. By using the parameter set from the optimization model, comparisons of model predictions to field data for temperature, chlorophyll a, dissolved oxygen and nutrients showed that the algorithm converged on a set of model parameters that led to reasonable agreement between field data and model predictions.

In comparison to the most similar and recent research, Yongtai Huang and Lei Liu (2010) calibrated water quality model (CE-QUAL-W2) of Lake Maumelle in central Arkansas with Hybrid Genetic Algorithm and Neural Network Approach for temperature and concentrations of DO, ammonium (NH4), nitrate plus nitrite (NO3+NO2), TP, and chlorophyll a (Chla). After 2000 iterations, they achieved the best solution with the average dimensionless objective function of 0.5 for the same six state variables that is two times higher than the average dimensionless objective function of the best solution (F(x)=0.3) achieved in the proposed study. This comparison can give us an idea that how the proposed method was successful in finding the accurate parameter and decreasing time consumed in optimization. However, the judgment would be more reasonable if comparison was done by different method but the same case study and same data.

Once the model is calibrated, the model can then be used to forecast strategies to improve water quality. Since phosphorus has been determined as the limiting nutrient (Kuo et al., 2006), to improve water quality in the reservoir, phosphorus loads should be controlled. Since the majority of the nutrients reaching the Karkheh Reservoir are from agriculture in the watershed, the model can then be used to forecast the effect of applying proper agricultural and soil conservation management techniques in the watershed. The proposed simulation- optimization scheme achieves the best solution with 1500 iterations. The CE-QUAL-W2 model of Karkheh reservoir can be converted to a model with 6 or 7 branches. So, calibration results of a simple model vs. a complex model can be investigated in the terms of time efficiency and accuracy in the further steps.

As mentioned previously, the accuracy of calibration results of Karkheh Reservoir model is highly dependent on initial condition. So using field data of other months or even model of other water bodies as a new bench mark can be led to the more fairly judgment about the performance of proposed optimization method in the calibration of water quality and hydrodynamic model.

This procedure also can be applied in multi-site simulation calibration process if data be available for other monitoring sites. It can be helpful to make sure calibration procedure is done uniformly in whole water body. For simultaneous multi-site automatic calibration, two types of calibration methods can be applied; finding the weighted summation of objective function values calculated at each monitoring site which is the single-objective optimization method or using multi-objective evolutionary algorithms to optimize the different objective functions calculated at multiple sites simultaneously, and finding a set of multiple Pareto optimal solutions.

Using single objective optimization method can lead to bias of the objective function value at one site when optimizing objective function values at other sites. On the other hand, by using the multi-objective optimization method, we encounter several objective function values at each monitoring site. Therefore, the use of multi-site observed data to evaluate model performance deserves further research in the future.

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Appendix A

Control File of CE-QUAL-W2 model of Karkheh Reservoir:
PSU W2 Model Version 3.7

```
TITLE C ..............................TITLE..................................
        Karkhe River
        Water Quality Simulation
        Default hydraulic coefficients
        Default light absorption/extinction coefficients
        Temperature simulation
        Eutrophician study
        The Data was provided by Ab-Niroo
        Simuldation was done during Ordibehesht until Azar
        1384 /2/27 or 2005


GRID        NWB    NBR    IMX    KMX   NPROC  CLOSEC
              1      1     66     55      2     OFF

IN/OUTFL    NTR    NST    NIW    NWD    NGT    NSP    NPI    NPU
              0      2      0      1      0      1      0      0

CONSTITU    NGC    NSS    NAL    NEP   NBOD    NMC    NZP
              0      1      1      0      1      0      0

MISCELL    NDAY SELECTC HABTATC ENVIRPC AERATEC INITUWL
            171     OFF     OFF     OFF     OFF     OFF

TIME CON  TMSTRT   TMEND    YEAR
         135.000 305.000    2005

DLT CON      NDT  DLTMIN DLTINTR
               1 1.00000     OFF

DLT DATE    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD    DLTD
DLTD
         135.000

DLT MAX   DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX  DLTMAX
DLTMAX  DLTMAX  DLTMAX
         86400.0

DLT FRN     DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF    DLTF
         0.50000
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DLT LIMI    VISC    CELC
WB 1          ON      ON

BRANCH G      US      DS     UHS     DHS     UQB     DQB   NLMIN   SLOPE  SLOPEC
BR1           2      65       0       0       0       0       1 0.00000 0.00000

LOCATION     LAT    LONG    EBOT      BS      BE    JBDN
WB 1     32.5000 48.1500 113.000       1       1       1

INIT CND     T2I    ICEI  WTYPEC   GRIDC
WB 1     -2.0000 0.00000   FRESH    RECT

CALCULAT     VBC     EBC     MBC     PQC     EVC     PRC
WB 1          ON      ON      ON      ON      ON     OFF

DEAD SEA   WINDC    QINC   QOUTC   HEATC
WB 1          ON      ON      ON      ON

INTERPOL   QINIC   DTRIC    HDIC
BR1           ON      ON      ON

HEAT EXCH  SLHTC    SROC  RHEVAP   METIC  FETCHC     AFW     BFW     CFW
WINDH
WB 1        TERM     OFF     OFF      ON      ON 9.20000 0.53000 2.00000 2.00000

ICE COVE    ICEC  SLICEC  ALBEDO   HWICE    BICE    GICE  ICEMIN   ICET2
WB 1         OFF  DETAIL 0.25000 10.0000 0.60000 0.07000 0.05000 3.00000

TRANSPOR   SLTRC   THETA
WB 1    ULTIMATE 0.55000

HYD COEF      AX      DX    CBHE    TSED      FI   TSEDF   FRICC      Z0
WB 1     1.00000 1.00000 0.30000 10.0000 0.01500 1.00000   CHEZY 0.00100

EDDY VISC    AZC   AZSLC   AZMAX     FBC       E   ARODI STRCKLR BOUNDFR
TKECAL
WB 1          W2     IMP 1.00000       3 9.53500 0.43000 24.0000 10.0000     IMP

N STRUC     NSTR DYNELEV
BR1           2     OFF

STR INT    STRIC   STRIC   STRIC   STRIC   STRIC   STRIC   STRIC   STRIC
STRIC
BR 1          ON      ON
```

```
STR TOP    KTSTR   KTSTR   KTSTR   KTSTR   KTSTR   KTSTR   KTSTR   KTSTR
KTSTR
BR1          30      18

STR BOT    KBSTR   KBSTR   KBSTR   KBSTR   KBSTR   KBSTR   KBSTR
KBSTR   KBSTR
BR1          35      27

STR SINK   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC   SINKC
SINKC
BR1       POINT   POINT

STR ELEV    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR    ESTR
BR1      162.000 182.300

STR WIDT    WSTR    WSTR    WSTR    WSTR    WSTR    WSTR    WSTR    WSTR
WSTR
BR1      50.0000 50.0000

PIPES      IUPI    IDPI    EUPI    EDPI    WPI   DLXPI    FPI  FMINPI   WTHLC
DYNPIPE


PIPE UP    PUPIC   ETUPI   EBUPI   KTUPI   KBUPI


PIPE DOWN  PDPIC   ETDPI   EBDPI   KTDPI   KBDPI


SPILLWAY    IUSP    IDSP     ESP    A1SP    B1SP    A2SP    B2SP   WTHLC
SP 1          65       0 220.000 10.0000 1.50000 20.0000 1.00000    DOWN

SPILL UP   PUSPC   ETUSP   EBUSP   KTUSP   KBUSP
SP 1     DENSITY 220.000 0.00000       2      40

SPILL DOWN PDSPC   ETUSP   EBUSP   KTDSP   KBDSP
SP 1     DENSITY 0.00000 0.00000       2       3

SPILL GAS GASSPC    EQSP  AGASSP  BGASSP  CGASSP
SP 1         OFF       0 0.00000 0.00000 0.00000

GATES      IUGT    IDGT    EGT    A1GT    B1GT    G1GT    A2GT    B2GT    G2GT
WTHLC
```

GATE WEIR GTA1 GTB1 GTA2 GTB2 DYNVAR GTIC

GATE UP PUGTC ETUGT EBUGT KTUGT KBUGT

GATE DOWN PDGTC ETDGT EBDGT KTDGT KBDGT

GATE GAS GASGTC EQGT AGASGT BGASGT CGASGT

PUMPS 1 IUPU IDPU EPU STRTPU ENDPU EONPU EOFFPU QPU WTHLC DYNPUMP

PUMPS 2 PPUC ETPU EBPU KTPU KBPU

WEIR SEG IWR IWR IWR IWR IWR IWR IWR IWR IWR

WEIR TOP KTWR KTWR KTWR KTWR KTWR KTWR KTWR KTWR KTWR

WEIR BOT KBWR KBWR KBWR KBWR KBWR KBWR KBWR KBWR KBWR

WD INT WDIC WDIC WDIC WDIC WDIC WDIC WDIC WDIC WDIC
ON

WD SEG IWD IWD IWD IWD IWD IWD IWD IWD IWD
45

WD ELEV EWD EWD EWD EWD EWD EWD EWD EWD EWD
177.500

WD TOP KTWD KTWD KTWD KTWD KTWD KTWD KTWD KTWD KTWD
24

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WD BOT     KBWD    KBWD    KBWD    KBWD    KBWD    KBWD    KBWD
KBWD    KBWD
           26

TRIB PLA    PTRC    PTRC    PTRC    PTRC    PTRC    PTRC    PTRC    PTRC    PTRC
       DENSITY

TRIB INT    TRIC    TRIC    TRIC    TRIC    TRIC    TRIC    TRIC    TRIC    TRIC
           ON

TRIB SEG     ITR     ITR     ITR     ITR     ITR     ITR     ITR     ITR     ITR
           34

TRIB TOP   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT   ELTRT
ELTRT
       230.000

TRIB BOT   ELTRB   ELTRB   ELTRB   ELTRB   ELTRB   ELTRB   ELTRB   ELTRB
ELTRB
       178.000

DST TRIB    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC    DTRC
DTRC
BR 1        OFF

HYD PRIN  HPRWBC  HPRWBC  HPRWBC  HPRWBC  HPRWBC  HPRWBC
HPRWBC  HPRWBC  HPRWBC
NVIOL       OFF
U           OFF
W           OFF
T           ON
RHO         OFF
AZ          OFF
SHEAR       OFF
ST          OFF
SB          OFF
ADMX        OFF
DM          OFF
HDG         OFF
ADMZ        OFF
HPG         OFF
GRAV        OFF

SNP PRINT   SNPC    NSNP   NISNP
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```
WB 1       ON      7      4

SNP DATE    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD    SNPD
SNPD
WB 1    135.000 183.400 206.400 227.400 247.400 275.400 305.400

SNP FREQ    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF    SNPF
WB 1    1000.00 1000.00 1000.00 1000.00 1000.00 1000.00 1000.00

SNP SEG     ISNP    ISNP    ISNP    ISNP    ISNP    ISNP    ISNP    ISNP    ISNP
WB 1         36      43      52      64

SCR PRINT   SCRC    NSCR
WB 1       ON      1

SCR DATE    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD    SCRD
SCRD
WB 1    50.0000

SCR FREQ    SCRF    SCRF    SCRF    SCRF    SCRF    SCRF    SCRF    SCRF    SCRF
WB 1    10.0000

PRF PLOT    PRFC    NPRF   NIPRF
WB 1      OFF      1      4

PRF DATE    PRFD    PRFD    PRFD    PRFD    PRFD    PRFD    PRFD    PRFD
PRFD
WB 1    130.000

PRF FREQ    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF    PRFF
WB 1    1.00000

PRF SEG     IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF    IPRF
WB 1         36      43      52      64

SPR PLOT    SPRC    NSPR   NISPR
WB 1      OFF      1      1

SPR DATE    SPRD    SPRD    SPRD    SPRD    SPRD    SPRD    SPRD    SPRD
SPRD
WB 1    50.0000

SPR FREQ    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF    SPRF
WB 1    1.00000
```

```
SPR SEG    ISPR    ISPR    ISPR    ISPR    ISPR    ISPR    ISPR    ISPR    ISPR
WB 1         63

VPL PLOT    VPLC    NVPL
WB 1         ON       1

VPL DATE    VPLD    VPLD    VPLD    VPLD    VPLD    VPLD    VPLD    VPLD
VPLD
WB 1     63.5000

VPL FREQ    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF    VPLF
WB 1     1.00000

CPL PLOT    CPLC    NCPL TECPLOT
WB 1        OFF       1     OFF

CPL DATE    CPLD    CPLD    CPLD    CPLD    CPLD    CPLD    CPLD    CPLD
CPLD
WB 1     63.5000

CPL FREQ    CPLF    CPLF    CPLF    CPLF    CPLF    CPLF    CPLF    CPLF    CPLF
WB 1     1.00000

FLUXES     FLXC    NFLX
WB 1         ON       6

FLX DATE    FLXD    FLXD    FLXD    FLXD    FLXD    FLXD    FLXD    FLXD
FLXD
WB 1     135.000 183.000 206.000 247.000 275.000 305.000

FLX FREQ    FLXF    FLXF    FLXF    FLXF    FLXF    FLXF    FLXF    FLXF    FLXF
WB 1     50.0000 50.0000 50.0000 50.0000 50.0000 50.0000

TSR PLOT    TSRC    NTSR   NITSR
             ON       1       1

TSR DATE    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD    TSRD
TSRD
         50.0000

TSR FREQ    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF    TSRF
         1.00000

TSR SEG    ITSR    ITSR    ITSR    ITSR    ITSR    ITSR    ITSR    ITSR    ITSR
             64
```

```
TSR LAYE    ETSR    ETSR    ETSR    ETSR    ETSR    ETSR    ETSR    ETSR    ETSR
        0.00000

WITH OUT    WDOC    NWDO   NIWDO
            OFF       1       1

WITH DAT    WDOD    WDOD    WDOD    WDOD    WDOD    WDOD    WDOD
WDOD    WDOD
        0.00000

WITH FRE    WDOF    WDOF    WDOF    WDOF    WDOF    WDOF    WDOF
WDOF    WDOF
        0.00000

WITH SEG    IWDO    IWDO    IWDO    IWDO    IWDO    IWDO    IWDO    IWDO
IWDO
              0

RESTART     RSOC    NRSO    RSIC
            OFF       0     OFF

RSO DATE    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD    RSOD
RSOD


RSO FREQ    RSOF    RSOF    RSOF    RSOF    RSOF    RSOF    RSOF    RSOF
RSOF


CST COMP     CCC    LIMC     CUF
             ON      ON       3

CST ACTIVE   CAC
TDS           ON
ISS1          ON
PO4           ON
NH4           ON
NO3           ON
DSI          OFF
PSI          OFF
FE           OFF
LDOM          ON
RDOM          ON
LPOM          ON
```

```
RPOM        OFF
BOD1        ON
BODP1        ON
BODN1        ON
ALG1        ON
DO         ON
TIC        ON
ALK         ON
LDOM-P      OFF
RDOM-P      OFF
LPOM-P      OFF
RPOM-P      OFF
LDOM-N      OFF
RDOM-N      OFF
LPOM-N      OFF
RPOM-N      OFF

CST DERI   CDWBC   CDWBC   CDWBC   CDWBC   CDWBC   CDWBC   CDWBC
CDWBC   CDWBC
DOC       CDWBC
POC         OFF
TOC         OFF
DON         OFF
PON         OFF
TON         OFF
TKN         OFF
TN         OFF
DOP         OFF
POP         OFF
TOP         OFF
TP         OFF
APR         OFF
CHLA         ON
ATOT        OFF
%DO         OFF
TSS         OFF
TISS        OFF
CBOD        OFF
pH         OFF
CO2         OFF
HCO3        OFF
CO3         OFF

CST FLUX   CFWBC   CFWBC   CFWBC   CFWBC   CFWBC   CFWBC   CFWBC
CFWBC   CFWBC
```

```
TISSIN     CFWBC
TISSOUT     OFF
PO4AR        ON
PO4AG        ON
PO4AP        ON
PO4ER        ON
PO4EG        ON
PO4EP        ON
PO4POM       ON
PO4DOM       ON
PO4OM        ON
PO4SED       ON
PO4SOD       ON
PO4SET       ON
NH4NITR     ON
NH4AR       ON
NH4AG       ON
NH4AP       ON
NH4ER       ON
NH4EG       ON
NH4EP       ON
NH4POM      ON
NH4DOM      ON
NH4OM       ON
NH4SED      ON
NH4SOD      ON
NO3DEN      ON
NO3AG       ON
NO3EG       ON
NO3SED      ON
DSIAG       OFF
DSIEG       OFF
DSIPIS      OFF
DSISED      OFF
DSISOD      OFF
DSISET      OFF
PSIAM       OFF
PSINET      OFF
PSIDK       OFF
FESET       OFF
FESED       OFF
LDOMDK      OFF
LRDOM       OFF
RDOMDK      OFF
LDOMAP      OFF
```

```
LDOMEP      OFF
LPOMDK      OFF
LRPOM       OFF
RPOMDK      OFF
LPOMAP      OFF
LPOMEP      OFF
LPOMSET     OFF
RPOMSET     OFF
CBODDK      OFF
DOAP        ON
DOAR        ON
DOEP        ON
DOER        ON
DOPOM       ON
DODOM       ON
DOOM        ON
DONITR      ON
DOCBOD      ON
DOREAR      ON
DOSED       ON
DOSOD       ON
TICAG       OFF
TICEG       OFF
SEDDK       OFF
SEDAS       OFF
SEDLPOM     OFF
SEDSET      ON
SODDK       ON

CST ICON   C2IWB   C2IWB   C2IWB   C2IWB   C2IWB   C2IWB   C2IWB   C2IWB
C2IWB
TDS      -1.0000
ISS1     -2.0000
PO4      -2.0000
NH4      -2.0000
NO3      -2.0000
DSI      -2.0000
PSI      -2.0000
FE       -2.0000
LDOM     0.10000
RDOM     0.10000
LPOM     0.10000
RPOM     0.10000
BOD1     0.10000
BODP1    0.00000
```

```
BODN1    0.00000
ALG1     -2.0000
DO       -2.0000
TIC      130.000
ALK      130.000
LDOM-P   0.00050
RDOM-P   0.00050
LPOM-P   0.00050
RPOM-P   0.00050
LDOM-N   0.00800
RDOM-N   0.00800
LPOM-N   0.00800
RPOM-N   0.00800

CST PRIN  CPRWBC  CPRWBC  CPRWBC  CPRWBC  CPRWBC  CPRWBC
CPRWBC  CPRWBC  CPRWBC
TDS           ON
ISS1          ON
PO4           ON
NH4           ON
NO3           ON
DSI          OFF
PSI          OFF
FE           OFF
LDOM         OFF
RDOM         OFF
LPOM         OFF
RPOM         OFF
BOD1          ON
BODP1         ON
BODN1        OFF
ALG1          ON
DO            ON
TIC          OFF
ALK          OFF
LDOM-P       OFF
RDOM-P       OFF
LPOM-P       OFF
RPOM-P       OFF
LDOM-N       OFF
RDOM-N       OFF
LPOM-N       OFF
RPOM-N       OFF
```

```
CIN CON   CINBRC  CINBRC  CINBRC  CINBRC  CINBRC  CINBRC  CINBRC
CINBRC  CINBRC
TDS           ON
ISS1         ON
PO4           ON
NH4           ON
NO3           ON
DSI          OFF
PSI          OFF
FE           OFF
LDOM         OFF
RDOM         OFF
LPOM         OFF
RPOM         OFF
BOD1          ON
BODP1         ON
BODN1         ON
ALG1          ON
DO            ON
TIC          OFF
ALK          OFF
LDOM-P       OFF
RDOM-P       OFF
LPOM-P      OFF
RPOM-P      OFF
LDOM-N      OFF
RDOM-N      OFF
LPOM-N      OFF
RPOM-N      OFF

CTR CON   CTRTRC  CTRTRC  CTRTRC  CTRTRC  CTRTRC  CTRTRC  CTRTRC
CTRTRC  CTRTRC
TDS          OFF
ISS1         OFF
PO4          OFF
NH4      CTRTRC
NO3          OFF
DSI          OFF
PSI          OFF
FE           OFF
LDOM         OFF
RDOM         OFF
LPOM         OFF
RPOM         OFF
BOD1        OFF
```

```
BODP1       OFF
BODN1       OFF
ALG1        OFF
DO          OFF
TIC         OFF
ALK         OFF
LDOM-P      OFF
RDOM-P      OFF
LPOM-P      OFF
RPOM-P      OFF
LDOM-N      OFF
RDOM-N      OFF
LPOM-N      OFF
RPOM-N      OFF

CDT CON   CDTBRC  CDTBRC  CDTBRC  CDTBRC  CDTBRC  CDTBRC
CDTBRC  CDTBRC  CDTBRC
TDS         OFF
ISS1        OFF
PO4         OFF
NH4         OFF
NO3         OFF
DSI         OFF
PSI         OFF
FE          OFF
LDOM        OFF
RDOM        OFF
LPOM        OFF
RPOM        OFF
BOD1        OFF
BODP1       OFF
BODN1       OFF
ALG1        OFF
DO          OFF
TIC         OFF
ALK         OFF
LDOM-P      OFF
RDOM-P      OFF
LPOM-P      OFF
RPOM-P      OFF
LDOM-N      OFF
RDOM-N      OFF
LPOM-N      OFF
RPOM-N      OFF
```

```
CPR CON   CPRBRC  CPRBRC  CPRBRC  CPRBRC  CPRBRC  CPRBRC  CPRBRC
CPRBRC  CPRBRC
TDS          OFF
ISS1         OFF
PO4          OFF
NH4          OFF
NO3          OFF
DSI          OFF
PSI          OFF
FE           OFF
LDOM         OFF
RDOM         OFF
LPOM         OFF
RPOM         OFF
BOD1         OFF
BODP1        OFF
BODN1        OFF
ALG1         OFF
DO           OFF
TIC          OFF
ALK          OFF
LDOM-P       OFF
RDOM-P       OFF
LPOM-P       OFF
RPOM-P       OFF
LDOM-N       OFF
RDOM-N       OFF
LPOM-N       OFF
RPOM-N       OFF

EX COEF    EXH2O    EXSS    EXOM    BETA     EXC    EXIC
WB 1     0.22000 0.01000 0.40000 0.45000     OFF     OFF

ALG EX       EXA     EXA     EXA     EXA     EXA     EXA
        0.20000

ZOO EX       EXZ     EXZ     EXZ     EXZ     EXZ     EXZ
        0.00000

MACRO EX     EXM     EXM     EXM     EXM     EXM     EXM
        0.00000

GENERIC    CGQ10   CG0DK   CG1DK     CGS
CG 1     0.00000 0.00000 0.00000 0.00000
```

```
S SOLIDS     SSS    SEDRC    TAUCR
SS# 1    1.00000     OFF 1.00000

ALGAL RATE     AG       AR       AE       AM       AS     AHSP     AHSN    AHSSI     ASAT
ALG1      1.15000 0.04000 0.04000 0.03500 0.04500 0.01000 0.02600 0.00000  85.000

ALGAL TEMP    AT1      AT2      AT3      AT4      AK1      AK2      AK3      AK4
ALG1      5.00000 25.0000 35.0000 40.0000 0.10000 0.99000 0.99000 0.10000

ALG STOI    ALGP    ALGN    ALGC    ALGSI    ACHLA    ALPOM    ANEQN     ANPR
ALG1      0.00500 0.08000 0.45000 0.18000 0.122000 0.80000        2 0.00100

EPIPHYTE    EPIC    EPIC    EPIC    EPIC    EPIC    EPIC    EPIC    EPIC    EPIC
EPI1    MP    AT1

EPI PRIN    EPRC    EPRC    EPRC    EPRC    EPRC    EPRC    EPRC    EPRC    EPRC
EPI1          OFF

EPI INIT    EPICI    EPICI    EPICI    EPICI    EPICI    EPICI    EPICI    EPICI    EPICI
EPI1      0.00000

EPI RATE       EG       ER       EE       EM       EB     EHSP     EHSN    EHSSI
EPI1      0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

EPI HALF     ESAT      EHS    ENEQN     ENPR
EPI1      0.00000 0.00000        0 0.00000

EPI TEMP      ET1      ET2      ET3      ET4      EK1      EK2      EK3      EK4
EPI1      0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

EPI STOI       EP       EN       EC      ESI    ECHLA     EPOM
EPI1      0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

ZOOP RATE      ZG       ZR       ZM     ZEFF    PREFP  ZOOMIN     ZS2P
Zoo1      1.50000 0.10000 0.01000 0.50000 0.50000 0.01000 0.30000

ZOOP ALGP  PREFA    PREFA    PREFA    PREFA    PREFA    PREFA    PREFA
PREFA    PREFA
Zoo1      0.00000

ZOOP ZOOP  PREFZ    PREFZ    PREFZ    PREFZ    PREFZ    PREFZ    PREFZ    PREFZ
PREFZ
Zoo1      0.00000

ZOOP TEMP     ZT1      ZT2      ZT3      ZT4      ZK1      ZK2      ZK3      ZK4
```

```
Zoo1     0.00000 15.0000 20.0000 36.0000 0.01000 0.90000 0.99000 0.10000

ZOOP STOI     ZP      ZN      ZC
Zoo1     0.01500 0.08000 0.45000

MACROPHY  MACWBC  MACWBC  MACWBC  MACWBC  MACWBC
MACWBC  MACWBC  MACWBC  MACWBC
Mac1         OFF

MAC PRIN  MPRWBC  MPRWBC  MPRWBC  MPRWBC  MPRWBC  MPRWBC
MPRWBC  MPRWBC  MPRWBC
Mac1         OFF

MAC INI  MACWBCI MACWBCI MACWBCI MACWBCI MACWBCI MACWBCI
MACWBCI MACWBCI MACWBCI
Mac1     0.00000

MAC RATE     MG     MR     MM    MSAT    MHSP    MHSN    MHSC    MPOM
LRPMAC
Mac1     0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

MAC SED     PSED    NSED
Mac1     0.00000 0.00000

MAC DIST    MBMP    MMAX
Mac1     0.00000 0.00000

MAC DRAG  CDDRAG     DMV    DWSA   ANORM
Mac1     0.00000 0.00000 0.00000 0.00000

MAC TEMP     MT1     MT2     MT3     MT4     MK1     MK2     MK3     MK4
Mac1     0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

MAC STOICH    MP      MN      MC
Mac1     0.00000 0.00000 0.00000

DOM       LDOMDK  RDOMDK   LRDDK
WB 1     0.10000 0.00100 0.01000

POM       LPOMDK  RPOMDK   LRPDK    POMS
WB 1     0.08000 0.00100 0.00100 0.50000

OM STOIC    ORGP    ORGN    ORGC   ORGSI
WB 1     0.00500 0.08000 0.45000 0.18000
```

```
OM RATE     OMT1    OMT2    OMK1    OMK2
WB 1     4.00000 25.0000 0.10000 0.99000

CBOD        KBOD    TBOD    RBOD   CBODS
BOD 1    0.10000 1.02000 1.85000 0.00000

CBOD STOIC  BODP    BODN    BODC
BOD 1    0.00400 0.06000 0.32000

PHOSPHOR    PO4R   PARTP
WB 1     0.02000 0.00000

AMMONIUM    NH4R   NH4DK
WB 1     0.01000 0.26500

NH4 RATE   NH4T1   NH4T2   NH4K1   NH4K2
WB 1     5.00000 25.0000 0.10000 0.99000

NITRATE    NO3DK    NO3S FNO3SED
WB 1     0.07800 0.01500 0.00000

NO3 RATE   NO3T1   NO3T2   NO3K1   NO3K2
WB 1     5.00000 25.0000 0.10000 0.99000

SILICA      DSIR    PSIS   PSIDK  PARTSI
WB 1     0.10000 0.00000 0.30000 0.20000

IRON         FER     FES
WB 1     0.50000 2.00000

SED CO2     CO2R
WB 1     1.00000

STOICH 1   O2NH4    O2OM
WB 1     4.57000 1.40000

STOICH 2    O2AR    O2AG
ALG1     1.10000 1.40000

STOICH 3    O2ER    O2EG
EPI1     0.00000 0.00000

STOICH 4    O2ZR
Zoop1    1.10000
```

```
STOICH 5    O2MR    O2MG
Mac1     0.00000 0.00000

O2 LIMIT   O2LIM
        0.10000

SEDIMENT    SEDC  SEDPRC   SEDCI    SEDS    SEDK    FSOD    FSED   SEDBR
DYNSEDK
WB 1          ON      ON 0.00000 0.10000 0.43000 0.65500 0.65500 0.01000     OFF

SOD RATE   SODT1   SODT2   SODK1   SODK2
WB 1     4.00000 30.0000 0.10000 0.99000

S DEMAND     SOD     SOD     SOD     SOD     SOD     SOD     SOD     SOD     SOD
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000 0.30000
        0.30000 0.30000 0.30000

REAERATION  TYPE    EQN#   COEF1   COEF2   COEF3   COEF4
WB 1        LAKE       5 0.00000 0.00000 0.00000 0.00000

RSI FILE.................................RSIFN................................
       rsi.npt - not used

QWD FILE.................................QWDFN................................
       qwd_dasht.npt

QGT FILE.................................QGTFN................................
       qgt.npt - not used

WSC FILE.................................WSCFN................................
       wsc.npt

SHD FILE.................................SHDFN................................
       shd.npt

BTH FILE.................................BTHFN................................
WB 1    bth_1.npt

MET FILE.................................METFN................................
```

```
WB 1    met_1.npt

EXT FILE.................................EXTFN................................
WB 1    ext_1.npt - not used

VPR FILE.................................VPRFN................................
WB 1    vpr_1.npt

LPR FILE.................................LPRFN................................
WB 1    lpr_1.npt

QIN FILE.................................QINFN................................
BR1     qin_br1.npt

TIN FILE.................................TINFN................................
BR1     tin_br1.npt

CIN FILE.................................CINFN................................
BR1     cin_br1.npt

QOT FILE.................................QOTFN................................
BR1     qot_br1.npt

QTR FILE.................................QTRFN................................
TR1     qtr_tr1.npt - not used

TTR FILE.................................TTRFN................................
TR1     ttr_tr1.npt - not used

CTR FILE.................................CTRFN................................
TR1     ctr_br1.npt - not used

QDT FILE.................................QDTFN................................
BR1     qin_br1.npt

TDT FILE.................................TDTFN................................
BR1     tdt_br1.npt

CDT FILE.................................CDTFN................................
BR1     cdt_br1.npt

PRE FILE.................................PREFN................................
BR1     pre_br1.npt

TPR FILE.................................TPRFN................................
```

```
BR1     tpr_br1.npt

CPR FILE.................................CPRFN................................
BR1     cpr_br1.npt

EUH FILE.................................EUHFN................................
BR1     euh_br1.npt

TUH FILE.................................TUHFN................................
BR1     tuh_br1.npt

CUH FILE.................................CUHFN................................
BR1     cuh_br1.npt

EDH FILE.................................EDHFN................................
BR1     edh_br1.npt

TDH FILE.................................TDHFN................................
BR1     tdh_br1.npt

CDH FILE.................................CDHFN................................
BR1     cdh_br1.npt

SNP FILE.................................SNPFN................................
WB 1    snp_br1.opt

PRF FILE.................................PRFFN................................
WB 1    prf_1.opt

VPL FILE.................................VPLFN................................
WB 1    W2Linkage1.w2l

CPL FILE.................................CPLFN................................
WB 1    cpl_1.opt

SPR FILE.................................SPRFN................................
WB 1    spr_1.opt

FLX FILE.................................FLXFN................................
WB 1    flx_1.opt

TSR FILE.................................TSRFN................................
        tsr.opt
WDO FILE.................................WDOFN................................
        wdo.opt
```

Appendix B

PSO code

```
    subroutine pso


    USE DFPORT
    USE DFLIB
    USE MSIMSL

    REAL, allocatable:: x(:,:),pbest(:,:),gbest(:),NO1DAY(:)
    REAL, allocatable:: velocity (:,:),fx(:,:),w(:),velocity_p(:,:)
    REAL, allocatable:: iij(:),objectivefun2(:),funct(:)
    REAL, allocatable:: objectivefun(:),matr(:,:),bound_min(:)
    REAL, allocatable:: vmax(:),vmin(:),bound_max(:)

    DIMENSION:: DEPTH1(500),Temprature1(500),depth11(50,50)
    DIMENSION:: DEPTH2(500),Temprature2(500),depth22(50,50)
    DIMENSION:: kj(50),temprature11(50,50),temprature22(50,50)

    integer:: r,particle,var,iterationmax,p,m,j,num_particle,iiii
        integer:: num_iter,num_iter1,a

    real:: iter,itermax,S,perv
   !****************************************
        open(unit=7, file ="input_pso.txt",status ="old")
    open(unit=3, file ="output.txt",status ="unknown")
    OPEN(2555,FILE='DECVAR3.DAT',STATUS='UNKNOWN')
    open(2252,file='COEEFICIENT.DAT', status='unknown')
    open(888,file='check2.dat')
    open(114, file='objfun.dat',status='unknown')
    open(666,file='realdata.npt',status='old')
    open(555, file='modelRes.dat', status='unknown')
    open(113, file='dec.dat', status='unknown')
        open (22222, file='checkObj.dat', status='unknown')
        open (4, file='variable.dat', status='unknown')
        open (5, file='velocity.dat', status='unknown')
        open(unit=1, file ="for diagram.dat",status ="unknown")


!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

    read(7,*)iterationmax
    read(7,*)p
```

```
      read(7,*)w1
      read(7,*)w2
      read(7,*)c1
      read(7,*)c2
      read(7,*)NDAY
         read(7,*)a
         read(7,*)b
      m = 2 + NDAY



!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

      ALLOCATE ( x(p,m),pbest(p,m),gbest(m),matr(p,m),bound_max(m))
      ALLOCATE ( velocity(p,m),fx(p,m),w(iterationmax),iij(p))
      ALLOCATE ( funct(p),velocity_p(p,m),NO1DAY(m),vmax(m),vmin(m))
         ALLOCATE ( objectivefun2(p),objectivefun(p),bound_min(m))

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

      WRITE(*,*)'ENTER NUMBER OF SEGMENTS'
      READ(*,*)IMX
      write(*,*)'Enter the number of water body:'
      read(*,*)NWB

      do r=1,iterationmax
        if(r.eq.1)then
          call input
             call initial
            else
             call inertia_weight
             rewind(114)
                 call main
        endif
      enddo
```

```
!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

    CONTAINS



!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

!@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@

   subroutine input()

   bound_min(1) = 0.25
   bound_max(1) = 0.35
   bound_min(2) = 0.4
   bound_max(2) = 0.5
       bound_min(3) = 0.65
   bound_max(3) = 0.75
       bound_min(4) = 0.75
   bound_max(4) = 0.85

   do var=1,m
         vmax(var) = bound_max(var) - bound_min(var)
     vmin(var) = -vmax(var)
   end do

       return
   end subroutine input


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      subroutine inertia_weight()

      itermax = iterationmax                  !this changing variables happend beacause if
mathmatical operation be done on 2 integers the answer is integer.
      iter = r
      w(r) = (w1 - w2)*(itermax - iter)/itermax + w2

      return
      end subroutine inertia_weight


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      subroutine initial()

      CALL RANDOM_SEED()
      OPEN(222,FILE='VARS.DAT',STATUS='UNKNOWN')



      do particle = 1,p
        objectivefun2(particle)=0
        iii = 0

            do var = 1,2

              CALL RANDOM_NUMBER(S)
              x(particle,var) = bound_min(var) + (bound_max(var)
     &                  - bound_min(var))* S
              pbest(particle,var) = x(particle,var)
          write(222,'(f8.2)') x(particle,var)
              write(4,*) x(particle,var)
          velocity_p(particle,var) = vmax(var)
        end do
```

```
          do i=1,NWB
            WRITE(2252,'(2F8.2)')(x(particle,var), var=1,2)
      enddo
      rewind(2252)

          do var = 3,m

            CALL RANDOM_NUMBER(S)
            x(particle,var) = bound_min(var) + (bound_max(var)-
   &             bound_min(var))* S
            X(particle,var)=X(particle,var)*100
            X(particle,var)=NINT(X(particle,var))
            X(particle,var)=X(particle,var)/100

            pbest(particle,var) = x(particle,var)

            write(222,*) x(particle,var)
                 write(4,*) x(particle,var)
        velocity_p(particle,var) = vmax(var)
      end do

          do var = 3,m

            IF (particle==1) THEN
              WRITE(*,*)'ENTER THE NUMBER OF DAY IN IT:'
              READ(*,*) NO1DAY(var)
            ENDIF
            WRITE(2555,*)NO1DAY(var)

            DO i=1,IMX
              WRITE(2555,*)x(particle,var)
            ENDDO

      end do

          rewind(222)
          REWIND(2555)
      CALL CE_QUAL_W2
          rewind(2252)
          rewind(2555)

      read(333,*)iij(particle)
          write(888,*)iij(particle)
          kk=1                              !kk= number of controling point in optimizer
```

```
      jj1=1                               !jj1 = depth
      rewind(555)

      if (particle ==1) then
        iii=iij(particle)
   write(888,*)iii
endif
      if (particle ==p) then
        iiii=iij(particle)
endif

      if (particle>1) then
        iii=(iij(particle)-iij((particle-1)))
        write(888,*)iii
      endif

open (221133,file='check333.dat', status='unknown')

      do jk=1,iii
        read(555,'(F9.2,f10.2)')DEPTH1(jk),Temprature1(jk)
        if (jk>1) then
          if (Depth1(jk)<Depth1(jk-1)) then
               kj(kk)=jj1-1
               kk=kk+1
               jj1=1
          endif
        endif
        depth11(kk,jj1)=depth1(jk)
        temprature11(kk,jj1)=temprature1(jk)
        jj1=jj1+1
      enddo

      rewind(555)
read (666,'(F8.0,f8.2)')(depth2(j),Temprature2(j), j=1,a)
      rewind(666)
      jj2=1
      kk=1

      do jk=1,a
        if (jk>1) then
          if (Depth2(jk)<Depth2(jk-1)) then
              kk=kk+1
              jj2=1
          endif
        endif
```

```
              depth22(kk,jj2)=depth2(jk)
              temprature22(kk,jj2)=temprature2(jk)
          write (221133,'(F8.0 , F8.2)')depth22(kk,jj2),
     &                temprature22(kk,jj2)
              jj2=jj2+1
            enddo

            check1=1
            ij=1
        k=0
13          k=k+1
            lL=1

14          if ((k<b).and.(lL==kj(k))) then
          go to 13
            endif

15          check1=abs(depth11(k,lL)-depth22(k,ij))

            if (check1<=0.5) then
              objectivefun2(particle)=objectivefun2(particle)+
     &     abs((temprature11(k,lL)-temprature22(k,ij)))
              if ((k==b).and.(lL==kj(b))) then
                goto 16
              endif
              lL=lL+1
              ij=1
              go to 14
18          endif
            ij=ij+1
            if (((ij<=31)).and.(k<=b)) then
              go to 15
            endif
16          close(2252)

          end do
          do particle =1,p
            WRITE(114,*) objectivefun2(particle)
            funct(particle) = objectivefun2(particle)
      end do
      rewind(114)

          do particle=1,p
            read(222, *)(x(particle,var), var=1,m)
            rewind(222)
```

```
  write(113,'(<m>F8.2)')(x(particle,var), var=1,m)
    end do

    rewind(4)
    do particle=1,p
      read(4, *)(x(particle,var), var=1,m)
      if (particle.eq.1)then
      perv = objectivefun2(particle)
      do var=1,m
                      gbest(var) = x(particle,var)
      end do
                    num_particle = particle
   end if
       if(objectivefun2(particle).le.perv) then
         perv = objectivefun2(particle)
     do var=1,m
                gbest(var) = x(particle,var)
      end do
              num_particle = particle
       end if
   num_iter = 1
       num_iter1 = 1
end do

do particle=1,p
  do var=1,m
    write(3,*)'pbests=',particle,var,pbest(particle,var)
  end do
end do

write(3,*)'------------------'

    do var=1,m
      write(3,*)'gbests=',num_particle,var,gbest(var),num_iter
      write(1,*)'gbests and its obj=',num_particle,var,gbest(var),
&    num_iter,(objectivefun2(particle), particle=1,p)
    end do
write(3,*)'------------------'
    write(1,*)'------------------'

return
end subroutine initial
```

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      subroutine main()

      OPEN(222,FILE='VARS.DAT',STATUS='UNKNOWN')

      do particle = 1,p
        objectivefun2(particle)=0
            do var = 1,2

                   CALL RANDOM_NUMBER  (S)
              CALL RANDOM_NUMBER  (S1)

                   velocity(particle,var) = w(r)*velocity_p(particle,var)+
     &             c1*S* (pbest(particle,var)- x(particle,var)) + c2*S1*
     &        (gbest(var)- x(particle,var))

          if (velocity(particle,var).lt.vmin(var)) then
            velocity(particle,var) = vmin(var)
              end if

              if (velocity(particle,var).gt.vmax(var)) then
                velocity(particle,var) = vmax(var)
                   end if

                   velocity_p(particle,var) = velocity(particle,var)

              x(particle,var) = x(particle,var) + velocity(particle,var)

              if ((x(particle,var).lt.bound_min(var)).or.(x(particle,var).
     &             gt.bound_max(var))) then
                     CALL RANDOM_NUMBER(S)
                     x(particle,var) = bound_min(var) +
     &                    (bound_max(var)-bound_min(var))*S
                   end if

                   write(222,'(f8.2)') x(particle,var)
```

```
                write(4,*)x(particle,var),particle,r
           matr(particle,var) = x(particle,var)

     end do

     do i=1,NWB
           WRITE(2252,'(2F8.2)')(x(particle,var), var=1,2)
     enddo

     rewind(2252)

        do var=3,m

                CALL RANDOM_NUMBER  (S)
           CALL RANDOM_NUMBER  (S1)

       velocity(particle,var) = w(r)*velocity_p(particle,var)+ c1*
&                    S* (pbest(particle,var)- x(particle,var)) +
&               c2*S1*(gbest(var)- x(particle,var))

       if (velocity(particle,var).lt.vmin(var)) then
         velocity(particle,var) = vmin(var)
           end if

           if (velocity(particle,var).gt.vmax(var)) then
              velocity(particle,var) = vmax(var)
                end if

                velocity_p(particle,var) = velocity(particle,var)

           x(particle,var) = x(particle,var) + velocity(particle,var)
           X(particle,var)=X(particle,var)*100
           X(particle,var)=NINT(X(particle,var))
           X(particle,var)=X(particle,var)/100

           if ((x(particle,var).lt.bound_min(var)).or.(x(particle,var).
&                gt.bound_max(var))) then
                   CALL RANDOM_NUMBER(S)
                   x(particle,var) = bound_min(var) + (bound_max(var)-
&                          bound_min(var))*S
                end if

                write(222,'(f8.2)') x(particle,var)
                write(4,*) x(particle,var),particle,r
           matr(particle,var) = x(particle,var)
```

```
      enddo

      do var = 3,m
        WRITE(2555,*)NO1DAY(var)

        DO i=1,IMX
          WRITE(2555,*)x(particle,var)
        ENDDO
      end do

rewind(222)
      REWIND(2555)
CALL CE_QUAL_W2
      rewind(2252)
      rewind(2555)

read(333,*)iij(particle)
      write(888,*)iij(particle)
      kk=1                                    !kk= number of controling point in optimizer
      jj1=1                                   !jj1 = depth
      rewind(555)
      if (particle==p) then
        iiii=iij(particle)
      endif

      if (particle ==1) then
        iii=iij(particle)-iiii
   write(888,*)iii
endif

      if (particle>1) then
        iii=(iij(particle)-iij((particle-1)))
        write(888,*)iii
      endif

      do jk=1,iii
        read(555,'(F9.2,f10.2)')DEPTH1(jk),Temprature1(jk)
        if (jk>1) then
          if (Depth1(jk)<Depth1(jk-1)) then
            kj(kk)=jj1-1
                    kk=kk+1
                    jj1=1
          endif
        endif
        depth11(kk,jj1)=depth1(jk)
```

```
         temprature11(kk,jj1)=temprature1(jk)
         jj1=jj1+1
        enddo
        rewind(555)
     read (666,'(F8.0,f8.2)')(depth2(j),Temprature2(j), j=1,a)
        rewind(666)
        jj2=1
        kk=1

        do jk=1,a
          if (jk> 1) then
             if (Depth2(jk)<Depth2(jk-1)) then
                kk=kk+1
                 jj2=1
             endif
          endif
         depth22(kk,jj2)=depth2(jk)
         temprature22(kk,jj2)=temprature2(jk)
         jj2=jj2+1
        enddo

        check1=1
        ij=1
     k=0
133     k=k+1
        lL=1

144     if ((k<b).and.(lL==kj(k))) then
      go to 133
        endif

155     check1=abs(depth11(k,lL)-depth22(k,ij))

        if (check1<=0.5) then
          objectivefun2(particle)=objectivefun2(particle)+
   &            abs((temprature11(k,lL)-  temprature22(k,ij)))
          if ((k==b).and.(lL==kj(b))) then
            goto 188
          endif
          lL=lL+1
          ij=1
          go to 144
        endif
        ij=ij+1
        if (((ij<=31)).and.(k<=b)) then
```

```
          go to 155
         endif
188      close(2252)
         objectivefun(particle)= objectivefun2(particle)
       end do

       do particle =1,p
166      WRITE(114,*) objectivefun2(particle)
     Write (22222,*)objectivefun2(particle),particle,r
       end do

       rewind(114)

       do particle=1,p
         read(222, *)(x(particle,var), var=1,m)
         rewind(222)
     write(113,'(<m>F8.2)')(x(particle,var), var=1,m)
   end do
   close(222)

       do particle=1,p
         if(objectivefun2(particle).le.perv) then
           perv = objectivefun2(particle)
      do var=1,m
                      gbest(var) = matr(particle,var)
        end do
                      num_particle = particle
              num_iter = r
     end if

          do var =1,m
        if(objectivefun(particle).le.funct(particle)) then
               funct(particle) = objectivefun(particle)
               pbest(particle,var) = matr(particle,var)
               num_iter1=r
             end if
     end do

   enddo

   do particle=1,p
     do var=1,m
      write(3,*)'pbests=',particle,var,pbest(particle,var),num_iter1
      write(5,*)velocity(particle,var),particle,var,r
         end do
```

```
      end do

      write(3,*)'------------------'
      do var=1,m
         write(3,*)'gbests=',num_particle,var,gbest(var),num_iter
       write(1,*)'gbests and its obj=',num_particle,var,gbest(var),
     &    num_iter,(objectivefun2(particle), particle=1,p)
      end do
      write(3,*)'------------------'
        write(1,*)'------------------'

        return
      end subroutine main


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      end subroutine pso
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