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APPLICATION OF EXPERT SYSTEMS TECHNOLOGY IN WATER QUALITY MODELING

Thomas O. Barnwell, Jr [*], Linfield C. Brown[**] and Wiktor Marek[***]

[*]*U.S. Environmental Protection Agency, College Station Road, Athens, Georgia 30613, U.S.A.*
[**]*Department of Civil Engineering, Tufts University, Medford, Massachusetts 02155, U.S.A.*
[***]*Department of Computer Sciences, University of Kentucky, Lexington, Kentucky 40506, U.S.A.*

ABSTRACT

Computerized modeling is becoming an integral part of decision making in water pollution control. Expert systems is an innovative methodology that can assist in building, using, and interpreting the output of these models. This paper reviews the use and evaluates the potential of expert systems technology in environmental modeling and describes elements of an expert advisor for the stream water quality model QUAL2E. Some general conclusions are presented about the tools available to develop this system, the level of available technology in knowledge-based engineering, and the value of approaching problems from a knowledge engineering perspective.

KEYWORDS

Water quality modeling, QUAL2E, systems analysis, expert systems.

INTRODUCTION

Computerized modeling is becoming an integral part of decision making in water pollution control. Problems increasingly involve complex interactions among elements of the environment and large, multi-media modeling systems must be built to understand these interactions. Expert systems is an innovative methodology that can assist in building, using, and interpreting the output of these models. In this paper, we review the use and evaluate the potential of expert systems technology in environmental modeling and describe elements of an expert advisor for the stream water quality model QUAL2E. QUAL2E has a long history of use both in the United States and worldwide and is a proven, effective modeling tool for analyzing the dissolved oxygen balance in a stream or river. Because of this widespread usage, a body of experience and empirical knowledge about the computer program and its supporting science has been gained that is ideal for codification in an expert system.

EXPERT SYSTEMS

Expert (or knowledge-based) systems is an emerging technology that holds the promise of assisting in the solution of many complex environmental problems. It is a branch of the field of artificial intelligence in which the symbolic manipulations of mathematical logic are applied to a knowledge base to simulate the problem-solving skills of a human expert in a specific problem domain. The term artificial intelligence (AI) was first applied to the study of how computers might replicate human reasoning. Although many AI-spawned technologies have reached the market -- for example, image-pattern recognition, speech recognition, and robotics -- most of them use numerical algorithms to process information and only a few exploit symbolic processing (Denning, 1986). AI technologies that encompass symbolic logic processing to manipulate a body of knowledge and draw inferences from user responses to questions regarding a specific problem context are known as "knowledge-based" or "expert" systems. The objective of an expert system is to provide the user with an intelligent assistant to solve a given problem or achieve a specific goal.

There is an important practical distinction between expert systems and traditional software. Expert systems use as a knowledge base the wisdom of one or more individuals that reflects state-of-the-art information or a particular type of knowledge or interest. The distinction, and the most important concept in the new technology, is a clear separation of the knowledge base and the reasoning process. As a consequence, the logical structure of the knowledge is separate from the actual control of program execution. Modification and maintenance of the knowledge base is easier as it is distinct from program control.

Whereas traditional computer programs use algorithmic solutions to problem-solving, expert systems use heuristic, or rule-of-thumb strategies akin to the thought process of humans. Traditional programs solve problems through a repetitive process often employing field convergence; expert systems use inferential processes. The knowledge in a traditional program is normally buried in the computer code and not explicitly available; expert system knowledge and logic are directly available to the developer for the modification process and, in particular, to the user wishing to better understand the system's reasoning process.

Two types of expert systems development tools are available today. The first are computer languages such as LISP or PROLOG that can be used in expert systems development, just as languages like FORTRAN and BASIC are used for conventional programming. The second are development tools called expert systems "shells" that are rapidly becoming the accepted and easiest way to implement an expert system.

The traditional development tool in expert systems has been LISP (LISt Processor), a computer language like FORTRAN or BASIC. LISP was developed in the 1950s and has been extensively used in AI research in the United States. LISP is designed to process symbolic data rather than the numerical data that more familiar languages (i.e., FORTRAN) process. Another language used in AI is PROLOG (PROgramming in LOGic). PROLOG was developed in Europe and is designed to manipulate logical expressions. PROLOG is receiving increasing attention in the United States and appears to be emerging as a significant development tool.

An alternative to the LISP and PROLOG languages are expert systems "shells." Shells are designed to facilitate the rapid development of knowledge systems and typically incorporate specific strategies for knowledge representation, inference, and control of the reasoning process. Shells essentially implement a subset of a language (i.e., LISP or PROLOG) that is important for an application. Shells are designed around a syntax for representing rules and a specific type of inference engine. Shells tend to be more limited than languages but are more efficient for problems for which they are applicable because they contain a significant amount of tested and debugged code. An excellent overview of the subject of expert systems, which includes a review of available shells, is Harmon and King (1985).

An expert system has three major characteristics -- (a) a data base where knowledge, axioms, and rules of inference are stored, (b) an algorithm using symbolic logic processing for constructing proofs, and (c) a user interface for expressing queries from the program and providing information to the system.

The process of building a knowledge base, which forms the most important part of an expert system, is called "knowledge engineering." In many engineering or regulatory applications, the knowledge base of an expert system closely resembles the information contained in a user manual or guidance document. This knowledge base must be formalized in a way that allows use of a particular tool. The knowledge base contains both objective information, a set of widely agreed upon facts, and subjective sets of rules of judgment that an expert might employ in solving a problem -- in this case, applying the QUAL2E program to a specific problem.

The inference engine of an expert system allows the system to search rapidly and efficiently through the knowledge base to solve the problem at hand. The reasoning and explanation features of an expert system are determined by the inference engine. Ease of use of an expert system depends primarily on the sophistication of the user interface. Detailed menus, queries, and user responses as well as graphics capabilities are important considerations.

In the early days of expert systems, the knowledge engineer was required not only to elicit information from experts, compile knowledge bases, and encode this information, but also to construct the inference engine that interprets these data and schedules the knowledge interface with the user. Consequently, programs were written where all facets of the expert system were integrated, making debugging difficult and rendering the knowledge base less explicit than desired. With the realization that diverse problem areas could effectively use common knowledge representation strategies (such as rule-based systems), there ensued a rapid development of the software packages known as "shells." These stand-alone inference engines are essentially expert systems without the knowledge base included. There are a variety of expert systems shells on the market today.

For a specific problem application, it is important that the inference engine match the framework of the knowledge base representation. A typical inference engine will include most of the following attributes: explanation facilities such as retrospective reasoning, hypothetical reasoning or counterfactual reasoning; knowledge extraction and consistency checking; debugging aids like trace facilities and automated testing; and input/output facilities such as menus, operating system accessibility, and run-time knowledge acquisition.

A user interface interacts directly with the user, asks for information from the user, and ultimately solves the problem by manipulation of the knowledge base through communication with the inference engine. Some expert system shells provide the capability to compile the knowledge base and inference engine into a delivery system.

In preparation for the QUAL2E project, a number of expert system shells were evaluated and the M.1 shell by Teknowledge was chosen for system development. M.1 has many of the desirable features of an expert system shell discussed above.

THE POTENTIAL OF EXPERT SYSTEMS

Most expert system shells are based on a limited set of related knowledge representation schemes -- either rule-based or frame-based representations. This codification of knowledge into a unique set of structures has enormous implications to many professions and is perhaps the main reason for the intense current interest in expert systems.

Large, complex models require extensive human interaction for their successful implementation. An expert system has the potential to act as an intelligent user interface to a complex simulation model, relieving the user of the tedium of preparing rigidly formatted input data and advising the user on the selection of appropriate parameter values, especially under conditions of uncertainty. Such a model preprocessor might offer alternate parameter selection techniques and provide advice on the technique that is most appropriate for the level of information the user is able to supply. A preliminary expert system with these capabilities (HYDRO) was developed by Gaschnig et al. in 1981. HYDRO has prototype advisors for 16 parameters in the U S EPA-developed Hydrologic Simulation Program-FORTRAN (HSPF). The objective of the study was to modify an existing expert system (PROSPECTOR) to address problems involving judgmental expertise requiring computation of numerical quantities. Although never implemented as an operating system, HYDRO served as a useful paradigm for the work with QUAL2E described later in this paper.

The proliferation of personal computers and the expectations raised by the usability of commercial systems such as data base managers and spreadsheets on them are forcing environmental modelers to rethink their approach to model development, particularly their models' interactions with users. The general availability of a knowledge-based expert system containing the experience and expertise of model developers and skilled users would be of enormous benefit to those skilled in the physical and biological sciences but less skilled in the art of modeling and interacting with the computer. Personnel intimately involved in regulation, for example, often lack detailed computer skills.

In spite of the pessimistic views of some (eg., Dreyfus and Dreyfus, 1986), knowledge-based expert systems have been or are being developed in the fields of accounting, agriculture, chemistry, computer systems, electronics, geology, law, manufacturing, mathematics, medicine, meteorology, military science, physics, process control, and space technology (Waterman, 1986). Expert systems are becoming a popular topic in many engineering and scientific conferences, thus indicating widening acceptance of the tool. For example, in the October 1984 issue of Civil Engineering, Fenves et al. discussed the potential of expert systems in civil engineering. The article mentioned only one such application -- HYDRO -- in a sidebar. In the May 1986 issue of Civil Engineering, Godfrey discussed five examples of expert systems, only two of which were described as "available." The first symposium at a professional conference on expert systems in civil engineering was held in April 1986 (Kostem and Maher, 1986). In the proceedings of this symposium , there is much discussion of ongoing work in the field and it is clear that many professionals are pursuing the application of this technology. The symposium consisted of 24 papers covering a broad range of applications in civil engineering, again indicating growing interest in and acceptance of this new tool by the profession. Recently, Environmental Science and Technology contained a review of expert systems applications for environmental problems (Huschton, 1987). This review identified 21 systems under active development but concluded that few are in actual use today. The October 1987 issue of the American Society of Civil Engineers' new Journal of Computing in Civil Engineering is devoted to the topic of expert systems. Manuscripts in the issue cover the topics of expert system shells, geotechnical engineering, construction engineering, structural engineering, and water resource management.

This brief review demonstrates that the science of expert systems and its associated engineering discipline, knowledge engineering, are new fields. It is not intended to imply that applications in civil engineering or environmental sciences are atypical. Rather, it is believed that this interest in expert systems is very typical of a wide range of professional disciplines from engineering to the sciences to the business world. It is clear from this intense interest that many people view expert systems as a potentially useful and valuable tool for analyzing and solving problems.

AN OVERVIEW OF QUAL2E

The computer program QUAL2E permits simulation of several water quality constituents in a branching stream system using a finite difference solution to the one-dimensional advective-dispersive mass transport and reaction equation. The equations include a hydrologic balance in terms of flow (Q), a heat balance in terms of temperature (T), and a materials balance in terms of concentration (C). Both advective and dispersive transport are considered in the materials balance. The specific equations and solution technique are described in detail in the QUAL2E computer program documentation (Brown and Barnwell, 1987) and a number of applications of the computer program are summarized in Barnwell, Brown and Whittemore (1987). The processes included in QUAL2E are summarized below without specific references; the reader is encouraged to refer to the documentation for details.

Mass Transport

Mass transport in the QUAL2E computer program is handled in a relatively simple manner. The forcing function used for estimating transport is the streamflow rate, which is assumed to be steady-state. Stream velocity, cross-sectional area, and depth are computed from streamflow by either of two methods: discharge coefficients or Manning's equation for a trapezoidal cross-section. Both methods require estimation of a dispersion constant and Manning's n. The discharge coefficients method requires, in addition, specification of coefficients and exponents in equations of the form:

$$X = a\,Q^{b} \qquad \ldots\ldots\ldots\ldots \quad 1$$

where X is velocity or depth, Q is stream volumetric flow rate, and a and b are coefficients and exponents that are different for velocity and depth. The method using Manning's equation requires specification of the slope of the energy grade line and three channel properties -- two side slopes and bottom width -- for each reach.

Constituent Reactions and Interrelationships

One of the most important considerations in determining the assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. The QUAL2E computer program includes the major interactions of the nutrient cycles, algal production, benthic and carbonaceous oxygen demand, atmospheric reaeration, and their effect on the dissolved oxygen balance. These interactions are summarized in Figure 1. In addition, the computer program includes a heat balance for the computation of temperature and mass balances for conservative minerals, coliform bacteria, and nonconservative constituents such as radioactive substances. Chlorophyll *a* is modeled as the indicator of planktonic algae biomass in QUAL2E. As shown in Figure 1, the nitrogen cycle is composed of four compartments: Organic nitrogen, Ammonia nitrogen, Nitrite nitrogen, and Nitrate nitrogen. The phosphorus cycle is similar to, but simpler than, the nitrogen cycle, having only two compartments. Ultimate carbonaceous biochemical oxygen demand (BOD) is modeled as a first-order degradation process in QUAL2E, which also takes into account removal by settling.

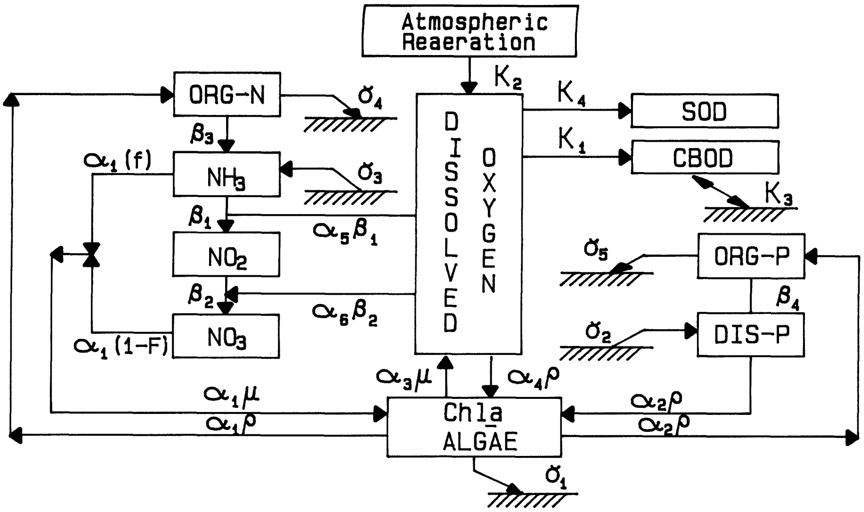

Figure 1. Constituent Interactions in QUAL2E

The processes discussed above represent the primary internal sinks of dissolved oxygen in the QUAL2E computer program. The major source of dissolved oxygen, in addition to that supplied from algal photosynthesis, is atmospheric reaeration. QUAL2E provides eight options for estimation of the reaeration coefficient, including several commonly used equations and two arbitrary methods of specification. In addition, the capability to estimate oxygen input from reaeration due to dams is included.

Water temperature is computed from a heat balance that estimates the net energy flux through the air-water interface from the net short-wave solar radiation, net long-wave atmospheric and back radiation, convective inputs and losses, and evaporative losses. Solar radiation may either be input or estimated from latitude, time of year, and climatologic factors.

The processes represented in QUAL2E are comprehensive and provide a flexible capability to fit the computer program to a wide variety of physical situations. On the other hand, this flexibility can be a curse to the inexperienced user because it requires a number of decisions related more to the structure of the computer program than the general theory of modeling. While the general theory may be familiar to most, model structure is specific to the computer program being used and its rational may not be obvious to those not familiar with the conditions under which the model was developed or previously successfully applied.

AN EXPERT ADVISOR FOR QUAL2E

It is useful to distinguish between levels of user assistance. A user interface often includes a help function to explain the shorthand used to represent information in the crowded confines of an 80 character by 25 line computer screen. This function, illustrated in Figure 2, is typically invoked by typing "HELP" when entering data. Explanatory text is then displayed that provides additional information on the subject of interest. In the example, if the user cannot decipher "Mann. n" in the input table, a request for "HELP" will display the explanation at the bottom of the figure and perhaps even a table of suggested values. This facility may even be used to place an entire users manual online at the disposal of the user. Some might consider a context-sensitive help facility to be an expert system and we agree that there may not be a clear distinction between what is called "help" and "advice" here. In fact, our inclination is to use the term "advisor" rather than "expert system" to avoid arguments over what constitutes an expert system.

In developing an expert system, as in any serious system development, it is important to consider the intended audience. One must determine the skills and knowledge required to operate the system. It seems reasonable to expect that a minimum set of qualifications be required to perform any task. As a trivial example, we might assume that the user will be able to determine the latitude and longitude of the river basin in question. A system could be built that would estimate these coordinates from other information, such as state and

```
 ________________________________________________________________
|                                                                |
|          DATA TYPE 5: HYDRAULIC DATA (COEFFICIENTS)            |
|                                                                |
|   Reach   Dispn  Q Coeff   Q Expo  Q Coeff   Q Expo    Mann.   |
|   Order   Const  Velocity Velocity  Depth    Depth      n      |
|   <---><-----><------><------><------><------><----->          |
|                                                                |
|     1.    300.    .250      .30      .45      .56     HELP     |
|     2.    none    none     none     none     none     none     |
|     3.    none    none     none     none     none     none     |
|     4.    none    none     none     none     none     none     |
|     5.    none    none     none     none     none     none     |
|                                                                |
| Min  0.    5.6     0.0      0.0      0.0      0.0      .010    |
| Max 50.  6000.    none      2.0     none     none      .500    |
| Def none ADVICE   none   ADVICE     none   ADVICE    ADVICE    |
|                                                                |
| HELP>> Mannings "n" is a coefficient that is a measure of the  |
|        resistance to flow in a stream channel.                 |
|________________________________________________________________|
```

Figure 2. HELP -- The First Level of Assistance

county, but the person who would require such assistance would not, in the author's opinion, be qualified to operate the model. More realistic expectations of the user include the ability to distinguish among levels of waste treatment (primary, secondary, or advanced treatment) and some familiarity with stream hydraulics. We do not expect, however, this familiarity to extend, for example, to knowledge of expected values of the exponents in equation 1. But we do expect the user to be able to calibrate the equation given an estimate of the exponents and observations of stream flow, velocity, and depth.

Thus it was decided to design the QUAL2E Advisor for users with a BS or MS degree in environmental sciences or engineering. Users with these credentials will be familiar with the general theory and objectives of environmental modeling but may not have the skills and knowledge to implement QUAL2E. They are normally well trained in the physical and biological sciences but are less skilled in the art of water quality modeling and interacting with the computer. We believe that the general availability of a knowledge-based expert system containing the experience and expertise of model developers and skilled users will be of enormous benefit to people in this group.

For purposes of this project, model users were classified as novices, general users, advanced users, or experts, as illustrated in Figure 3. We use the terms education, experience, and expertise to distinguish among levels of proficiency, perhaps because we agree in part with Dreyfus and Dreyfus (1986) that these systems may be more properly called "competent" rather than "expert." Given this framework, the QUAL2E Advisor is intended to provide the general user with the experience and knowledge of the advanced user, rather than to serve as an educational tool for the novice or to provide expertise to the advanced user.

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============================================
CLASSES OF          METHOD OF INCREASING
QUAL2E USERS        PROFICIENCY
------------        -----------------------
Novice        0
              |     Education/Training
General       v  0
                 |  Experience/Expert System
Advanced         v  0
                    | Expertise
Expert              v
============================================
```

Figure 3 - Target Audience for QUAL2E Advisor

For the novice, workshops for training are already in place. The objective of these workshops is to increase the proficiency of the novice to that of a general user. Although education and training are features of some expert systems, a system with the level of detail required would be beyond the exploratory purposes of this project. The QUAL2E Advisor is intended for modelers with restricted access to expertise; it is not targeted at the advanced user. Identifying exceptional conditions and dealing with them properly is the true mark of expertise. To anticipate all possible exceptional conditions that can arise in applying QUAL2E is beyond the scope of this project.

In preparing a simulation, a variety of information must be supplied. The 24 QUAL2E input forms given in the QUAL2E Users Manual (Brown and Barnwell, 1987) are summarized below. The information required to run the program can be categorized into four general types as shown. (The number of individual inputs in each category are in parentheses.)

1. Choices of options	(22)
2. Generally measured "forcing functions"	(31)
3. Generally estimated or calibrated "coefficients"	(66)
4. System definition inputs	(10)

Category 1 includes such straightforward options as the constituents to be simulated and other, more difficult options such as the choice of a functional relationship between light level and algal growth. Category 2 includes model variables that are generally measured such as stream and wasteload flow rates and constituent concentrations in headwaters, waste discharges, and incremental inflows. Category 3 includes model inputs that are generally estimated rather than measured directly. Category 4 specifies the manner in which the real river is represented in QUAL2E as a network of discrete elements. These classifications are somewhat arbitrary and represent a convenient grouping of input requirements. For example, some options such as choice of a reaeration prediction method were classified as a coefficient rather than an option. A detailed report on a prototype advisor system is available from the first author (Barnwell, Brown, and Marek, 1986). Development of advice for a small subset of the input related to stream hydraulics is described below.

As previously discussed, one must carefully consider the audience for an expert system. Expertise is a relative concept; one person's expert is another's competent technician. A criterion we have used to select inputs for expert "advice" is to focus on those that are estimated rather than measured. In deciding which inputs are appropriate for advice, we have chosen those inputs from the third category, "coefficients" and the fourth, "system definition." In general, option choices do not require expertise although some, such as choice of a functional relationship between algal growth and light, do. Inputs such as forcing functions clearly should be measured as they are system specific. The issue here is more one of modeler responsibility than expertise. Estimation of missing data requires a degree of experience and expertise that we do not yet feel comfortable in encoding in an expert system.

HYDRAULIC ADVISOR

To illustrate the development of of a set of rules, or a knowledge base, for various QUAL2E inputs, we will consider here the development of advice for the input shown in Figure 4, the hydraulic inputs of the program. A good description of channel geometry and flow conditions is important in properly using QUAL2E. The hydraulic input, summarized in Figure 4, defines the relationship between velocity, depth and streamflow. Both velocity and depth are sensitive in almost all applications of QUAL2E. Velocity determines the residence, or reaction, time of pollutants in the system and many rate coefficients are dependent on depth. Reaches are usually chosen so that travel time is short in order to maintain constant rate coefficients. Thus errors in travel time can be magnified in importance.

DISPERSION CONSTANT		MANNING'S n	
Trapezoidal Channels Option		Discharge Coefficients Option	
BOTTOM WIDTH	SIDE SLOPE 1	COEFFICIENT FOR VELOCITY	COEFFICIENT FOR DEPTH
CHANNEL SLOPE	SIDE SLOPE 2	EXPONENT FOR VELOCITY	EXPONENT FOR DEPTH

Figure 4 - Information Required for Hydraulic Calculations

The first choice the user must make is the option to use for calculating velocity and depth from streamflow. Two methods are provided and a third method is available but not described in the user manual. The choice of hydraulics option is a global choice and applies to the entire river being modeled, whereas the hydraulic input is reach variable.

Trapezoidal Channels

The method called "Trapezoidal Channels" requires detailed knowledge of the geometric properties of the stream channel for use in Manning's equation:

$$V = \frac{1}{n} R^{2/3} S^{1/2} \qquad (2)$$

where V is velocity (mps), R is hydraulic radius (m), S is slope of the energy grade line (m/m), and n is a roughness coefficient. Manning's equation is often combined with the continuity equation,

$$Q = V A \qquad (3)$$

where Q is streamflow (cms), and A is cross-sectional area (sq m), and expressed as:

$$Q = \frac{1}{n} A R^{2/3} S^{1/2} \qquad (4)$$

This equation is commonly used in civil engineering practice and is described in any stream hydraulics text (e.g. Chow, 1959). The area (A) and hydraulic radius (R) are calculated from the channel bottom width, two side slopes, and depth. A precondition for the equation to be applicable is that flow must be mainly uniform although its use has been extended to gradually varied flows. It cannot be used in portions of lakes and reservoirs where discharge and channel geometry vary rapidly.

Discharge Coefficients

The second option for computing depth and velocity from streamflow, called "Discharge Coefficients," is based on empirical observations of the velocity-depth-streamflow relationship (Leopold and Maddox, 1953). The equations relate velocity, channel width, and depth to streamflow through power functions:

$$V = a Q^{b} \qquad (5)$$

$$D = c Q^{d} \qquad (6)$$

$$W = e Q^{f} \qquad (7)$$

where D is average depth (m), W is average width (m), and a, b, c, d, e, and f are empirical coefficients or exponents. Given that area is a function of average width (W) and average depth (D),

$$A = D W \qquad (8)$$

it is clear from equation 3 that:

$$Q = V A = V D W = (aQ^{b}) (cQ^{d}) (eQ^{f}) = (a c e) Q^{b + d + f}$$

and, therefore, the following relationships hold:

$$a c e = 1 \qquad (9)$$

$$b + d + f = 1 \qquad (10)$$

QUAL2E only requires specification of the relationships for velocity (eq. 5) and depth (eq. 6) but the coefficients for equation 7 are implicitly specified by equations 9 and 10.

These options can be put into perspective by noting that, for a given specific channel cross-section, the coefficients (a, c, e) and exponents (b, d, f) can be derived from equation 2. For example, if a channel of rectangular cross-section is assumed, then width (W) is not a function of streamflow (Q), the exponent (f) is zero (0.00) and the coefficient (e) is the width of the rectangular channel (W). By noting that hydraulic radius (R) is approximately equal to depth (D) for wide streams and that A = D W, the discharge coefficients for rectangular cross sections can be derived by substituting equation 8 into equation 4 thusly:

$$Q = \frac{1}{n} A R^{2/3} S^{1/2} = \frac{1}{n} S^{1/2} W D D^{2/3} = \frac{1}{n} S^{1/2} W D^{5/3} \qquad (11)$$

Solving equation 11 for D gives

$$D = c\,Q^{3/5} = c\,Q^{0.60} \quad \ldots\ldots \quad 12$$

where $c = [\, n \,/\, W\, S^{1/2}\,]^{3/5}$ for rectangular channels. This implies that

$$V = a\,Q^{2/5} = a\,Q^{0.40} \quad \ldots\ldots \quad 13$$

where $a = [\, n\, W^{2/3} \,/\, S^{1/2}\,]^{-3/5}$ for rectangular channels.

Having shown that Manning's equation is a subset of the Discharge Coefficients option, we can further investigate its use with information that can be readily collected in a reconnaissance survey. Leopold et al. (1964) have noted that stream channels in humid regions tend towards a rectangular cross-section because cohesive soils promote steep side slopes whereas noncohesive soils encourage shallow-sloped, almost undefined banks.

Channel Cross-Section	Exponent for Velocity (b)	Exponent for Depth (d)	Exponent for Width (f)
Rectangular	0.40	0.60	0.00
Average of 158 US Gaging Stations	0.43	0.45	0.12
Average of 10 Gaging Stations on Rhine River	0.43	0.41	0.13
Ephemeral Streams in Semiarid US	0.34	0.36	0.29

Figure 5. - Comparison of Hydraulic Exponents

Figure 5 compares hydraulic exponents for a rectangular channel with data reported by Leopold et al. (1964). Note that the average velocity exponent is relatively constant for all channel cross sections. The major variation occurs as a decrease in the depth exponent and concomitant increase in the width exponent as channel cross-sections change from the steep side slopes characteristic of cohesive soils to the shallow slopes of arid regions with noncohesive soils. Discharge Coefficients is perhaps the more useful of the two options as it is more flexible and can encompass the Manning equation for trapezoidal channels and other channel shapes as well. From a computational standpoint, the Discharge Coefficients option is more efficient as Manning's equation requires an iterative solution for depth of flow.

Special Case of Discharge Coefficients

The third option that can be used is a special case of the Discharge Coefficients option. QUAL2E does not require the consistency implied by equations 9 and 10. Thus, both the velocity and depth exponents (b and d) can be chosen arbitrarily to replicate specific situations. If these exponents are chosen to be zero (0.00), then Q to the zero power is equal to one (1.0) and the coefficients a and c must be the velocity and depth. This special case is useful if the user is not interested in extrapolating water quality beyond conditions where velocity and depth are known or in investigating the sensitivity of water quality to changes in streamflow.

Selecting a Hydraulic Option

As discussed above, there are three options for computing hydraulics in QUAL2E. The Trapezoidal Channels option requires that two special conditions be met: 1) information must be available on channel geometry for the entire system being modeled and, 2) there can be no hydraulic conditions that would cause rapidly varying backwater effects such as found in lakes or reservoirs. If these conditions cannot be met, the Discharge Coefficients option must be chosen. In addition, the user may prefer to enter observed velocity and depth directly rather than compute these variables from streamflow; in which case the special case of Discharge Coefficients is an appropriate choice.

Once the option is selected, observed data must then be entered for the Trapezoidal Channels option or the coefficients and exponents must be estimated for the Discharge Coefficients option. Our recommended approach is to estimate the exponents (b and d) and then calibrate the coefficients (a and c) to observed velocity and depth. The exponents may be chosen based on observations of channel shape noted in a reconnaissance survey. If cross sections are largely rectangular with vertical banks, the first set of exponents shown in Figure 5 should be useful. If channels have steep banks typical of areas with cohesive soils, then the second set of exponents is appropriate. If the stream is in an arid region with typically noncohesive soils and shallow sloping banks, then the last set of exponents is recommended.

The key property of the channel that should be noted in a reconnaissance survey is the condition of the bank slopes or the extent to which width would increase with increasing streamflow. Clearly the bank slopes and material in contact with the streamflow at the flow rate(s) of interest are the main characteristics to note in a reconnaissance. Figure 5 gives general guidance but it should be noted that values are derived for bankful flows. Even in streams with vertical banks, the low flows may be in contact with a sand bed having shallow-sloped, almost nonexistent banks more representative of ephemeral streams in semiarid areas.

Manning's n

Regardless of the hydraulic option selected, an estimate of Manning's n must be made. In the case of the Trapezoidal Channels option, Manning's n is likely to be important as it is the only calibration coefficient in the velocity-depth-streamflow relationship. If Discharge Coefficients are chosen, then Mannings n is not used in computing velocity and depth but appears in the calculation of a longitudinal dispersion coefficient (discussed below). Hence, it is less sensitive if the Discharge Coefficients option is chosen.

Descriptor	Description
Material Involved	Earth, Rock cut, Fine gravel, Coarse gravel
Degree of Irregularity	Smooth, Minor, Moderate, Severe
Variations of Cross Section	Gradual, Alternating occasionally, Alternating frequently
Relative Effect of Obstructions	Negligible, Minor, Appreciable, Severe
Vegetation	Low, Medium, High, Very High
Degree of Meander	Minor, Appreciable, Severe

Figure 6 - Cowan's' Method for Estimation of Manning's n.

There is no exact method for selecting Manning's n (Chow, 1959). Chow describes estimation of this coefficient as "a matter of intangibles" and reviews the factors affecting its value. He describes a method attributed to Cowan (1956) for estimating Manning's n based on a detailed qualitative description of the channel summarized in Figure 6. From these descriptors, which can be obtained in a reconnaissance survey, an estimate for the coefficient can be calculated. Cowan's method is valid for channels less than 15 feet deep and is recommended in the advisor if a high degree of confidence is desired in the estimate of Manning's n.

Reach Description	Manning's n
Clean and straight	0.025
Winding with pools and shoals	0.040
Winding with pools, shoals and aquatic weeds	0.080
Very weedy, winding and overgrown with vegetation	0.120

Figure 7 - Descriptive Method for Manning's n

An alternative method, given in Figure 7, is available for users who cannot provide the detailed description required by Cowan's' method. These values are taken from the QUAL2E documentation (Brown and Barnwell, 1987). If neither method can be used, a default value of 0.020 is suggested. Of course, lesser degrees of confidence should be assigned to these less accurate methods.

Dispersion Constant

The final estimate required for the hydraulics input is the dispersion constant, K. This constant is used to compute the longitudinal dispersion coefficient as shown in equation 14,

$$D_l = 3.82\ K\ n\ V\ D^{5/6} \qquad (14)$$

where D_l is the dispersion coefficient (ft^2/sec) and K is the dispersion constant.

The theoretical and empirical basis for K is described in the QUAL2E documentation (Brown and Barnwell, 1987) and by Fischer et al.,1979. Typically, K is not a sensitive parameter in typical QUAL2E applications to free-flowing streams. Therefore, a high degree of confidence is not necessary in an initial estimate. The dispersion constant will be important, however, in applications in tidal areas or in large shallow lakes, but application of QUAL2E in these situations requires special expertise and is not recommended for novice or general users.

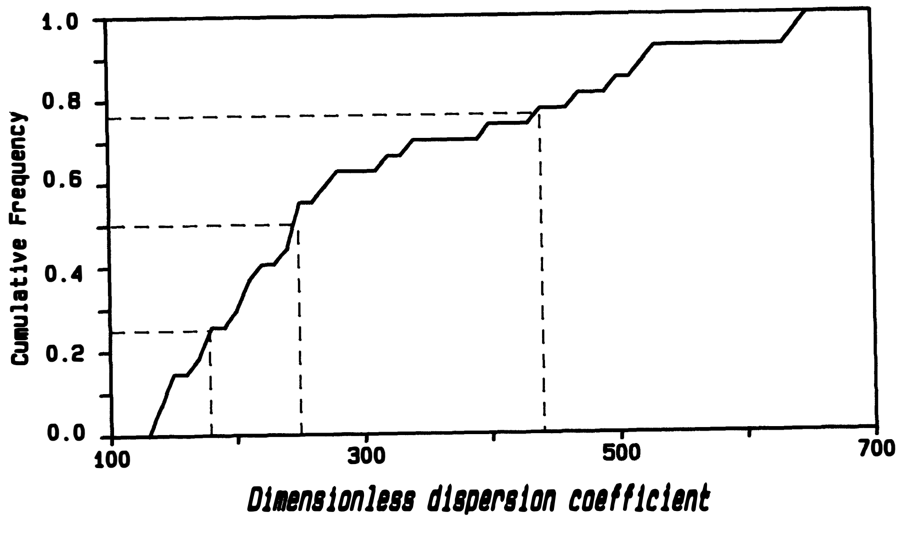

Figure 8 - Distribution of the Dispersion Constant

Figure 8 summarizes data reported in the QUAL2E documentation as guidance for estimating the dispersion constant. Much analysis has been focused on K but it has proven difficult to relate to quantitative stream physical properties such as width/ depth ratios (see Bowie et al., 1985, pp 48-55). For the QUAL2E Advisor, we have chosen to estimate K based on the degree of meander of the stream. We choose the lower 25th percentile value (175) from Figure 8 if the stream is relatively straight, the 50th percentile (250) if the stream meanders appreciably, and the 75th percentile (475) if meander is severe. Although this approach is qualitative, we believe it is reasonable based on the relative importance of the constant and the fact that meander should be related to the magnitude of turbulent eddies that induce longitudinal dispersion. If meander cannot be estimated, K is related to the reach descriptions of Figure 8. A default of 250 is used if these descriptions are not available.

SUMMARY

Clearly, application of expert systems technology offers several benefits to environmental modeling. The process of knowledge engineering (the applied side of expert systems) will improve the modeling process by producing a different perspective on modeling and by improving man-machine interaction. The most significant benefit, however, is that expert systems will increase the level of sophistication and proficiency of the average model user. This is done not through the extension of the user's knowledge (although it may be assumed that at least some users, realizing the improvement of performance, may become more involved in the modeling process), but by providing users with a better tool that is an extension of QUAL2E. A significant benefit to be gained from the application of this technology to the model developer is a better understanding of the model itself. By approaching the application of the model from the perspective of the knowledge engineer, considerable insight into the model is gained and the codification of rules for application of the model reveals many subtle linkages between inputs that may not be obvious. The development of the Advisor certainly proved valuable to the authors in developing a better understanding of this particular model.

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