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# A review on integration of artificial intelligence into water quality modelling

Kwok-wing Chau
*Department of Civil & Structural Engineering, Hong Kong Polytechnic University, Hunghom, Kowloon, Hong Kong*
Email: cekwchau@polyu.edu.hk

ABSTRACT
With the development of computing technology, numerical models are often employed to simulate flow and water quality processes in coastal environments. However, the emphasis has conventionally been placed on algorithmic procedures to solve specific problems. These numerical models, being insufficiently user-friendly, lack knowledge transfers in model interpretation. This results in significant constraints on model uses and large gaps between model developers and practitioners. It is a difficult task for novice application users to select an appropriate numerical model. It is desirable to incorporate the existing heuristic knowledge about model manipulation and to furnish intelligent manipulation of calibration parameters. The advancement in artificial intelligence (AI) during the past decade rendered it possible to integrate the technologies into numerical modelling systems in order to bridge the gaps. The objective of this paper is to review the current state-of-the-art of the integration of AI into water quality modelling. Algorithms and methods studied include knowledge-based system, genetic algorithm, artificial neural network, and fuzzy inference system. These techniques can contribute to the integrated model in different aspects and may not be mutually exclusive to one another. Some future directions for further development and their potentials are explored and presented.

## INTRODUCTION

In the analysis of the coastal water process, numerical models are frequently used to simulate the flow and water quality problems. The rapid development of numerical models provides a large number of models to be used in engineering problems or environmental problems. Up to now, a variety of flow and water quality models are available and the techniques become quite mature. The numerical technique can be based on finite element method, finite difference method, boundary element method, and Eulerian-Lagrangian method. The time-stepping algorithm can be implicit, explicit or characteristic-based. The shape function can be of first order, second order or higher order. The modelling can be simplified into different spatial dimensions, i.e., 1-dimensional model, 2-dimensional depth-averaged model, 2-dimensional layered model, 3-dimensional model, etc [1-8]. The analysis of coastal hydraulics and water quality generally involves heuristics and empirical experience and it is effected through some simplifications and modelling techniques on the basis of the experience of specialists [9]. However, the accuracy of the prediction is to a great extent dependent on the accuracy of the open boundary conditions, model parameters used, and the numerical scheme adopted [10].

Usually, selecting a suitable numerical model to solve a practical water quality problem is a highly specialised task, requiring detailed knowledge on the application and limitation of models. Ragas et al. [11] have compared eleven UK and USA water quality models used in discharge permitting and found that model selection is a complicated process of matching model features with the particular situation. Yet, conventionally, the emphasis has been placed on algorithmic procedures to solve specific coastal problems. These numerical models, being insufficiently user-friendly, lack knowledge transfers in model interpretation. This results in significant constraints on model uses and large gaps between model developers and practitioners. It is a difficult task for novice application users to select an appropriate numerical model due to varying factors, such as the water depth, water velocity, grid spacing, etc. It is usual that, especially for non-expert users, the length of procedures for model manipulation depends largely on their experience. As a result, it is desirable to establish the bridge between model developers and application users. Therefore as the design aid or training tool for engineers or students, it is necessary to include some features to provide help for selections of models. Due to the complexity of the numerical simulation of flow and/or water quality, there is an increasing demand to integrate artificial intelligence (AI) with these mathematical models in order to assist selection and manipulation. Moreover, the development of numerical modelling system reinforces the trend to incorporate more and more features based on the advanced computer technology.

Over the past decade, there has been a widespread interest in the field of AI [12-15]. AI techniques have rendered it possible to simulate human expertise in narrowly defined domain during the problem-solving by integrating descriptive knowledge, procedural knowledge, and reasoning knowledge. The advance in AI techniques allow the development of these intelligent management systems by employing some shells under the established development platforms such as MathLab, Visual Basic, C++, etc. Hence it is extremely important and timely to review and evaluate the state-of-the-art on its application to water quality modelling. In this paper, the development and current progress of integration of AI into water quality modelling are reviewed.

## NEED TO INTEGRATE WITH ARTIFICIAL INTELLIGENCE

In the following section, the need for the integration of artificial intelligence into hydrodynamic and water quality modelling is explained in terms of the existing problems, reasons and tendency.

### *Problems in Numerical Modelling*

Numerical modelling can be delineated as a process that transforms knowledge regarding physical phenomena into digital formats, simulates for the behaviours, and translates the numerical results back to a comprehensible knowledge format [16]. However, an inherent problem in modelling is the requirement of model manipulation, particularly during the set-up of the model, since a slight change of the parameters may lead to quite different results. Knowledge of model manipulation includes real physical observations, the mathematical description of water movement or water quality, the discretization of governing equations for physical and chemical processes, schemes to solve the discretized equations effectively and accurately, and output analysis. Experienced modellers can determine a model failure based on the comparison of the simulated results with real data as well as a heuristic judgement of the key environmental behaviour. The knowledge mentioned above may be used unconsciously. However, many model users do not possess the requisite knowledge to glean their input data, build algorithmic models and evaluate their results. This may produce inferior design and cause under-utilization, or even total failure, of these models.

### *Reasons for Integration with AI*

The ultimate goal of model manipulation in coastal engineering is to acquire satisfactory simulation. However, since a computer is used and the memory and speed of a computer are often limited, a balance should be struck between the modelling accuracy and speed. It is noticeable that modellers usually keep certain fundamental parameters unchanged during the manipulation process. For instance, when researchers were used to two-dimensional coastal modelling, they varied only the bottom friction coefficient [17]. In water quality modelling, Baird and Whitelaw [18] reported that the algal behaviour was related intimately to both its respiration rate and the water temperature. Model users will consider sunlight intensity variation within the water column when simulating the eutrophication phenomenon [19]. These examples reflect that human intelligence uses existing knowledge to reduce the number of choices in order to raise the effectiveness of model manipulation. Each time, they tend to alter merely one or two parameters. This is because if they modify many parameters at the same time, they may easily get lost in the manipulation direction. To this end, AI techniques are capable to mimic this behaviour as well as to complement the deficiency.

### *Tendency in Modelling*

Abbott [20] and Cunge [21] introduced the notion of “generations” of modelling to describe the trend of development. The third generation modelling, being a system to solve specific domain problems, can only be apprehended by the modeller and special users well trained over a long period. It has incorporated very few features to facilitate other users and for other problems. Typical examples are some sophisticated 2-dimensional or 3-dimensional finite difference numerical models on tidal flow and on a particular water quality phenomenon [4,17,19]. The fourth generation modelling has become much more useful to a much wider range of end-users, by furnishing menu of parameter specification, automatic grid formation, pre-processing and post-processing features, and features of management of real collected data for modelling, etc. These tools act as intelligent front-ends to support the handling of the simulation models for specific hydrological or water quality problems [22-23]. Yet they do not address the core problem of knowledge elicitation and transfer [24]. Ragas et al. [11] suggested, though they did not actually implement, the development of an expert system for model selection in order to deal with uncertainty in model predictions, after compared a number of UK and USA models. Nowadays, the fifth generation modelling system [20,24,25] is acknowledged to have the features of integrating AI technology and computational hydrodynamics into a single system to furnish assistance for non-experienced user.

## INTEGRATION WITH ARTIFICIAL INTELLIGENCE

The information revolution during the last decade has fundamentally altered the traditional water quality planning, modelling, and decision-making methodologies. Furthermore, the general availability of sophisticated personal computers with ever-expanding capabilities has given rise to an increasing complexity in terms of computational ability in the storage, retrieval, and manipulation of information flows. With the recent advancements in AI technology, there is an increasing demand for a more integrated approach in addition to the need for better models. Justification for this claim comes from relatively low utilization of models in the industry when compared to the number of reported and improved models. It is expected that this enhanced capability will both increase the value of the decision-making tool to the users and expedite the water quality planning and control process. Table 1 lists the categorization and application of the algorithms studied here including knowledge-based system, genetic algorithm, artificial neural network, and fuzzy inference system. It can be observed that these techniques can contribute to the integrated model in different aspects and may not be mutually exclusive to one another.

Knowledge-based systems (KBSs)

KBSs are interactive computer programs that mimic and automate the decision making and reasoning processes of human experts in solving a specific domain problem, through delivering expert advice, answering questions, and justifying their conclusions. The schematic view of a typical KBS is shown in Figure 1. The knowledge base is a collection of general facts, rules of thumb, and causal models of the behaviour specific to the problem domain. The inference mechanism guides the decision making process by using the knowledge base to manipulate the context. The context contains facts that reflect the current state of the problem, constructed dynamically by the inference mechanism from the information provided by the user and the knowledge base. The knowledge acquisition module serves as an interface between the experts and the KBS and provides a means for entering domain specific knowledge into the knowledge base. The user interface is responsible for translating the interactive input as specified by the user to the form used by the KBS. The explanation module provides explanations of the inferences used by the KBS, namely, why a certain fact is requested and how a conclusion was reached. During the past decade, the potential of AI techniques for providing assistance in the solution of engineering problems has been recognized. KBSs are considered suitable for solving problems that demand considerable expertise, judgment or rules of thumb. KBSs have widespread applications in different fields and are able to accomplish a level of performance comparable to that of a human expert [26,27].

Recently, some literatures about study into the feasibility of integrating KBS with the numerical modelling can be found [28-29]. Most of this kind of the fifth generation numerical modelling system in coastal area only refers to a one-dimensional modelling system for river network or river planning due to the simplicity of knowledge and selection procedure. Chau and Yang [13] implemented an integrated expert system for fluvial hydrodynamics. Jamieson and Fedra [30] developed a decision-support system for efficient river basin planning and management. Ghosh Bobba et al. [31] applied environmental models through an intelligent system to different hydrological systems. Booty et al. [32] presented the design and implementation of an environmental decision support system for toxic chemicals in the Great Lakes using spatial algorithms, models, statistics, KBSs, and other information technologies. These works are, however, limited to one-dimensional modelling systems, and represent only a minute portion of knowledge in this field. Their knowledge bases include heuristic rules for model selection but not for model manipulation. However, even for that simplest case, the symbolic programming for the knowledge representation and selection procedure required enormous effort. For two or three-dimensional modelling, the integration of KBS and problem solution in a single system will become much more complex. The basic requirement is that the system should be able to provide expert advice on selection of the most appropriate model as well as the entailed model parameters under that particular scenario. Since the numerical modelling programs have often been developed in some traditional programming languages such as Fortran, Pascal, C, etc., it is considered not cost-effective to re-write and replace these well-proven and validated programs whose development involved long hours of concerted effort.

To introduce the KBS technology into the modelling system is a method to make the system capable of providing advice to parameter selection or model selection, and to make the system to have the intelligent features of “usage wizard” if the program is written in some embedded forms of code. The architecture of a prototype integrated system [33] is shown in Figure 2. The expert system shell, Visual Rule Studio [34], which runs as an ActiveX Designer under the windows-based programming language environment Microsoft Visual Basic 6.0, was employed. Visual Rule Studio is a hybrid expert system shell that couples the advantage of both production rules and objected programming paradigm. All the usual control objects of the common interface under Windows environments such as command button, picture box, etc., are furnished.

Genetic algorithms (GAs)

GAs belong to the class of stochastic search procedures known as evolutionary algorithms that use computational models of natural evolutionary processes in developing computer-based problem solving systems [35]. This form of search evolves throughout generations by improving the features of potential solutions. GAs, being search techniques based on the mechanism of natural genetics and biologically-inspired operations, can be employed as an optimization method so as to minimize or maximize an objective function. They apply the concept on the artificial survival of the fittest coupled with a structured information exchange using randomized genetic operators taken from the nature to compose an efficient search mechanism. GAs work in an iterative fashion to generate and test a population of strings. This process mimics a natural population of biological creatures where successive generations of creatures are conceived, born, and raised until they are ready to reproduce.

GAs are not limited by assumptions about search space, such as continuity or existence of derivatives. Through a variety of operations to generate an enhanced population of strings from an old population, GAs exploit useful information subsumed in a population of solutions. Various genetic operators that have been identified and used in GAs include, namely, crossover, deletion, dominance, intra-chromosomal duplication, inversion, migration, mutation, selection, segregation, sharing, and translocation. A variety of applications has been presented since the early works and GAs have clearly demonstrated their capability to yield good solutions even in cases of highly complex, multiple-parameter problems [36-37].

In mathematical simulation for flow prediction and water quality management, the inappropriate use of any model parameters, which cannot be directly acquired from measurements, may introduce large errors or result in numerical instability. GA can be used to determine an appropriate combination of parameter values in this domain. The percentage error of peak value, peak time, and total volume of flow and water quality constituents are important performance measures for model prediction. The parameter calibration is based on field data of tidal as well as water quality constituents collected over several years' span with other years' records to verify these parameters. Sensitivity analysis on crossover probability, mutation probability, population size, and maximum number of generations can be performed to determine the most befitting algorithm parameters. Moreover, GAs can be applied to the evolution of models with more transparent knowledge representations, which facilitates understanding of model predictions and model behaviour. It may also help in determining the patterns, regularities and relationships, which exist and drive a certain phenomenon, such as algal abundance. Bobbin and Recknagel [38] established inducing explanatory rules for the prediction of algal blooms by GA. Ng and Perera [39] employed GA for calibration of river water quality model. Cho et al. [40] used GA to optimize regional wastewater treatment in a river water quality management model. Chau [41] implemented GA to calibrate flow and water quality modelling and the results demonstrated that its application was able to mimic the key features of the flow and water quality process and that the calibration of models was efficient and robust. Yet, up to now, a comprehensive investigation on the application of GA on flow and water quality modeling is still outstanding.

Artificial neural networks (ANNs)

ANNs are based on our present understanding of the brain and its associated nervous systems. They use highly simplified models composed of many processing elements connected by links of variable weights to form black box representations of systems [42]. Figure 3 shows the architecture of a typical ANN comprising three layers of interconnected nodes or neurons, each of which is connected to all the neurons in the ensuing layer. An input layer is the layer where data are presented to the neural network whilst an output layer holds the response of the network to the input. One or more intermediate layers, termed hidden layers, may exist between the input layer and the output layer, in order to enable these networks to represent and compute complicated associations between patterns. All hidden and output neurons process their inputs by multiplying each input by its weight, summing the product, and then processing the sum using a nonlinear transfer function to generate a result. Amongst others, the S-shaped sigmoid curve is one of the most commonly used transfer functions [43].

These models have the ability to deal with a great deal of information and to learn complex model functions from examples, i.e. by training using sets of input and output data. The greatest advantage of ANNs over other modelling techniques is their capability to model complex, non-linear processes without having to assume the form of the relationship between input and output variables. Learning in ANNs involves adjusting the weights of interconnections. Areas addressed by ANN techniques include pattern matching, combinatorial optimization, data compression, and function optimization. As a developing and promising technology, the capability of an ANN to cope with uncertainty in complex situations has been seized upon for wide ranging applications in recent years [44-45].

ANNs have found application in water quality modelling [46, 47]. Kralisch et al. [48] employed an ANN approach for the optimization of watershed management to maintain a reasonable balance between water quality demand and consequent restrictions for the farming industry. Maier et al. [49] used ANNs to predict optimal alum doses and treated water quality parameters. However, most of the studies were undertaken for limnological systems [50-53] or riverine systems [54-55] whilst report on ANN modelling of a coastal system has been very scarce [56]. Moreover, in most of the studies, the effectiveness of ANN as a predictive tool has not been fully addressed. For example, the water quality dynamics at the current time were often linked via the model with other environmental variables at the same time, which rendered them useless in real prediction. Most of them employed almost all possible environmental parameters as input variables without considering the optimal choice amongst them. Moreover, insufficient attention has been given to extract some knowledge from the learning process. Thus, a lot of works can be further pursued in the application of this technique to this domain problem.

Fuzzy inference systems

Zadeh et al. [57] pioneered the development of fuzzy logic, which is very useful in modelling complex and imprecise systems. Under the fuzzy set theory, elements of a fuzzy set are mapped to a universe of membership values using a function-theoretic form belonging to the close interval from 0 to 1. An important step in applying fuzzy methods is the assessment of the membership function of a variable, which parallels the estimation of probability in stochastic models. Membership functions in fuzzy set theory, which are appropriate for modelling preferences of the decision maker, can be obtained on the basis of the actual statistical surveys. The fuzzy logic based modelling is a simple approach, which operates on an ‘if-then’ principle, where ‘if’ is a vector of fuzzy explanatory variables or premises in the form of fuzzy sets with membership functions and the ‘then’ is a consequence also in the form of fuzzy set.

An optimization problem, in general, is expressed as a formulation maximizing or minimizing an objective under a set of constraints. If the objective or the constraints are vague, then the problem can be referred to as a fuzzy optimization problem. Fuzzy logic has been used in a number of applications but generally as a refinement to conventional optimization techniques in which the usual crisp objective and some or all of the constraints are replaced by the fuzzy constraints [36,58].

Fuzzy set theory concepts can be useful in water quality modelling, as they can provide an alternative approach to deal with those problems in which the objectives and constraints are not well defined or information about them is not precise. Chang et al. [59] used the fuzzy synthetic evaluation approach to identify river water quality. Chen and Mynett [60] employed data mining techniques and heuristic knowledge in modelling the fuzzy logic of eutrophication in Taihu Lake. Liou et al. [61] applied two-stage fuzzy set theory to river quality evaluation in Taiwan. Marsili-Libelli [62] described the design of a bloom predictor based on the daily fluctuations of simple water quality parameters such as dissolved oxygen, oxidation–reduction potential, pH and temperature. Individual applications of this technique have been recorded in an isolated manner. Moreover, most of the studies were undertaken for fresh water riverine systems whilst application to a coastal system has been very scarce. Much more efforts can be performed in order to stretch its full application in this area.

## FUTURE DIRECTIONS

One of the promising directions is the hybrid combinations of two or more of the above methods to produce an even more versatile water quality modelling system. Moreover, progresses in AI are made in parallel in two areas: basic capabilities of tools; and, real applications in solving water quality problems. Research is currently underway in developing better AI tools, which may have capabilities to furnish better knowledge representational schemes, alternative inference techniques, and alternative mechanisms for addressing uncertain or incomplete data. Better and more user-friendly interfaces to database management systems, graphical displays, and knowledge acquisition modules will enhance the applicability of modelling systems in real practice. Since prototype systems are being developed under this context, demands for better AI tools will be increased, which may in turn lead to better techniques for applying AI technology. More importantly, the prototype systems will be moving out of the laboratory and into real practice. Continued work will enhance the technology and applications of AI in water quality modelling.

## CONCLUSIONS

Existing water quality models are insufficiently user-friendly and often result in significant constraints on their uses. It is a difficult task for novice application users to select an appropriate numerical model. As such, it is instrumental to incorporate the existing heuristic knowledge of model manipulation and to furnish intelligent manipulation of calibration parameters. The recent advancement in AI technologies provides a way to bridge the existing gap between the model developer and practitioner. This study has reviewed the current state-of-the-art and progress on the integration of AI into water quality modelling. Attempts on the integration of various AI technologies, including KBS, GA, ANN, and fuzzy inference system, into numerical modelling systems have been found. These techniques can contribute to the integrated model in different aspects and may not be mutually exclusive to one another. This can provide substantial assistance to novice users of these algorithmic models to determine whether or not digital sets generated by numerical modelling represent real phenomena. Some future directions for further development and their potentials are explored and presented. It is believed, with the ever heightening capability of AI technologies, that further development of numerical modelling in this direction will be promising.

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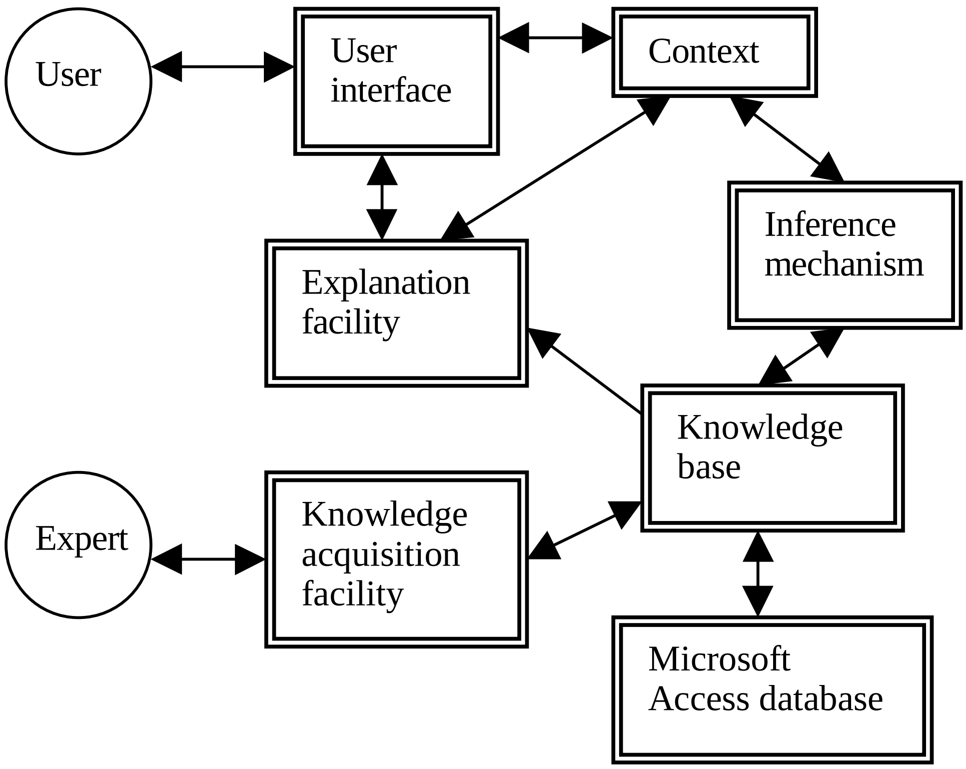


Figure 1. Schematic view of a typical KBS

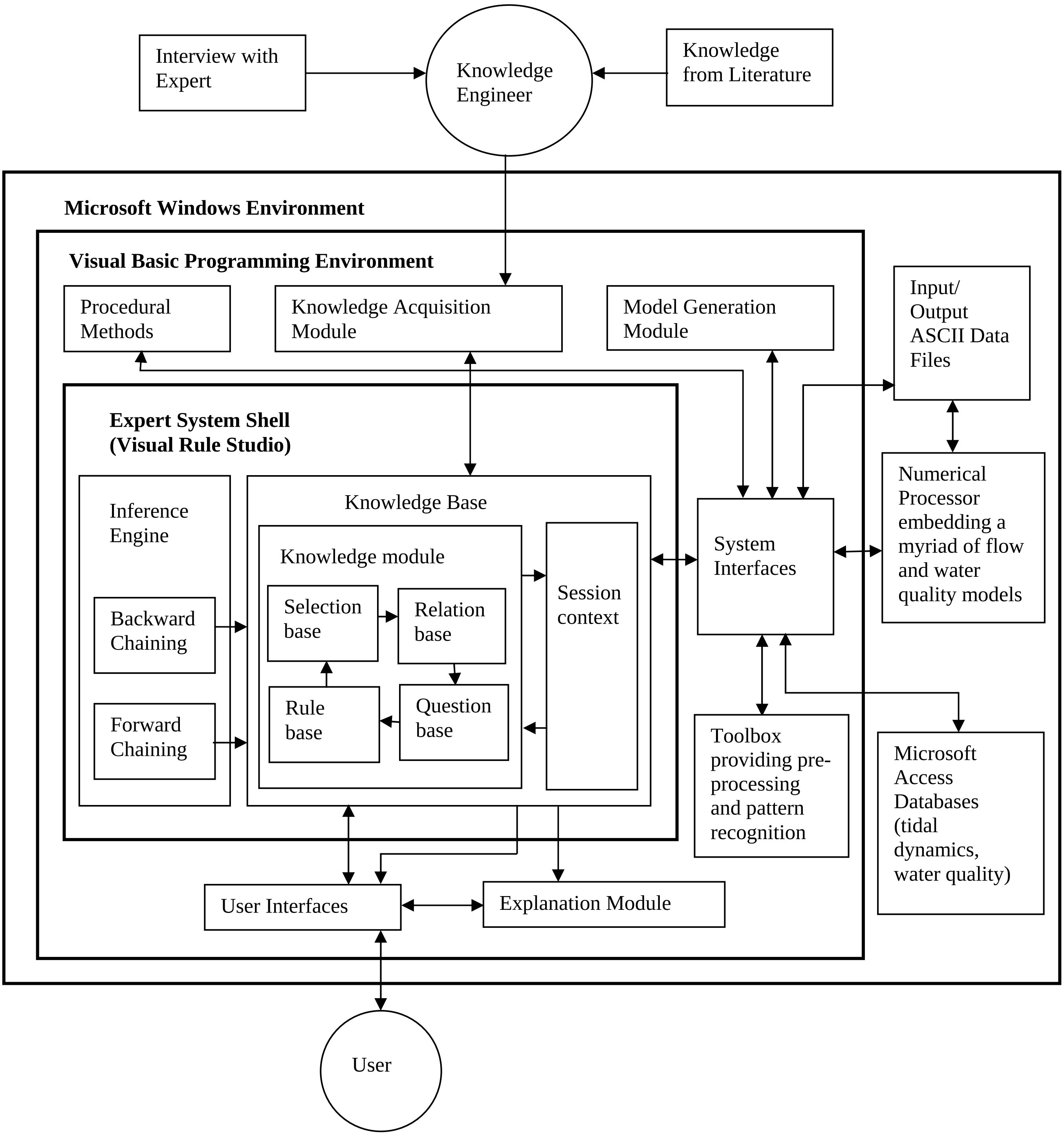


Figure 2 Architecture of a prototype KBS on manipulation of numerical flow and water quality model [32]

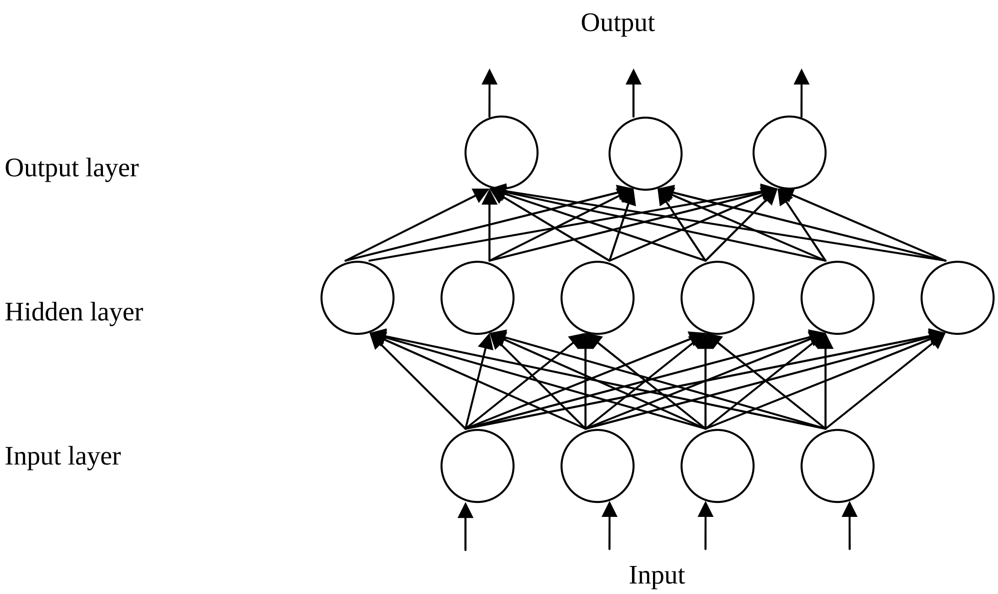


Figure 3 Architecture of a typical ANN

Table 1. Categorization of various AI techniques

| Technique | Algorithm | Domain | Applications in water quality/hydrodynamics |
|---|---|---|---|
| Knowledge-based systems | symbolic and logical reasoning | mimic and automate the decision making and reasoning processes of human experts in solving problem | selection and manipulation of various numerical models on hydrodynamics/water quality |
| Genetic algorithms | evolutionary algorithm using selection, reproduction, crossover, mutation | use computational models of natural evolutionary processes in developing computer-based problem solving systems | optimization of calibration of the parameters of numerical models on hydrodynamics/water quality |
| Artificial neural networks | data driven modelling approach with highly interconnected processing elements | constitute an information-processing paradigm that is inspired by biological nervous systems in simulating underlying relationships that are not fully understood | 1. determination of underlying physical/ biological relationships that are not fully understood<br>2. optimized calibration of the parameters of numerical models on hydrodynamics/water quality |
| Fuzzy inference systems | map elements of a fuzzy set to a universe of membership values | modelling complex and imprecise systems when objective or the constraints are vague using a function-theoretic membership form belonging to the close interval from 0 to 1 | quantification of the semantemes of the expertise and determine the confidence factors of the semantemes |