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Stepwise Automatic Calibration of Large-Scale Water Quality Model for Evaluation of Thermal Stratification and Eutrophication in Water Reservoir

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Abstract

This research addresses the essential need for assessing and managing water quality in reservoirs, which play a pivotal role in various socioeconomic aspects. To achieve this, a stepwise automatic calibration approach is proposed, specifically targeting the CE-QUAL-W2 model. This two-dimensional hydrodynamic and water quality model is widely employed in studies worldwide. Calibration, a fundamental aspect of model development, is complex and traditionally relies on manual, trial-and-error methods, which can be time-consuming and require substantial expertise. In this study, an alternative approach is introduced, incorporating the JAYA optimization algorithm, which reduces the complexity associated with fine-tuning optimization parameters. Furthermore, a clustering framework is adopted, grouping related variables for independent calibration. The research is conducted on the Dez reservoir in southwest Iran, using a two-step calibration process. The first step focuses on hydrodynamics, while the second step addresses water quality variables, including phosphate, ammonium, nitrate, and dissolved oxygen. The proposed methodology applied to Dez reservoir and tested against the observed data, where it demonstrates promising results.

Keywords: Automatic Calibration, JAYA optimization, Thermal Stratification, CE-QUAL-W2.

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1. Introduction

Reservoirs are complex systems that serve multiple purposes, including water supply, power generation, and flood control [1, 2]. However, the rapid growth of industry and population has resulted in the introduction of various pollutants to water bodies, leading to the degradation of more than 30% of the world's aquatic biodiversity [3]. Reservoirs are particularly vulnerable to contamination, as they receive wastewater discharges and river floods from upstream areas, making them potential sinks for pollutants. Moreover, climate change which affects the inflow to

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the reservoir, may exacerbate the water quality [4]. Therefore, it is crucial to evaluate the water quality and hydrodynamics of reservoirs, which tend to be more stable than rivers [5], to support socioeconomic development [6] and effective water resource management.

Over the past two decades, the integration of monitoring programs and water quality modeling has provided effective tools for managing water quality in impounding reservoirs [7]. Various models have been employed for simulating water quality in reservoirs, such as onedimensional models (e.g., WQRRS [8]), two-dimensional models (e.g., CE_QUAL-W2), and three-dimensional models (Water Quality Analysis Simulation Program (WASP) [9]). In this study, we employed a 2D (longitudinal-vertical) hydrodynamic and water quality model, which was previously known as LARM (laterally averaged reservoir model) and is currently referred to as CE-QUAL-W2 [10], which developed by the U.S. Army Corps of Engineers and has been widely used in studies across the globe [11].

In CE-QUAL-W2, like any mathematical simulation model, a fundamental and critical aspect of developing a reliable model that can consistently replicate natural processes involves appropriately its parameterization. Some of these parameters cannot be directly measured and are associated with collective phenomena and needs to be, therefore, calibrated. However, the process of calibrating the unknown parameters of the model is complex and not straightforward. Traditionally, calibration is done through a trial-and-error approach, where the parameters of the model are manually adjusted until the desired accuracy is achieved. The modelers select the most suitable parameters based on their expert knowledge, the goodness-of-fit measures associated with each parameter set, and subjective judgment [e.g., 12, 13]. Manual calibration offers the benefit of utilizing expert knowledge and comprehension of physical and biological processes, which is crucial for achieving a reasonable solution [14]. However, this method can be timeconsuming and may not always result in the optimal choices for the parameters. Additionally, it requires a significant amount of experience and expertise from the user.

An alternative method for parameter determination in numerical models is the use of automatic calibration techniques, which rely on advanced optimization algorithms to determine the optimal parameter values. Incorporating automatic optimization techniques can provide a means of simultaneously calibrating multiple model parameters while accounting for the interdependencies between them and their impact on the overall goodness-of-fit. Such methods can streamline the parameterization process, allowing for the identification of the most suitable parameter values and minimizing the time and effort required for calibration. Additionally, these methods can help improve model accuracy and reliability, leading to better predictions and more informed decision-making in various scientific fields.

The automatic calibration approach has been widely adopted in water quality modeling, facilitating the parameter determination of complex models and improving their predictive capabilities. Der Yang et al (2000) [15] created a nonlinear calibration model that utilized the least squares method to estimate the biological parameters of algae, aiming at minimize the average difference between the observed data, derived from satellite images, and the simulated data. In a calibration setting, the genetic algorithm (GA) was employed as a tool for parameter optimization in water quality models [16]. [17] linked the QUAL2E model with a GA to calibrate and verify the model's efficacy for different observation of river water quality data. In order to calibrate the hydrodynamic and water quality model CE-QUAL-W2, Ostfeld and Salomons (2005) [18] utilized a hybrid algorithm that combined the genetic algorithm (GA) and k-nearest neighbor approach. This approach achieved excellent results in less time than using only the GA. Afshar et al. [19] used a particle swarm optimization (PSO) algorithm to automatically calibrate the CE-QUAL-W2 model. In a similar vein, Afshar et al. (2013) [20]

proposed a multi-objective particle swarm optimization (MOPSO) model for automatic calibration of CEQUAL-W2 to predict physical, chemical, and biological behaviors of a water body. The authors concluded that the proposed approach may provide a wide version of all possible calibration solutions for better decision making to select the best solution from the Pareto front.

Recently, [21] introduced new automated calibration framework for three-dimensional lake hydrodynamic models, which reduces the calibration time and provides a more accessible option for a wide range of users. The framework has been tested on two different lakes, and the models showed a 50% reduction in mean absolute errors over the baseline. [22] described the use of the Sequential Uncertainty Fitting algorithm to automatically calibrate CE-QUAL-W2 model. The results showed that the developed method has high potential for matching the simulated temperature and water surface elevation with the measured data and that SUFI-2 algorithm had a better convergence rate compared to particle swarm optimization (PSO) algorithm. A new Repetitive parameterization and optimization (Rep-OPT) strategy was proposed by [23], which uses multiple optimization steps with expert knowledge to identify the right calibration parameters, resulting in excellent model fit. [24] investigated the use of Bayesian calibration to aid in the characterization of faulty model setups and calibration parameter combinations for complex hydrodynamic flow patterns in reservoirs and lakes. The study used a Gaussian process emulator to considerably speed up the calibration process and demonstrates that Bayesian calibration can describe the quality of calibration and correctness of model assumptions through geometric characteristics of posterior distributions.

Most of the previous studies have employed evolutionary optimization algorithms for the automatic calibration of hydrodynamic and water quality models. While these studies achieved positive outcomes, the utilization of such optimization algorithms can be troublesome due to the presence of fine-tuning parameters inherent in evolutionary algorithms. These algorithms involve multiple fine-tuning parameters, including population size, mutation rate, and crossover rate, which significantly impact their performance. Determining the optimal values for these parameters is challenging and requires considerable time and effort. It should be noted that no universally optimal parameter values exist for all optimization problems, as different problems may necessitate varying parameter settings. A common approach to address this issue involves a trial-and-error process, where the optimization algorithm is executed with different parameter configurations until the best-performing parameters are identified. However, this approach may not always yield the most favorable outcomes and is computationally demanding especially in automatic calibration water quality models in which large-scale simulation models are included. Furthermore, most of the prior studies employed a single-step automatic calibration approach where all variables within the model were determined through solving a single optimization problem. However, the simultaneous calibration of water surface elevation, hydrodynamic model, and water quality variables expands the search space of the optimization problem, posing challenges in finding an optimal solution. As an alternative, a clustering approach can be adopted, grouping highly related variables together, allowing for the determination of optimal parameter values for each cluster independently.

The purpose of this study is to overcome the shortcomings of existing approaches by developing and presenting an effective and trustworthy method for calibrating the widely used CE-QUAL-W2 water quality simulation model. This is accomplished by using the JAYA optimization algorithm, which does away with the requirement for fine-tuning optimization process parameters. A subset of variables is identified at each phase of the calibration process, thus narrowing the search space and cutting down on the number of iterations needed. The

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identification of the thermal modeling parameters is the first step in the calibration process. Next comes the identification of the water quality variables. The online integration of the simulation and optimization models facilitates transfer data between them.

2.1. Case Study

The Dez reservoir, situated in the Zagros Mountains of southwest Iran (between 31°35′51″– 34°7′46″ N and 48°9′15″–50°18′37″ E), was formed in 1963 by the construction of the Dez dam, towering at a height of 203 meters. Initially, the reservoir volume stood at approximately 3300 million cubic meters (MCM), but sedimentation has gradually reduced it to 2600 MCM over its 60-year operational period. The reservoir spans a length of 65 kilometers and operates within a water level range of 300 m to 352 m above sea level. Dez dam station records an average annual rainfall of 474 millimeters, with peak rainfall occurring in January and February and the lowest amounts in July and September. The reservoir primarily serves the purposes of drinking water supply, agricultural demand, and hydropower generation. Refer to Figure 1 for the geographical location of the Dez dam Basin along with the streams within the basin and measurement stations. Water quality variables such as temperature, total dissolved solids (TDS), phosphate concentration, ammonium concentration, and nitrate concentration were measured in-situ at these stations and various depths across different seasons throughout the year. Figure 1 shows the location of the dam and its reservoir.



Figure 1. Location of Dez dam in the region

2.2. Stepwise Automatic Calibration

This study introduces a methodological advancement in the calibration of the CE-QUAL-W2 model, employing a systematic stepwise approach. The proposed calibration strategy leverages a clustering framework, wherein closely interrelated variables are grouped together, and the optimal parameter values for each cluster are ascertained independently. In the initial phase, a selection of pertinent water quality variables is undertaken. This investigation seeks to model various variables, namely temperature, total dissolved solids (TDS), phosphate (PO₄), ammonium (NH₄), nitrate (NO₃), and dissolved oxygen (DO). Subsequently, these variables are partitioned into distinct clusters, with a specific emphasis on variables exhibiting physical interdependencies. In this particular study, we delineate two distinct clusters for analysis as



and

 $Z_2 = \{PO_4, NH_4, NO_3, DO\}$

The present challenge entails a two-step automatic calibration process. In the initial step, the calibration procedure focuses on variables within the set Z_1 , while in the subsequent step, the calibration is directed towards variables belonging to the set Z_2 .

Based on an extensive review of the literature, the foremost parameters exerting significant influence on the temperature and total dissolved solids (TDS) profiles of the reservoir were meticulously identified and subsequently designated as decision variables within the optimization framework. In the initial phase of the calibration process, the following parameters were considered for calibration: wind sheltering coefficient (WSC), evaporation coefficients (AFW, BFW, CFW), floor heat exchange coefficient (CBHE), substrate sedimentation temperature (TSED), extinction coefficient for pure water (EXH2O), extinction due to inorganic suspended solids (EXSS), extinction due to organic suspended solids (EXOM), and solar radiation absorbed at the water surface (BETA). These parameters represent the focal points of our calibration efforts in the first step.

In the subsequent step of the calibration process, the following parameters were identified as the decision variables for optimization: floor heat exchange coefficient (CBHE), evaporation coefficients (AFW, BFW, CFW), substrate sedimentation temperature (TSED), sediment release rate of phosphorus (PO4R), sediment release rate of ammonium (NH₄R), ammonium decay rate (NH₄DK), nitrate decay rate (NO₃DK), denitrification rate from sediments (NO₃S), fraction of first-order sediment concentration (FSEDK), and the fraction of the zero-order sediment oxygen demand (FSOD). These variables constitute the focal elements of the optimization problem in the subsequent calibration step.

The flowchart depicting the proposed stepwise automatic calibration process is presented in Figure 2. The simulation module within this algorithm employs the CE-QUAL-W2 model, while the optimization component leverages the JAYA optimization algorithm to fulfill its objectives.

3.1. Simulation Model

CE-QUAL-W2 is a sophisticated two-dimensional longitudinal/vertical hydrodynamic and water quality model developed by the United States Environmental Protection Agency (EPA). Its initial iteration, known as LARM, was first applied in 1975 to model a branchless reservoir. Over time, CE-QUAL-W2 has undergone multiple iterations, incorporating enhancements and corrections to accommodate a wide range of aquatic systems, including reservoirs, lakes, estuaries, and rivers.

This comprehensive model is proficient in simulating various facets of water bodies, encompassing hydrodynamics, temperature dynamics, and a multitude of water quality parameters. These water quality parameters include, but are not limited to, inorganic suspended solids, phytoplanktons, ammonia, phosphorus, nitrate, stable and unstable dissolved organic matter, and dissolved gases.

CE-QUAL-W2's core computational framework is grounded in a finite-difference approximation method applied to the equations governing fluid motion in laterally averaged form. These equations comprise the free surface wave equation, momentum equations in both the z and x directions, the equation governing continuity of component transfer, and the equation



of state. Consequently, the model offers the capability to compute critical variables such as free surface elevation, pressure, density, vertical and horizontal velocities, as well as concentrations of various constituents, as detailed in [10].

The model's robustness hinges on the integration of multiple data sources, including geometric data, meteorological data, boundary conditions, initial conditions, inlet and outlet flow information, hydraulic parameters, and calibration data which intended to be optimally determined in this study.

3.2. Jaya Optimization Algorithm

The Jaya optimization algorithm is a meta-heuristic technique, introduced by Rao [25], specifically designed for solving both constrained and unconstrained continuous optimization problems. Similar to other meta-heuristic approaches, the Jaya algorithm iteratively explores the problem space, commencing with a randomly initialized population, with the goal of locating the optimal solution. In this context, let F(x) represent the objective function of the problem, and the Jaya algorithm seeks to either minimize or maximize this function.

At each iteration 'i', the algorithm considers 'm' decision variables (j=1,2,3...m) and 'n' candidate solutions. The algorithm identifies the best value among all candidate solutions for the objective function F(x) as $X_{j \ best \ i}$, and the worst value as $X_{j \ worst \ i}$. If, during iteration 'i', candidate variable $X_{j \ k \ i}$ is chosen for decision variable 'j', the algorithm modifies and updates this decision variable using the following equation:

$$X_{i,k,i}^{new} = X_{j,k,i} + r_{1,j,i} \left(X_{j,best,i} - |X_{j,k,i}| \right) - r_{2,j,i} \left(X_{j,worst,i} - |X_{j,k,i}| \right)$$
(1)

Here, $X_{j,best, i}$ represents the value of variable 'j' for the best candidate, and $X_{j,worst,i}$ represents the value of variable 'j' for the worst candidate. $X_{i,k,i}^{new}$ signifies the updated value of $X_{j,k,i}$, and $r_{1,j,i}$ and $r_{2,j,i}$ are two random numbers for variable 'j' during iteration 'i', each within the range [0,1]. The term $r_{1,j,i}(X_{j,best,i} - |X_{j,k,i}|)$ indicates a tendency to move closer to the best solution, while the term $r_{2,j,i}(X_{j,worst,i} - |X_{j,k,i}|)$ indicates a tendency to avoid the worst solution. The updated value $X_{i,k,i}^{new}$ is accepted if it yields a superior solution. All accepted solutions are retained at the end of the iteration, and these values serve as inputs for the subsequent iteration.

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Figure 2. Flowchart of the proposed algorithm for stepwise automatic calibration

The objective function in this research is defined to assess the collective error, quantifying the fitness between the observed field data and the model-generated results for either temperature or water quality variables. To facilitate the aggregation of diverse errors originating from various variables within the formulation of the comprehensive error function, it is imperative to normalize these errors, ensuring they share uniform orders of magnitude. Mathematically, this objective function is expressed as follows:

$$OF = \left(\sum_{j=1}^{M} \sum_{t=1}^{T} \sum_{i=1}^{N} \left(\frac{C_{j,t,i}^{model} - C_{j,t,i}^{obs}}{C_j}\right)^2\right)$$
(2)

Where $C_{j,t,i}^{model}$ and $C_{j,t,i}^{obs}$ are the water quality variables obtained from the model and field data, respectively. Also, *i*, *t*, and *j* denote the number of observed data in a station, the period of measuring data and all water quality variables, respectively.



4. Results and Discussion

CE-QUAL-W2 was utilized for investigating of thermal stratification and water quality variation in Dez reservoir. The model was calibrated using the proposed stepwise automatic calibration method. Considering the water quality variables in this study, two steps were determined. In the first step, the hydrodynamic simulation of the reservoir was performed in which the temperature variation and TDS concertation profiles determined and their affecting parameters were calibrated. To this end, the total number of iterations in Jaya optimization algorithm was set to 200 with the population size of 6. The resulting parameter values following calibration are presented in Table 1, while Figure 3 illustrates the convergence curve of the optimization algorithm, depicting the progression of the calibration process.



Figure 3. convergence curve of JAYA optimization algorithm in the first step of automatic calibration.

Coefficient	FORTRAN name	Range	Calibrated value
Wind sheltering coefficient for each segment of first and last day of calibration	(WSC)	0.7-1	1
Coefficient of bottom heat exchange	(CBHE)	0.3-1	0.31
Sediment temperature	(TSED)	9-15	15
A coefficient in the wind speed formulation	(AFW)	8-15	11.15
B coefficient in the wind speed formulation	(BFW)	0.3-0.9	0.89
C coefficient in the wind speed formulation	(CFW)	1-3	1.85
Light extinction coefficient for pure water	(EXH_2O)	0.28-0.6	0.25
Extinction coefficient for inorganic solids	(EXINOR)	0.01-0.1	0.02
Extinction coefficient for organic solids	(EXORG)	0.01-0.9	0.4
Fraction of incident solar radiation absorbed at water surface	(BETA)	0.3-0.7	0.6

Table 1. calibrated values in the first step of automatic calibration.

Figure 4 displays the monthly vertical temperature variations in the Dez reservoir. The temperature profiles corresponding to fall, winter, spring, and summer are exemplified by the temperature variations in November, February, May, and August, respectively. The figure further contrasts the outcomes of the simulation model with the observed data, thereby substantiating the precision and efficacy of the proposed algorithm. Evidently, the graphical representation indicates the development of thermal stratification during the spring and summer seasons. This observation underscores the accuracy and validity of the model's representation of the Dez reservoir's thermal behavior.



Figure 5 provides a representation of the TDS (Total Dissolved Solids) variation in the reservoir over the course of the simulation year. Notably, the figure reveals a satisfactory correlation between the results generated by the simulation model and the data obtained from experimental measurements. This alignment between the model and experimental data indicates a favorable level of agreement and supports the credibility of the simulation model's representation of TDS dynamics within the reservoir.



Figure 4. Temperature profiles compared to simulation model in Dez reservoir



Figure 5. TDS profiles compared to simulation model in Dez reservoir

The second step of the automatic calibration process focuses on characterizing the variation of water quality variables, specifically PO_4 , NH_4 , NO_3 , and DO_4 . It's noteworthy that the population size employed in the JAYA optimization algorithm remains consistent with the previous step. However, for this phase, the maximum number of iterations was extended to 250 to facilitate more thorough optimization. The convergence curve of the optimization algorithm is graphically depicted in Figure 6, providing insight into the progression of the calibration process.

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Figure 6. Convergence curve of JAYA optimization algorithm in the second step of automatic calibration.

The simulation model results, depicting the variations in phosphate, ammonium, nitrate, and dissolved oxygen (DO) across different depths within the reservoir, are showcased in Figures 7 to 10, respectively. These figures also feature a side-by-side comparison with the observed data. As evident in the figures, the simulation model effectively aligns with the observed data for phosphate, ammonium, and nitrate. However, a slight variance is noticeable between the measured DO data and the values generated by the simulation model. This variance may be attributed to factors such as the precision of the DO measurement experiments or potential limitations within the simulation model.

It's important to note that while the proposed simulation-optimization process did converge to a solution, as evidenced by Figure 6, the model's inability to attain a more precise match with the observed DO data suggests that further refinements may be needed to enhance the model's accuracy in representing DO dynamics within the reservoir.



Figure 7. Phosphate profiles compared to simulation model in Dez reservoir

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Figure 8. Ammonium profiles compared to simulation model in Dez reservoir



Figure 9. Nitrate profiles compared to simulation model in Dez reservoir



Figure 10. DO profiles compared to simulation model in Dez reservoir

5. Conclusion

This study presents a systematic and effective approach to calibrating the CE-QUAL-W2 water quality model, offering a solution to challenges associated with traditional manual calibration methods. Leveraging the JAYA optimization algorithm and a clustering framework, the proposed stepwise calibration process significantly reduces the complexity and time required for parameter determination. In the case study of the Dez reservoir, the calibration process successfully reproduces temperature and total dissolved solids (TDS) profiles, demonstrating the model's capacity to represent thermal stratification. Additionally, the study aligns well with observed data for phosphate, ammonium, and nitrate, albeit a slight variance in dissolved oxygen (DO) representation. The stepwise automatic calibration approach not only improves the accuracy of water quality modeling but also minimizes the effort and expertise required for calibration. While it has demonstrated its potential, further refinements may enhance the model's accuracy in representing DO dynamics within the reservoir. This research contributes to the advancement of water quality modeling, aiding in the effective management of vital water resources.



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