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Groundwater Model Approximation with Artificial Neural Network for Selecting Optimum Pumping Strategy for Plume Removal

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Abstract: Cleanup of contaminated aquifers by pumping and injection is one of the commonly used approaches for the remediation of groundwater contamination. Contaminant transport travel time in groundwater can be calculated using a method called 'particle-tracking' based on advection. The travel time of the contaminants is a highly non-linear and nonconvex function of pumping/injection rates and well locations. Global optimization (GO) techniques are therefore appropriate for finding an optimum pumping strategy. However, a pronounced disadvantage of these techniques is that they require running simulation models – in this case groundwater flow and particle tracking models - quite many times taking very long time to find an optimal solution. On the other hand, Artificial Neural Networks (ANN) are nowadays one of the widely used modelling techniques which can approximate a non-linear relationship between input and output data sets without considering physical processes and the corresponding equations of the system. As a result, an ANN model is much faster than a physically based model which it approximates. In this study, ANNs were trained to approximate the groundwater models MODFLOW and MODPATH using the data generated by these models. The resulting ANN models were then coupled with a GO tool, GLOBE, to find optimal pumping strategies. The experiments were carried out using different number of pumping wells and different GO algorithms.

1. Introduction

Management and cleanup of contaminated aquifers requires a long term strategy and huge amount of investments. The widespread occurrence of subsurface contamination problems has resulted in the development of various techniques for its remediation. The pump-and-treat method is one of the most commonly used methods for both large- and small-scale groundwater containment and cleanup. This method involves installing and operating a set of extraction/injection wells so that the contaminated groundwater is hydraulically contained and can be pumped out for subsequent treatment (Wang and Zheng[23]). During the last decade, the combination of optimization and simulation approach has been used extensively for the optimal design of pump-and-treat systems. In this approach the simulation is carried out with usual types of available groundwater models for flow and transport and the optimization is based on the standard linear programming and non-linear optimization tools. Some examples of the application of this approach are Bogacki and

Daniels[2]; Greenwald and Gorelick[7]; Chang et al.[3]; Gorelick et al.[6]; Willis and Yeh[24]. Several researchers also used randomized search techniques for optimization. For example, Wang and Zheng[23] used genetic algorithms (GA); Karatzas and Pinder[9, 10] presented an outer approximation method; Aral and Guan[1] used a differential GA and El Harrouni et al.[5] used GA and a dual reciprocity boundary element method.
Contaminant transport travel time in groundwater can be calculated using a method called ‘particle-tracking’ based on advection (Greenwald and Gorelick[7]; Jonoski et al.[8]). The travel time of the contaminants is a highly non-linear and nonconvex function of pumping/injection rates and well locations. Studies of Maskey et al.[11, 12] show the successful use of Global optimization (GO) techniques for finding an optimum pumping strategy. However, a pronounced disadvantage of these techniques is that they require running simulation models – in this case groundwater flow and particle tracking models - quite many times taking very long time to find an optimal solution. In order to reduce the computational time, different techniques can be applied including the hybrid use of artificial neural networks (ANNs) and GO algorithms (GOAs) (see Solomatine and Avila Torres[21]; Dibike et al.[4]). Some examples of the hybrid use of ANNs and GOAs were reported by Rogers et al.[18] and Rao and Jamieson[17]. The former used ANNs to predict selected outcomes of a groundwater contaminant transport model. Then, a GA was applied to search through possible alternatives evaluating the effectiveness of each alternative with predictions generated by the ANNs. Similarly, the latter made use of an ANN in association with a groundwater simulation model to determine the performance of different combinations of abstraction/injection wells, and thereafter, a GA to identify the least-cost solution offered by these combinations. Morshed and Kaluarachchi[14] also used ANN and GA, but in their work a GA and a back propagation algorithm were used to train two separate ANNs. In all these works, instead of particle tracking, concentration of the plume was used to estimate the state of the contamination.
This paper describes the approximation of groundwater flow and particle tracking models with ANNs for the optimal selection of pumping strategy for groundwater plume removal. The ANN, a widely used modelling technique, can approximate a non-linear relationship between input and output data sets without considering physical processes and corresponding equations of the system. As a result, an ANN model is much faster than a physically based model which it approximates. In this study, ANNs were trained for different pumping scenarios using the data generated by groundwater models MODFLOW and MODPATH, developed by USGS. The resulting ANN model was then coupled with a GO tool, GLOBE, to find an optimal pumping strategy. The experiments were carried out using different number of pumping wells and different GO algorithms. The results from the ANN models were compared with the results from the physically based models (MODFLOW and MODPATH).

2. Groundwater flow and particle tracking models

In the plume removal by pumping/injection system, pumping rates and well locations are major decision variables. For a given set of decision variables a flow model updates the hydraulic head (a state variable) and a particle-tracking model computes the particle travel time and path lines. The equation describing the three-dimensional movement of groundwater assuming constant density is expressed as:

$$\frac{\partial}{\partial x}(K_{xx}\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}(K_{yy}\frac{\partial h}{\partial y})+\frac{\partial}{\partial z}(K_{zz}\frac{\partial h}{\partial z})+q_s = S_s\frac{\partial h}{\partial t} \qquad (1)$$

where: K_{xx}, K_{yy} and K_{zz} are the principle components of the hydraulic conductivity along x, y and z coordinate axes; h is the hydraulic head; q_s is the source/sink term; S_s is the specific storage; and t is time.

The total cleanup time of a contaminant plume by pumping can be viewed as a function of the transport of particles defined at the plume boundary. When all particles have reached a pumping well, the plume is said to be removed. Hence, the travel time of the slowest particle is assumed to be the total cleanup time. Considering the transport by advection only, the time it takes for a particle to flow to a pumping well is given by the integral along the particle flow path ***S(q)*** as follows (Greenwald and Gorelick[7]):

$$t(q)=\int_s \frac{1}{v(q)}ds \qquad (2)$$

where: q = vector of pumping and injection rates; $t(q)$ = travel time of the particle; $v(q)$ = velocity in the direction of flow; ds = incremental distance in the direction of flow; and $S(q)$ = length of particle flow path. The non-linearity of this function (travel time and pumping rates) is mainly due to the facts that (1) the integration is to be evaluated over the flow path ***S(q)*** which is a function of pumping rates, and (2) the velocity over each incremental distance is a function of pumping rates, and velocity appears in the denominator of the integral.

In this study, the groundwater simulation codes MODFLOW (McDonald and Harbaugh[13]) and MODPATH (Pollock[16]), developed by U. S. Geological Survey, for flow and particle-tracking respectively have been used.

3. GOAs and optimization problem formulation

3.1 Global optimization algorithms

Global optimization is aimed at finding the best solution of constrained optimization problems which (may) have various local optima. A GO problem (GOP) with box constraints has been posed in Solomatine[19] as follows:

Find an optimizer x^* such that

$$f^* = f(x^*) = \min_{x\in X} f(x) \qquad (3)$$

where the objective function ***f (x)*** is defined in the finite interval (box) region of the n-dimensional Euclidean space as:

$$X = \{x \in \Re^n : a \le x \le b \qquad (componentwise)\} \qquad (4)$$

This constrained optimization problem can be transformed to an unconstrained optimization problem by introducing a penalty function with a high value outside the specified constraints. In cases when the exact value of an optimizer cannot be found, we speak about its estimate and, correspondingly, about its minimum estimate.
There are various algorithms oriented towards the search of global minima in GOPs (see Pinter[15]; Torn and Zilinskas[22]). In this study, a GO tool GLOBE developed at IHE, Delft has been used for optimization. The GLOBE now incorporates nine different algorithms. Three of them, namely GA, adaptive cluster covering (ACCO) and Controlled random search (CRS4) have been used in this study. Solomatine [19, 20] discussed all the GOAs used in the GLOBE system in detail.

3.2 Optimization problem formulation

Two separate optimization problems are formulated: (1) minimization of cleanup cost (establishment cost and operation plus maintenance cost of pumping and wells), and (2) minimization of cleanup time. In both cases the pumping rates and the well locations are decision variables. The upper and lower limits in pumping rates and the specified area for well locations are considered as constraints. In addition, in the case of cost minimization the limitation in cleanup time is also introduced as a constraint.

3.2.1 Optimization of cleanup time

If the aquifer cleanup time is to be minimized the objective function and the constraints can in general be defined as (Maskey et al.[11, 12]):

minimize: $$t = f(q_1, q_2, ...q_n, c_1, r_1, c_2, r_2, ...c_n, r_n) \tag{5}$$

subject to: q_{min} £ $(q_1, q_2, ...q_n)$£ q_{max}
c_{min} £ $(c_1, c_2, ... c_n)$ £ c_{max}
r_{min} £ $(r_1, r_2, ... r_n)$ £ r_{max}

where $\boldsymbol{t}$ = cleanup time; $\boldsymbol{q_1, q_2, ...q_n}$ = pumping rates in wells ***1, 2,...n***; $\boldsymbol{c_1, c_2, ...c_n}$ = column number (on grid) of wells ***1, 2, ... n***; $\boldsymbol{r_1, r_2, ... r_n}$ = row number (on grid) of wells ***1, 2, ... n***; $\boldsymbol{q_{min}, q_{max}}$ = minimum and maximum ranges in pumping rates; $\boldsymbol{c_{min}}$, $\boldsymbol{c_{max}}$ = ranges in column number for well locations; and $\boldsymbol{r_{min}}$, $\boldsymbol{r_{max}}$ = ranges in row number for well locations. In the experiments presented in this paper, only the pumping rates have been taken as decision variables keeping the positions of the wells fixed.

3.2.2 Optimization of cleanup cost

The well installment cost (capital cost) and the operation and maintenance cost per year (annual cost) can be expressed as a function of total pumping rates as:

$$\text{Capital cost} = C_1 \sum_{i=1}^{n} q_i^m \tag{6}$$

$$\text{Operation and maintenance cost per year} = C_2 Q^r \tag{7}$$

The constants $\boldsymbol{C_1}$ and $\boldsymbol{C_2}$ depend on the unit rates (per unit pumping rate) of capital cost and annual cost respectively. The coefficients $\boldsymbol{m}$ and $\boldsymbol{r}$ are generally less than unity and they account for the rate of change (generally decrease) in per unit capital and annual costs respectively with respect to the increase in total pumping rate. The $\boldsymbol{Q}$ is the total pumping rate of all wells and $\boldsymbol{q_i}$ are the pumping rates of individual wells with $\boldsymbol{n}$ being the number of wells. Thus, for the optimization of the total cost of well installment and pumping the objective function can be expressed as a function of pumping rates. Expressing the total cost in present worth the objective function and the constraints are defined as:

$$\text{minimize} \qquad C_1 \sum_{i=1}^{n} q_i^m + C_2 \sum_{k=1}^{t} \frac{C_3 Q^r}{(1+D)^k} \tag{8}$$

subject to $\quad t$ £ t_{max}

The constraints in pumping rates and position arrays apply similarly as in the optimization of cleanup time. In the above equation: $\boldsymbol{t}$ is the cleanup time in years, $\boldsymbol{D}$ is the discount rate (discounted from $\boldsymbol{k^{th}}$ year) and $\boldsymbol{C_3}$ is the coefficient that takes the value unity if $\boldsymbol{k}$ is a whole number and has the value of the fraction part of the $\boldsymbol{k}$ otherwise. The $\boldsymbol{t_{max}}$ is the maximum limit in cleanup time. If the resulting cleanup time is greater than the maximum limit the model generates a high value of the cost outside the constraint limit (a penalty) as an objective function value.

4 Neural network approximation of groundwater models

After enjoying much success in other areas of application, such as in the fields of pattern recognition and robotics, ANNs are now being applied more and more to problems of the aquatic environment (Dibike et al.[4], Solomatine and Avila Torres[21]). This wide range of applications follows from the property of ANN that it is possible to obtain a (very fast) prediction of system response without attempting to reach an understanding of, or to provide an insight into, the nature of the phenomena that are being modelled.

Multi–layer feed-forward networks (also known as multilayer perceptrons or MLPs) constitute one of the most widely used classes of ANNs. Each such ANN consists of an input layer, an output layer and one or more intermediate, 'hidden' layers as shown in

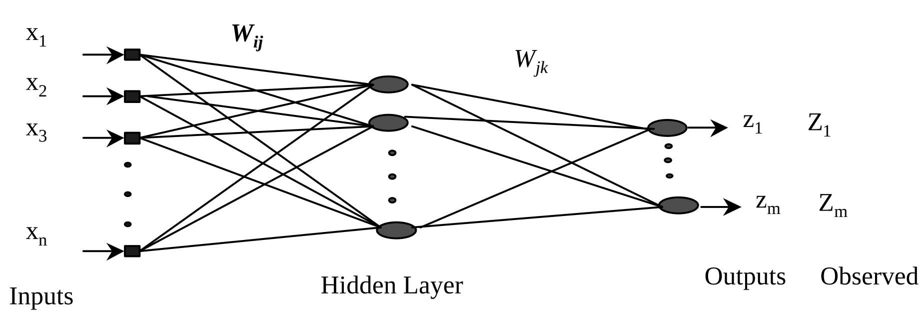
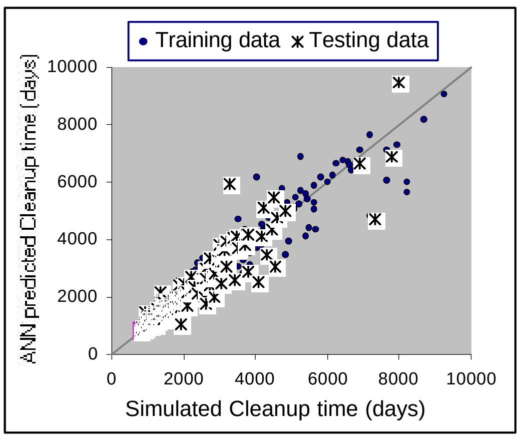


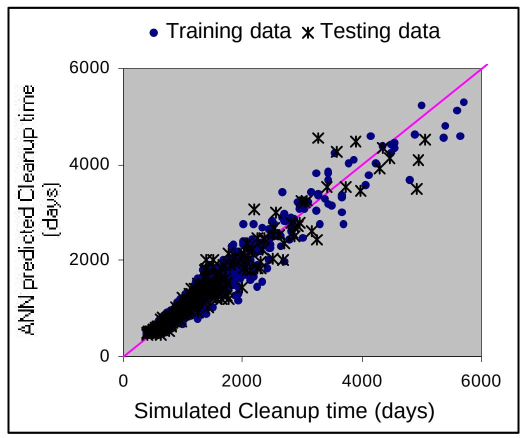
Figure 1: Multi-layer feed-forward network with one hidden layer.

Figure 1. Each unit in the hidden layer and the output layer has a (usually non-linear) transfer function such as sigmoid, tan-hyperbolic, etc. The most common learning rule for multilayer perceptrons is called the “back propagation rule”. In order to learn successfully, the output of the net should approach the desired output during training. This is achieved by adjusting the weights on the links between the units, and the generalized delta rule does this by calculating the value of the error function for a particular input, and then back-propagating the error from one layer to the previous one. Each unit in the net has its weight adjusted so that it reduces the value of an error function. These steps are repeated for each input pattern in the training set; in this way the error function is reduced and the network learns.

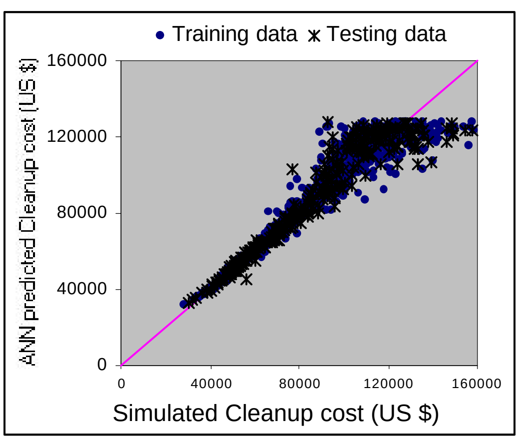
In this study, ANN is required to approximate the groundwater models MODFLOW and MODPATH for prediction of cleanup time (or cleanup cost). To do this, the network is



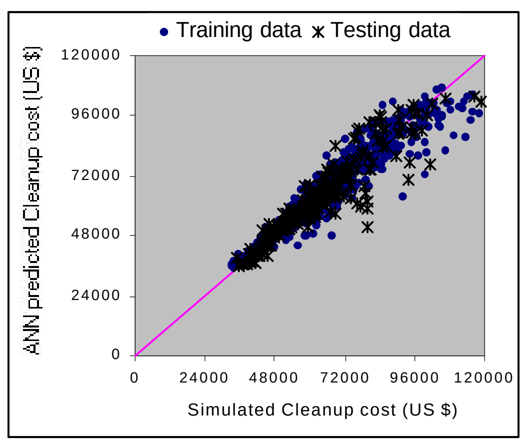
(a) Cleanup time, 2 pumps



(b) Cleanup time, 3 pumps



(c) Cleanup cost, 2 pumps



(d) Cleanup cost, 3 pumps

Figures 2(a-d): Scatter plots of network training and validation for different cases.

first trained with data generated by these models when applied to a hypothetical contaminated unconfined aquifer system. The inputs to the network consist of the pumping rates of a number of wells and the output is the corresponding cleanup time or cleanup cost calculated by the models. Four different cases with different output (time or cost) and different number of wells were considered. In each of these cases, relatively large number of data covering reasonable range of pumping rates is used to train and validate the networks. The scattered plots on Figs. 2(a-d) illustrate the networks training and validation performances for the different cases considered. The validation result shows that the trained ANNs predicted the model output (both cleanup time and cleanup cost) to a reasonable accuracy. It is important to note that the accuracy is higher especially in the lower range of these values where the accurate approximation of the models is critical for the next optimisation step. The mean absolute errors corresponding to the smallest 50 % of the prediction values during training and validation of the ANNs are shown in Table 1. Once the training is satisfactory, the resulting ANNs are converted in to executable codes and each NN model is then coupled with the GO tool (GLOBE) replacing the physically based model (MODFLOW and MODPATH) to find an optimal pumping strategy to minimise cleanup time or cleanup cost.

Table 1: ANN performance on the training and validation data

	Cleanup time (days) 2 pumping wells	Cleanup time (days) 3 pumping wells	Cleanup cost (US $) 2 pumping wells	Cleanup cost (US $) 3 pumping wells
Training MAE	104	46	1977	1940
Validation MAE	122	43	2164	1919
Correlation coeff.	0.965	0.977	0.956	0.957

5 Optimization and comparison of results

5.1 Coupling of simulation models with GLOBE

Using the GLOBE system as an optimiser requires coupling it with the simulation model so that they execute as a single application without the necessity of interactive input during computation. When MODFLOW and MODPATH (physically based models) are used as simulation models, two sets of executable programs are needed to couple them with GLOBE. The first program converts the GLOBE output file (searched values of parameters) as an input file to MODFLOW. The second program is required to read the output form MODPATH and to compute the objective function value to feed to GLOBE. Whereas, when the physically based models are replaced by an ANN model, the additional executable programs are not required. In fact, the ANN model is built in such a way that it takes input directly from the GLOBE output file and generates output in the format acceptable to GLOBE as input. In both cases, the coupled model starts from GLOBE and runs in a loop until the selected algorithms generate an acceptable solution and a stopping criterion is met.

5.2 Optimization of cleanup time

Using the coupled model as described in Sec. 5.1, the optimization of cleanup time was carried out using both physically based model and ANN model using three different GOAs. The comparison of results for 3 pumping wells and 4 pumping wells are shown in

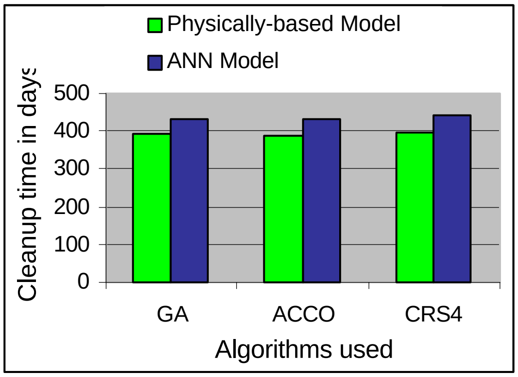


Figure 3(a): Optimal solutions (cleanup time) using physically based and ANN models for 3 wells.

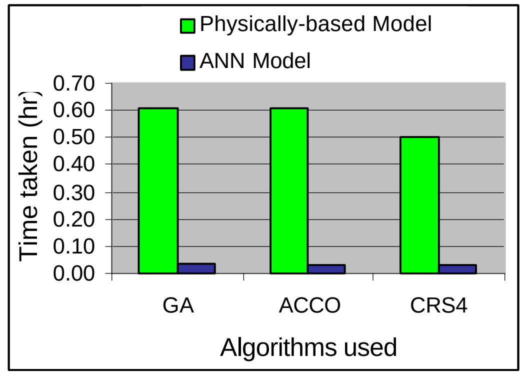


Figure 3(b): Running time taken for physically based and ANN models for 3 wells.

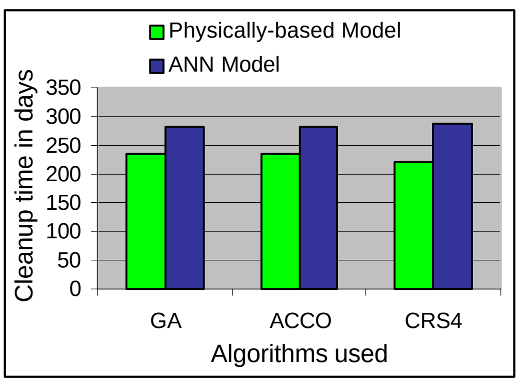


Figure 4(a): Optimal solutions (cleanup time) using physically based and ANN models for 4 wells.

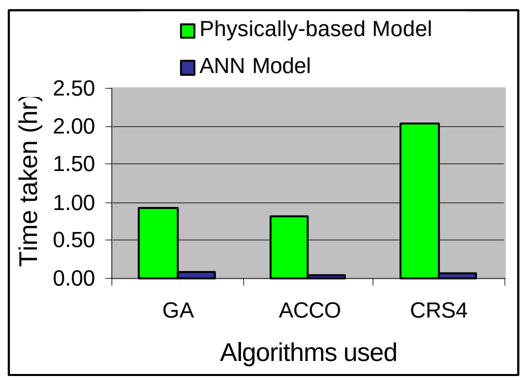


Figure 4(b): Running time taken for physically based and ANN models for 4 wells.

Figs. 3 (a-b) and 4 (a-b) respectively. In terms of the optimal solutions, the performance of ANN models is better in the 3 well case than in the 4 well case. This is due to the fact that in 4 well case the ANN was trained with courser data than in 3 well case. In both cases, all three algorithms produced more or less similar cleanup time. On the contrary, as seen in Figs. 3(b) and 4(b), the time taken to find the optimal solution by different algorithms are significantly different. These figures also show the relatively small running time taken to find the optimal solution when an ANN replaces the physically based models.

5.3 Optimization of cleanup cost

Similarly, optimization was carried out for cleanup cost using both physically based and ANN models. The comparison of results for two well case is shown in Figs. 5(a-b). The performance of ANN model is extremely good in this case. When GA was used, the ANN model gave even lower cleanup cost than the physically based model. However, it is important to note that the lower value of cleanup cost given by ANN does not necessarily mean that the ANN model is better. This could also be due to the error with which ANN replicates the physically based model.

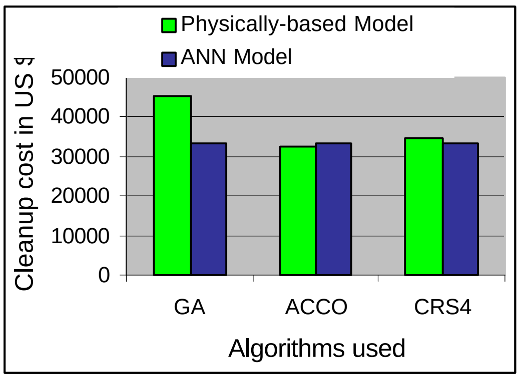


Figure 5(a): Optimal solutions (cleanup cost) using physically based and ANN models for 2 wells.

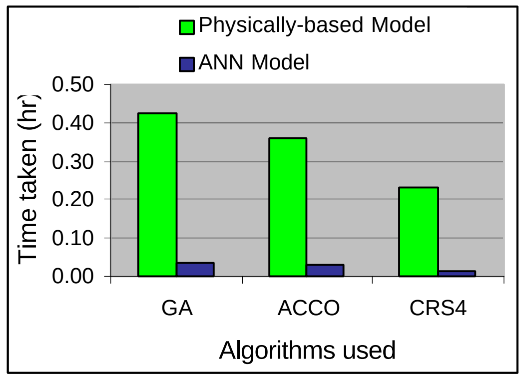


Figure 5(b): Running time taken for physically based and ANN models for 2 wells.

6 Conclusion

This study has demonstrated the potential applicability of ANN models in selecting optimal pumping strategy for contaminated aquifer cleanup. In very short time (17 times faster than the physically based model in average), the ANN model was able to give reasonably good solution. The validation result shows that the trained ANNs predicted the model output (both cleanup time and cleanup cost) to reasonable accuracy. This is true especially in the lower range of these values where the accurate approximation of the models is very important for the optimization purpose. The simplicity of the ANN model, both for its use and for coupling with GO tool, is another advantage of the ANN model. However, it is clear that the ANN must be trained with data consisting of finer interval of decision variables, in this case pumping rates, to achieve a better performance. This obviously requires more effort both for generating the data and for training the network. Further experiments are therefore recommended, particularly using higher number of pumping wells, for more comprehensive analysis of the performance of ANN models trained with different techniques, for example training with different algorithms, different number of hidden layers and more importantly using randomly generated data sampled from practically observable distributions.

The optimization process can also be made more accurate and faster by using the ANN model for finding the regions in the search space associated with the higher probability of finding the global minimum, and then using physically based model for further searching within these regions. Furthermore, the ANN models can also be used advantageously in the experiments aimed at evaluating the performances of different GO algorithms where the optimization process needs to be repeated a large number of times.

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