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ORIGINAL PAPER

Genetic algorithms and neural networks for solving water quality model of the Egyptian research reactor

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Abstract. The second Egyptian research reactor ETRR-2 became critical on 27th November, 1997. The National Center of Nuclear Safety and Radiation Control (NCNSRC) has the responsibility for the evaluation and assessment of safety of this reactor. Modern managements of water distribution system (WDS) need water quality models that are able to accurately predict the dynamics of water quality variations within the distribution system environment. Before water quality models can be applied to solve system problems, they should be calibrated. The purpose of this paper is to present an approach which combines both macro and detailed models to optimize the water quality parameters. For an efficient search through the solution space, we use a multi-objective genetic algorithm which allows us to identify a set of Pareto optimal solutions providing the decision maker with a complete spectrum of optimal solutions with respect to the various targets. This new combinative algorithm uses the radial basis function (RBF) metamodeling as a surrogate to be optimized for the purpose of decreasing the times of time-consuming water quality simulation and can realize rapidly the calibration of pipe wall reaction coefficients of chlorine model of large-scaled WDS.

Key words: genetic algorithm • neural networks • model calibration • water distribution system • water quality model

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Introduction

Modern managements of WDS need water quality models that are able to accurately predict the dynamics of water quality variations within the distribution system environment. Such models would have possible applications in predicting water quality degradation problems, calibrating system hydraulics, designing water quality sampling programs, optimizing the disinfection process, evaluating the water quality aspects of distribution network and storage-reservoir improvement projects, and assessing alternative operational and control strategies for maintaining and improving water quality in distribution systems [12].

Water quality models need to be calibrated before they can be applied to solve system problems. Effective water quality model demands accuracy of hydraulic models and its accurate parameters. So, the calibration of hydraulic model is the basis of calibration of water quality model. Water distribution model calibration is typically accomplished by adjusting network parameters so that model results match field measurements. Reference [16] used artificial neural networks (ANN) to perform the hydraulic model calibration, which obtained pipe's roughness from pressures and flow rates.

In the past, Refs. [4, 11] used genetic algorithm (GA) to calibrate the parameters of hydraulic models. In Ref. [9], calibration of water network model can be

integrated with leakage distribution in the process of hydraulic calibration. Reference [6] considered the uncertainties in measurement and estimation and provides a measure of the quality of the calibration. Reference [14] made full use of information from tracer studies as well as information from pressure surveys, which would be helpful to calibration of both hydraulic and water quality model.

The literature presented above is only a part of calibration of hydraulic model. Though the underlying philosophy of water quality calibration is the same as that of hydraulic calibration, the water quality calibration will cost more computing time than calibration of hydraulic model, even reaching more than a hundred times. Recently, some programs to calibrate water distribution models have been available and have occasionally been used on real water systems, such as the Darwin Calibrator of Haestad Methods [11, 17] using a GA solver to optimize relative parameters, it is difficult, however, to apply on a large-scale or a medium-scale real system for long computation time. Therefore, we have to seek a new method to calibrate the parameters of water quality model.

This paper is organized as follows. Section 'Background' provides a brief background discussion of this topic preparing for subsequent sections. It is followed by a specified description of the new method in section 'Methodology'. In section 'Case study' a large-scale water distribution network applies this method to optimize the parameter of water quality model. The final section concludes this method and restates the key traps in the optimal process.

Background

Water quality model

Most water quality models make use of one-dimensional advective-reactive transport to predict the changes in constituent concentrations due to transport through a pipe. It can be written as follows [17]:

$$\frac{\partial c}{\partial t} + \nu \frac{\partial c}{\partial x} = R(c) \tag{1}$$

where: c is the concentration of a constituent; t is the time; ν is the flow velocity; x is the distance and R represents the constituent reaction relationship. Water quality model used in this paper is based upon a parcel tracking algorithm. It tracks the change in water quality of discrete parcels of water as they move along pipes and mixe together at junctions between the fixed-length time steps. In order to do this, there is a need to know the rate at which the substance reacts and how this rate might depend on substance concentration. Reactions can occur within both the bulk flow and with the material along the pipe wall.

Bulk flow reactions occur in the main flow stream of a pipe or in a storage tank, unaffected by any processes that might involve the pipe wall. A water quality model simulates these reactions using the n-th order kinetics, where the instantaneous rate of reaction (R in unit of mass/volume/time) is assumed to be concentration-dependent, given as [17]:

$$R(c) = K_b c^n \tag{2}$$

where K_b is a bulk rate coefficient; c is the reactant concentration (mass/volume) and n is the reaction order. K_b has units of concentration raised to the $(1-n)$ power divided by time. It is positive for growth reactions and negative for decay reactions. It also considers reactions where a limiting concentration exists on the ultimate growth or loss of the substance. In this case the rate expression for a growth reaction becomes [17]:

$$R(c) = K_b(c_L - c)c^{(n-1)} \tag{3}$$

where c_L is the limiting concentration. Thus, there are three parameters (K_b, c_L and n) that are used to characterize bulk reaction rates. Different values of these parameters lead to different kinetic models. Bottle test is recommended for determining the bulk reaction coefficient such as a chlorine decay factor. It provides a good baseline value and reference for constructing a water quality model [17].

In addition to bulk flow reactions, constituent reactions occur with material on or near the pipe wall. The rate of this reaction is dependent on the concentration in the bulk flow and pipe wall conditions, given as:

$$R(c) = \frac{A}{V} K_w c^n \tag{4}$$

where K_w is a wall reaction rate coefficient; A/V is the surface area per unit volume within a pipe. It converts the mass reacting per unit of wall area to a per unit volume basis. n is the wall reaction order taking a value of either 0 or 1, so that the unit of K_w is either mass/area/time or length/time. Both K_w and n are site specific and need to be calibrated for water distribution pipes.

Water quality model with combined bulk and wall decay gives better results than a single decay coefficient. Reliability of wall demand K_w estimation results in a very low model error [17]. Combined bulk and wall decay are adopted in this paper.

Metamodeling

Metamodeling research has been published since 1970, it has been a major research field during the last decade [3, 4]. The basic idea of metamodeling is to construct an approximate model using function values at some sampling points, which are typically determined using experimental design methods [10]. The main purpose of metamodeling is to reduce the cost, time, and amount of effort required during a simulation analysis. It is usually a supplementary model that can be alternatively used to interpret a more detailed model. The goals of metamodeling cover understanding, prediction, optimization, and verification and validation [15]. Metamodels are constructed in three stages, i.e. estimation, analysis and validation. Its process can involve both qualitative and quantitative factors [7].

The most popular metamodeling approach in simulation involves the use of parametric polynomial regression models in response surface methods [4], which is formulated as follows:

$$Y = \sum_{j=1}^{m} \sum_{k=1}^{q} \beta_{kj} p_k(X_j) \tag{5}$$

where Y is the output vector; X is the input vector; m is the dimension of input vector; p is the polynomial order. Metamodel can be classified into parametric and nonparametric techniques [6]. The most popular types of metamodels are polynomial regression models, splines, kriging and neural networks [15]. The metamodel might model only a local portion of the simulated system or may encompass the complete simulated system, a global metamodel. Trade between accuracy and computational expense and between local and global information must be considered when developing a simulation metamodel.

The use of metamodels as surrogates for WDS simulation models has been very rare to date. Roughness coefficients [16] were optimized using a GA linked to the ANN. This metamodeling example in WDS optimization ran approximately at twice the speed of the hydraulic simulation model, suggesting that the ANN metamodeling technique has potential for increasing the computational efficiency of WDS optimization. ANNs are used as a surrogate model to optimize the drinking water distribution [6]. The neural networks may be used to obtain precalibrations or guides for a manual calibration, but they are insufficient when used as unique calibration tools [16].

Radial basis functions

Neural networks have seen an explosion of interest over the last few years, and are being successfully applied across an extraordinary range of problem domains, in areas as diverse as finance, medicine, engineering, geology and physics. In particular, neural networks are non-linear. It also keeps in check the curse of dimensionality problem which bedevils attempts to model non-linear functions with large numbers of variables. Neural networks can accommodate a combination of continuous variables and discrete numeric variables. Additionally, most neural network paradigms are global models, so a single neural network could be developed to model the entire simulation response surface.

Radial basis functions (RBF) were originally developed by Hardy to fit irregular topographic contours of geographical data [7, 14]. Radial basis function networks have an input layer, a hidden layer of radial units and an output layer of linear units. The mathematically represented of the RBF metamodel as follows:

$$f(x) = \sum_{i=1}^{n} w_i \varphi(\| x - x_i \|) \tag{6}$$

where n is the number of sampling points; x is the vector of input variables; x_i is the center of basis function φ, $||\bullet||$ is any l_p norm (typically is Euclidean norm, this kind of norm is used in this study) and w_i is the unknown weighting coefficient. Therefore, an RBF is actually a linear combination of n basis functions with weighted coefficients.

RBF can be expressed as matrix format:

$$f = A\lambda \tag{7}$$

where: $f = [f(x_1), \ldots, f(x_m)]^T$, $A_{ij} = \varphi(||x_i - x_j||)$, $i = 1,2,\ldots,m$; $j = 1,2,\ldots,n$

The coefficient vector λ is obtained by solving Eq. (7). An RBF using the aforementioned highly non-linear functions does not work well for linear responses. To solve this problem, we can augment an RBF by including a polynomial function such that.

$$f(x) = \sum_{i=1}^{n} w_i \varphi(\| x - x_i \|) + \sum_{j=1}^{m} c_j p_j(x) \tag{8}$$

where m is a total number of terms in the polynomial, and c_j ($j = 1,2,\ldots,m$) is the corresponding coefficient.

The advantage of RBF is found to be the best for overall performance on accuracy, robustness, problem types, sample size, efficiency, and simplicity compared to response surface method (RSM), kriging method (KM) and multivariate adaptive regression splines (MARS), based on evaluations of the coefficient of multiple determination (R2), relative average absolute error (RAAE) and relative maximum absolute error (RMAE) [8].

One of the disadvantages of RBF is that it is more expensive than RSM, because it uses a series of computationally expensive functions for a single model; therefore, it is less efficient in performing function evaluations. This drawback becomes apparent when solving multi-objective design optimization problems in which millions sometimes even billions of solutions need to be found in order to develop the Pareto Frontier. Another disadvantage of using RBF is that model fitness cannot be checked using ANOVA, because by definition an RBF passes exactly through all the design points [10].

Methodology

Water quality modeling of WDS is a time-consuming task, which has to solve the hydraulic equation firstly, i.e. the equations of continuity and energy, for transient analysis, the equations of momentum are necessary. The water quality computing step is shorter than the hydraulic one and the number of computing times will be greater than the hydraulic one. Additionally, water quality analysis must take an extended-period simulation, or it will be no-good for long-distance pipelines as the constituent cannot reach the relative node. From our previous experiences, a medium-scale network with 6000 nodes and 6000 pipes will cost near one minute time to make a 24 h simulation (15 min/step, 96 steps in all; normal computer configuration: 512M/1.7G). Optimization algorithms may require a few hundred to several thousands of model simulations to converge at a unique set of parameters. For example, an optimization using GA with 30 populations and 100 generations needs 3000 min (50 h). Thus, water quality simulation in each iterative program of specified optimization belongs to costly functions that is computationally challenging.

Because of the enormous computational cost involved, the analyst is typically willing to perform only a small number of function evaluations when optimizing such costly functions. Our goal, then, is to develop

global optimization algorithms of the number of function evaluations. A more practical type of optimization method for a computationally expensive function is one that is based on a metamodel presented as before (also known as response surface model or surrogate model). The purpose of the metamodel is to serve as an inexpensive approximation to the costly evaluation function that can help identify promising points for costly function evaluation.

Reference [5] presented a new framework, CORS (Constrained Optimization using Response Surface), for solving costly evaluation function optimization. The CORS method is a flexible framework and can be used to different fields. But it should be adjusted and reinforced according to the characters of applied objects.

Based on the framework of CORS method and the characters of water quality model of WDS, a new combinational algorithm, CORS-RBF-GA, is designed by us which combines the CORS framework, RBF network and GA to calibrate the parameters of water quality model. The flow chart of CORS is the same as the left side of Fig. 1 (step 1–6), the RBF network is the water quality metamodel, GA is the optimizing method of metamodel. In addition, the algorithm of CORS-RBF-GA is also reinforced by using the generalization checking and cluster analysis. The algorithm of CORS-RBF-GA is presented as follows.

Step 1 is to select initial evaluated points. Set and select a finite initial set of points $S = \{x_1,x_2,\ldots,x_k\}$ which are prepared for water quality simulation and fit the RBF network. S is a vector if only one parameter is calibrated, and a matrix with m rows (number of calibrated parameters) and k columns (number of points) when more than one parameter are present. The method of selecting evaluated points includes factorial design (grid), Latin hypercube and orthogonal arrays. The most known technique is the factorial design which requires fitness function evaluations at K_N design points,

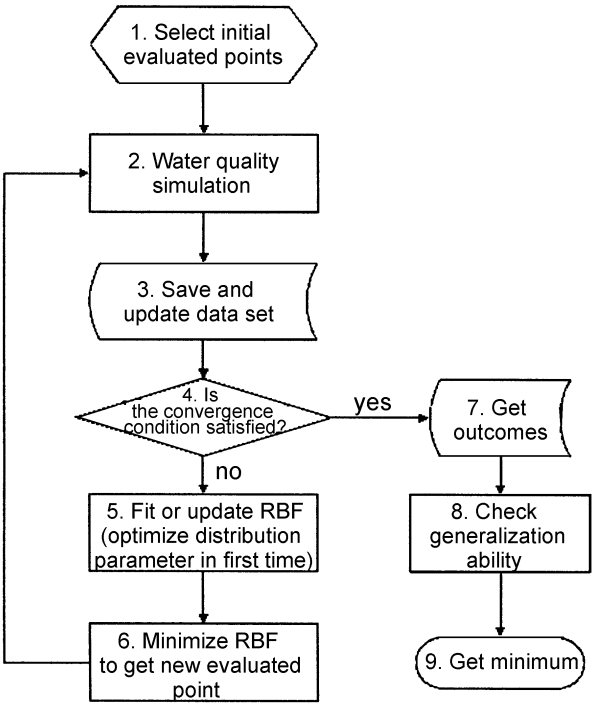

Fig. 1. Flow chart calibration of water quality of WDS.

where N is the number of design variables and K the number of levels defined between the lower and upper bounds of each variable. Usually, K is 2 or 3, depending on the effects we want to model [5]. After experimental comparison, we found that the number of experimental points should be beyond 100 for more than two parameters that should be calibrated.

Step 2 is to do water quality simulation. Data from water quality simulation can be used directly or changed to other forms, which typically are transformed into discrepancy between calculated data and measured data. These data will play a role as output of RBF network, while the evaluated points as input. Basis function employs the Gaussian function because MATLAB is based on this one. In this paper the predicted error, $f(x)$, is adopted to the output of RBF network and defined as follows in order to calibrated the parameters according to minimize the discrepancy. The data of boundary condition of WDS are manually treated firstly with the goal of focusing on this method singly.

$$f_1(x) = g_i(x) - m_1 \quad i = 1,\ldots,n \tag{9}$$

$$f(x) = \sum_{i=1}^{n} [\,|\, f_i(x) \,|\,] \tag{10}$$

where: $g_i(x)$ is the calculated value of number i monitoring node; m_i is the measured value of number i monitoring node; n is the total number of monitoring nodes. Note that the calculated values of monitoring nodes are zero in the early period of extended period simulation of WDS until the disinfectant pass through these nodes. So $f(x)$ must start to accumulate from the time that is above water age of every node.

Step 3 is to save evaluated points and the value of accumulated error. Evaluated points are saved into $S = \{x_1,x_2,\ldots,x_k\}$ and the values of error into $E = \{f(x_1),\ldots,f(x_k)\}$. When the following optimization produces new data, S adds one point after the last point and E adds the evaluated value with respect to the new added point. Note that to prevent oscillation in the RBF interpolation, the large error values should be replaced by the median of all available error function values [13].

Step 5 is to fit or update RBF. The RBF is an approximated metamodel as a surrogate of WDS, which is key part of the whole algorithm. Based on data set S and E, the former is input and the latter is output, new RBF network will be trained and updated in each iteration. For practical purposes, it should be intuitively clear that the rate of convergence is somehow dependent on how well the RBF model approximates the water quality model and also on how well we solve the optimization problem on the RBF network. In the first time, we should optimize the spread parameter of RBF which is so important that directly influences the degree of approximation. Quasi-Newton methods or GA [9] can be used to solve this optimization. After the optimized spread, a parameter has been found and a new RBF network should be trained again.

Step 6 can use the different optimization method, such as non-linear programing or GA, to find a minimized point in the surface of RBF function which will be the next evaluated point.

In a former research, we found that non-linear programing is easy to make a matrix close to singular or badly scaled, thus it will result in optimization terminated early. GA is recommended as a universal optimization method. Objective function and constraint conditions are presented as follows.

$$\text{Minimize } f(x) \tag{11}$$

Subject to:

$$\|x - x_j\| \geq \beta\Delta \quad j = 1,\ldots,k+i-1, \quad x_j \in S \quad 0 \leq \beta \leq 1 \tag{12}$$

$$0.5 \leq \frac{x(i)}{x(k)} \leq 1.5 \quad i,k = 1,\ldots,m \tag{13}$$

where $\Delta_i = \max \min \|x - x_j\|$, $\bar{x}$ is the cover points defined beforehand which covers the whole hypercube domain.

Function f is the RBF. $x(i)$ and $x(k)$ are the elements of the vector of x, m is the dimension of x. The purpose of the constraint is to drive the algorithm towards unexplored regions and prevent the algorithm from prematurely converging to some possibly undesirable points. To be able to perform both local and global search in this scheme, we use β to control the distance range from high values for global search to low values for local search. Detailed proved process can be referred to in [8]. Inequality constraints (13) restrict the grouping parameters (wall reaction coefficients), assuming that there are no great discrepancies among the parameters.

Steps 4 and 7 are identification of convergence condition and obtainment of optimized values via optimization of RBF metamodel. According to the following case study, we found that many combinations of wall reaction parameters can have a near the same influence on predictions of monitoring points in WDS. So, we have to select the point as the final result that has the best generalization ability among the options.

Step 8 utilizing the data from step 8 compares the generalization ability of given new evaluated points from RBF optimization, which computes individually the total predicted error of a given period of water quality behaviors. Step 9 is the end of methodology.

This method is realized in MATLAB programing language, and RBF network and GA call functions of corresponding toolbox. Water quality modeling is operated using EPANET programer's toolkit, the EPANET2.dll is incorporated into the main program.

Case study

The forced convection core cooling (FCCC) system will be responsible for removing heat produced by fuel elements, as well as other elements inside the core, while the reactor is in operation at powers greater than 500 kW. (In fact operation with natural convection cooling at powers as high as 800 kW is allowable from a thermohydraulic point of view, but considerations on the doses at pool surface limit the power to 500 kW, [1]).

The forced convection cooling will be achieved as a result of operation which makes up the primary cooling system. The pumps have an inertia flywheel which, should they come out of service, will permit maintaining for a certain period of time the required flow to dissipate core decay heat produced immediately after a reactor shutdown, and until such a time as natural convection core cooling will prove to be sufficient (NCCC).

The primary system, whose diagram is shown in Fig. 2, consists of a closed circuit through which the coolant is made to circulate driven by two centrifugal pumps (B), making it pass through the core in an upward flow and then through heat exchangers (H) where heat generated in the core is eventually transferred to the secondary system.

At the outlet of the chimney, the primary circuit branches off in two non-redundant trains at 50% each with similar characteristics. Each train has been provided with two identical pumps in parallel (one in stand by), plus a heat exchanger. Both trains return separately to the reactor pool and their piping will descend to the base of the core in order to inject coolant from below. In this manner, both natural convection as well as forced convection share the same upwards direction, thus avoiding flow inversion phenomena.

Since the upper part of the chimney is open in order to allow access to the core and coolant circulation by natural convection when the reactor is shutdown or operating at very low powers, a small water flow will be forced to descend through the chimney in order to diminishing the possible arrival of activated water from the core to pool water level. Due to this reason, at the heat exchangers outlet, a small flow from the primary will be diverted to the reactor pool cooling system (RPCS), through the interconnection system, and will then return to the reactor pool having first passed through a decay tank. This transfer from one circuit to another will enable to compensate the water taken from the pool through the chimney (see Fig. 2).

To enhance the accuracy of calibration, in this case we use a cluster analysis method, a hierarchical cluster analysis, to divide the whole pipes into six groups. Hierarchical cluster analysis attempts to identify relatively homogeneous groups of wall reaction coefficient are based on selected characteristics, which include pipe diameters, pipe materials, construction time, flow rates, flow velocity, location.

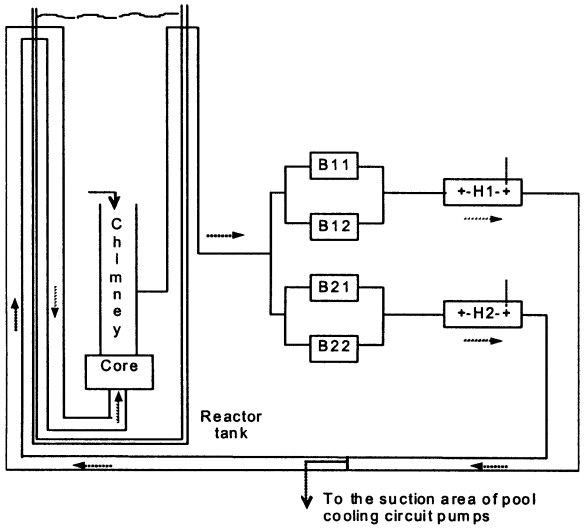

Fig. 2. Primary cooling system.

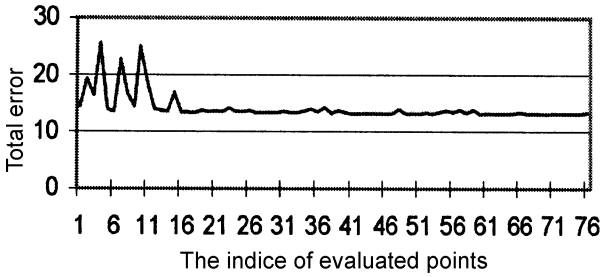

Fig. 3. The process of optimization via RBF approximation--optimization process.

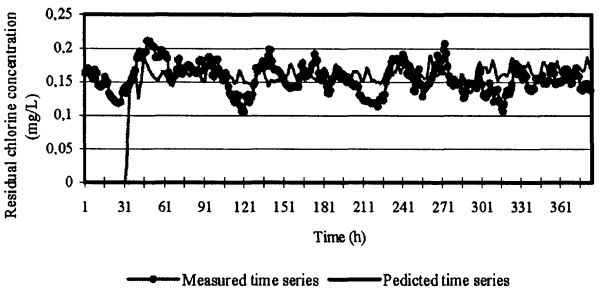

Fig. 4. One of the comparisons of predicted values and measured values.

Table 1. Computational comparison of times

Methods	Sampling data (h : min)	Training optimization (h : min)	Generalization checking	Total
GA		100 : 00		100 : 00
RBF	6 : 24	2 : 35	1 : 30	10 : 30

The initial evaluated points are obtained using a simple grid method. Using this method, the results presented in the paper can be obtained soon [2]. We select 100 data to train the RBF network and 28 data to optimize the spread parameter of RBF network. The following process shows the real optimization process in Fig. 3 that surges in the early stage and smoothes or coverage to the minimum in the latter. The RBF network stability is shorter because of the contribution of the spread parameter optimization. In the early stage the line surges a short time, then becomes gently inclined. But there are two unwilling juts in the range from no. 22 to 28. It testifies that some margin inputs, for example [–0.5, –6.0, –6.0, –3.5, –4.2, –6.0], will bring more total error because short age of initial fitting points cannot fit the RBF surface more accurate in margin region, while these can do well in the middle of network.

One of the comparisons of predicted values and measured values is shown in Fig. 4. From the figure you can find the predicted line is smoother than the measured one, there is a big difference in the early time of every day from 1 to 9 o'clock. According to simply research, we find that the possible reason is the influence of flow velocity the same as other research findings [8]. Another possible reason may be that the pipe water is still in the leading out thin branch pipe at the water quality monitoring station, which will be no refilling chlorine into this pipe at this period. While the simulation concentration is upstream pipeline relative to this monitoring location in WDS, this difference of position contribute to the simulating error. In order to solve this problem the deeper research should be executed in the future. Comparison of the computational times is listed in Table 1, which compares EPANET linked to GA and the new method presented in this paper. The total computing time of RBF metamodeling is only 10.3% of the one of EPANET linked to GA which is adopted normally. Every water quality simulation needs 3 min, and the sampling data are produced after water quality simulations based on every initial evaluated point. Thus, the sampling computing time should be 128 × 3 min, namely 6 h and 24 min. Optimization time of the former method is calculated by assuming GA parameters adopted normal values, 100 generations and 20 populations. Generalization ability checking is carried out during a 12 d long simulation and finds an optimal value in the end.

Conclusion

In this paper we performed a multi-objective optimization by means of genetic algorithms. The genetic algorithm adopted considers a population of chromosomes, each one encoding a different solution to the optimization problem. For a given solution, there are more than one objective to be evaluated, so that the performance of any given candidate solution is evaluated introducing the concepts of Pareto optimality and dominance. The proposed multi-objective genetic algorithm approach has been applied for determining the optimal test intervals of the components of a safety system in a nuclear research reactor. The optimization performed with respect to availability, economic and workers' safety objectives has shown potentials of the approach and the benefits which can derive from a more informative multi-objective framework.

This paper presents a new method, using RBF metamodeling as a surrogate to be optimized for the purpose of decreasing the times of time-consuming water quality simulation. The algorithm succeeds in calibrating the parameters of water quality model more efficiently than EPANET linked to GA. In order to assure the quality of optimization and avoid traps, key points should be restated and obeyed:

1. The sampling data should be adequate, in general, above 100.
2. The spread parameter should be optimized; this will enhance the fitting level.
3. The constraints between two parameters should add to the constraint conditions of main optimization.
4. Generalization ability checking can decrease the influence of local target value, namely measured value.

Although the new method can solve the problem of computational time, there also are some works to be researched more deeply in the future, such as considering data uncertainty the same as former hydraulic

calibration in the water quality calibration and quantification of other influence factors to bulk and wall reaction coefficients.

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