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

by

Nasim Shojaei

A thesis submitted in partial fulfillment of the
requirements for the degree of

Master of Science
in
Civil and Environmental Engineering

Thesis Committee:
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Portland State University
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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). CEQUAL-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

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

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

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

8: end loop

Where:

- $\vec{U}(0, \varphi_i)$ represents a vector of random numbers uniformly distributed in $[0, \varphi_i]$ which is randomly generated at each iteration and for each particle.
- $\otimes$ is component-wise multiplication.
- In the original version of PSO, each component of $\vec{v}_i$ is kept within the range $[-V_{\max}, +V_{\max}]$ ”

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 $\vec{U}(0, \varphi_1) \otimes (\vec{p}_i - \vec{x}_i)$ and $\vec{U}(0, \varphi_2) \otimes (\vec{p}_g - \vec{x}_i)$. 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 $[-V_{\max}, +V_{\max}]$. 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 $V_{\max}$, and to eliminate it altogether. So updated equations were proposed:

$$\begin{aligned}\vec{v}_i &\leftarrow \omega \vec{v}_i + \vec{U}(0, \varphi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0, \varphi_2) \otimes (\vec{p}_g - \vec{x}_i), \\ \vec{x}_i &\leftarrow \vec{x}_i + \vec{v}_i\end{aligned}\tag{2}$$

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 $1 - \omega$ 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., $V_{\max}$) 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 $V_{\max}$ parameter. One of the simplest methods of incorporating of the constriction coefficient based on Clerc and Kennedy (2002) research is:

$$\begin{aligned}\vec{v}_i &\leftarrow \chi(\vec{v}_i + \vec{U}(0, \phi_1) \otimes (\vec{p}_i - \vec{x}_i) + \vec{U}(0, \phi_2) \otimes (\vec{p}_g - \vec{x}_i)), \\ \vec{x}_i &\leftarrow \vec{x}_i + \vec{v}_i\end{aligned}\tag{3}$$

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, $\phi_1 = \phi_2 = 4.1$, 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 $\omega \leftrightarrow \chi$ and $\phi_i \leftrightarrow \chi\phi_i$. So, the optimal settings suggested by Clerc correspond to $\omega = 0.7298$ and $\phi_1 = \phi_2 = 1.49618$ 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 $X_i = (x_{i1} \dots x_{iD})$, and the velocity of that particle is $V_i = (v_{i1} \dots v_{iD})$. The best position of the i -th particle reached in a previous cycle is $P_i = (p_{i1} \dots p_{iD})$, and the best particle in the whole swarm is $P_g = (p_{g1} \dots p_{gD})$. The velocity and the position of the particle i in the iteration of $n+1^{\text{th}}$ are governed by

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

$$X_i^{n+1} = X_i^n + V_i^{n+1} \quad (6)$$

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 chl a 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 NH_4DK [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 $(\text{SOD rate}) \cdot (\text{NH}_4\text{R})$ in units of $\text{g NH}_4\text{-N/m}^2/\text{day}$ or if divided by the layer height in m in units of $\text{g NH}_4\text{-N/m}^3/\text{day}$. 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 $\text{mg NH}_4\text{-N/m}^2/\text{day}$ 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 (NO_3S), 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/m²/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/m²/day for Beaver Lake, Arkansas. Auer et al. (1993) found rates in a hypereutrophic lake from 9-21 mg/m²/day (mean 13 mg/m²/day). Kim et al. (2004) found rates in the summer between 20-24 °C up to 16 mg/m²/day.

Spears et al. (2007) showed that for a large shallow lake recovering from high nutrient that the maximum P release was 12 mg/m²/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/m²/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 $1.0 \text{ gO}_2 \text{ m}^{-2} \text{ day}^{-1}$.

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 1st 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).

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

$F(w_z)$; 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 km² surface area, 5×10^9 m³ 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 Karkheh 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:

$$Q = \alpha_1 \Delta H^{\beta_1} \quad (8)$$

Where:

α_1 = empirical parameter = 10

β_1 = empirical parameter = 1.5

Δh = $Z_u - Z_{sp}$, m

Z_u = upstream head, m

Z_{sp} = the spillway crest elevation, m

And for submerged conditions:

$$Q = \alpha_2 \Delta H^{\beta_2} \quad (9)$$

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):

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

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), NH₄-N, NO₃-N, and PO₄-P concentrations in the Karkheh reservoir simultaneously. This satisfactory agreement can be expressed mathematically as:

$$\begin{aligned} \text{Minimize } F(\mathbf{X}) = & f_T' \times w_T + f_{DO}' \times w_{DO} + f_{Chl\ a}' \times w_{Chl\ a} \\ & + f_{PO_4}' \times w_{PO_4} + f_{NH_4}' \times w_{NH_4} + f_{NO_3}' \times w_{NO_3} \end{aligned} \quad (11)$$

$$w_T + w_{DO} + w_{Chl\ a} + w_{PO_4} + w_{NH_4} + w_{NO_3} = 1 \quad (12)$$

$$\text{Subject to } x_{low} < x < x_{up} \quad (13)$$

Where, $F(X)$ 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, $\mathbf{X}$, 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):

$$RMSE = f_k(X) = \sqrt{\frac{\sum_{i=1}^M (c_{ik} - c_{ik}^*)^2}{M}} \quad (14)$$

$$f_k(x)' = f_k(x) / \bar{c}_k \quad (15)$$

Where, $f_k(\mathbf{x})$ represents the fitness function for each alternative combination of calibration parameters of vector $\mathbf{X}$ for variable k ; c_{ik}^* is the i^{th} field measurement of variable k ($i = 1, \dots, M$); c_{ik} is the simulated value corresponding to c_{ik}^* ; $f_k(x)'$ is the normalized dimensionless error functions; $\bar{c}_k$ is the average measurement for K^{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 $\mu\text{g/L}$. 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 Chl a simulation with observed data before calibration

Figure 26 b. Comparing Chl 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.

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 (NH_4), nitrate plus nitrite (NO_3+NO_2), 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 CTITLE.....

Karkhe River
Water Quality Simulation
Default hydraulic coefficients
Default light absorption/extinction coefficients
Temperature simulation
Eutrophician study
The Data was provided by Ab-Niroo
Simulation 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	

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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
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WB 1 W2 IMP 1.00000 3 9.53500 0.43000 24.0000 10.0000 IMP

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KBSTR KBSTR

BR1 35 27

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BR1 POINT POINT

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DYNPIPE

PIPE UP PUPIC ETUPI EBUPI KTUPI KBUPI

PIPE DOWN PDPIC ETDPI EBDPI KTDPI KBDPI

SPILLWAY IUSP IDSP ESP A1SP B1SP A2SP B2SP WTHLC
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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
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PUMPS 2 PPUC ETPU EBPu KTPU KBPU

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LDOM ON
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DO	ON
TIC	ON
ALK	ON
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LDOM-N	OFF
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PO4POM	ON
PO4DOM	ON
PO4OM	ON
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NH4AP	ON
NH4ER	ON
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DSISET	OFF
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PSINET	OFF
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LRDOM	OFF
RDOMDK	OFF
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CBODDK	OFF
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DODOM	ON
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DONITR	ON
DOCBOD	ON
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TICEG	OFF
SEDDK	OFF
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SEDSET	ON
SODDK	ON

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PO4		-2.0000						
NH4		-2.0000						
NO3		-2.0000						
DSI		-2.0000						
PSI		-2.0000						
FE		-2.0000						
LDOM		0.10000						
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LPOM		0.10000						
RPOM		0.10000						
BOD1		0.10000						
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 ALG1 -2.0000
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 TIC 130.000
 ALK 130.000
 LDOM-P 0.00050
 RDOM-P 0.00050
 LPOM-P 0.00050
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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

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DSI	OFF
PSI	OFF
FE	OFF
LDOM	OFF
RDOM	OFF
LPOM	OFF
RPOM	OFF
BOD1	OFF

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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
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	0.00000					

MACRO EX	EXM	EXM	EXM	EXM	EXM	EXM
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CG 1	0.00000	0.00000	0.00000	0.00000

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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
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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 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 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 (2222, 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

!@@
@@

!@@
@@

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

```
subroutine inertia_weight()
```

```
    itermax = iterationmax      !this changing variables happend beacause if
    mathematical 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
```

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

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

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

```
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 controlling point in optimizer

```

```

jj1=1                                !jj1 = depth
rewind(555)

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

if (particle>1) then
    iii=(ij(particle)-ij((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
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

```

!@@
@@

!@@
@@

!@@
@@

```
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 controlling 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 (2222,*)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

```

```

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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