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ROLE OF NUMERICAL SIMULATION IN ANALYSIS OF GROUND-WATER QUALITY PROBLEMS

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ABSTRACT

The increasing public awareness and concern about the hazards of toxic chemicals contaminating aquifers has created an increased need for predictive capabilities to analyze ground-water contamination problems. Several digital models to simulate the movement and concentration of ground-water contaminants have been documented recently. Most simulate the transport and dispersion of a nonreactive solute, but some include mathematically simple reaction terms to represent decay and sorption processes. For applications to field problems, these solute-transport models impose data requirements that, in general, exceed our practical capabilities to accurately describe the field properties and stresses of the hydraulic and chemical systems. Thus, interpretations based on model analyses must recognize the significance of uncertainties in input data. Models of ground-water systems should be regarded as just one tool among many that can be used in the analysis of a ground-water quality problem. Numerical simulation can help the analyst integrate available data, evaluate conceptual models, test hypotheses pertaining to flow and quality changes, and predict system responses to alternative stresses. The models do not replace field data, but they do offer a feedback mechanism that can help to guide the design of a more effective and more efficient data-collection program.

INTRODUCTION

About half of the population of the United States uses ground water for drinking or other domestic purposes, and approximately 40 percent of the Nation's agricultural irrigation water is supplied by ground water. But the long-term integrity and usability of the Nation's aquifers, particularly the shallow and therefore most utilized aquifers, are threatened by pollution caused by man's activities. Despite the large amount of data already collected on ground-water quantity and quality, the present extent and magnitude of ground-water contamination in the United States is uncertain. Nevertheless, there is an increasing public awareness about the hazards of toxic chemicals contaminating aquifers from which ground water discharges to water-supply wells, springs, streams, or lakes.

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In the United States, this awareness is reflected by recent actions at the Federal, State, and local levels of government. For example, the Chairman of an areawide Water Quality Board in Michigan recently stated, "Ground-water contamination is no longer a problem, it is a crisis" (Hazardous Waste News, v. 2, no. 2, Jan. 21, 1980, p. 15). On a national scope, the U.S. Environmental Protection Agency has just published a proposed Ground-Water Protection Strategy (U.S. Environmental Protection Agency, 1980) in which the stated national goal of the strategy is "... to assess, protect, and enhance the quality of ground waters to the levels necessary for current and projected future uses and for the protection of the public health and significant ecological systems." EPA adds that "... the long-term objective of the strategy is to prevent ground-water contamination before it occurs, rather than to clean it up after the fact."

Although prevention of ground-water contamination is undoubtedly the best cure, contamination is already serious in many places in the United States. In such places, even if the source of contamination were to be eliminated, contaminants already in the aquifer will continue to migrate and spread through the aquifer unless they are immobilized, neutralized, or removed. The magnitude of the problem is reflected by the results of several recent surveys of municipal and industrial waste-disposal sites in the United States (U.S. Environmental Protection Agency, 1980); they indicate that (1) 32,000 to 50,000 disposal sites may contain hazardous wastes; (2) of the approximately 57 million tons of hazardous liquid and solid industrial wastes generated in 1978, about 80 percent were disposed improperly in landfills or lagoons and pose a threat of ground-water contamination; (3) there may be as many as 100,000 abandoned industrial landfill sites; and (4) there are over 25,000 industrial surface impoundments and most of them are unlined. Pollution at a single site may be localized or may spread over a large area, depending on the nature and source of the pollutant and on the nature of the ground-water system. Of growing concern is the cumulative impact of pollution from diffuse sources, such as septic tanks, airblown debris, or agricultural applications, or from areas with a high density of point sources, on the water quality of regional ground-water flow systems. These numerous site-specific problems have created a need for general and transferable models to simulate and predict the movement of contaminants in flowing ground water. However, because of controversies that often arise over the origins and liabilities for sources of contamination, ground-water quality models and modeling analyses are undergoing increasingly greater scrutiny.

For ground-water contamination problems, needs for aquifer analysis frequently focus on one of two general types of situations-- (1) assessments of already contaminated sites, and (2) planning to minimize contamination hazards from future activities or waste-disposal operations. Both types of situations require the capability to predict the behavior of chemical contaminants in flowing ground water. Reliable and quantitative predictions of contaminant movement can only be made if the processes controlling convective transport, hydrodynamic dispersion, and chemical, physical, and biological reactions that affect solute concentrations in the ground are understood. These processes, in turn, must be expressed in precise mathematical equations having defined parameters. Although many of the processes that affect waste movement are individually well understood, their complex interactions may not be understood well enough for the net outcome to be reliably predicted. Analysis of ground-water contamination problems can be greatly aided by the application of deterministic numerical simulation models, which solve the equations describing ground-water flow and solute transport.

Figure 1 illustrates in a general manner the role of models in providing input to the analysis of ground-water contamination problems. The value of the modeling approach is its capability to integrate site-specific data with equations describing the relevant processes as a basis for predicting changes or responses in ground-water quality. Site-specific data include (1) hydraulic and chemical properties of the aquifer (derived from field and laboratory tests), (2) geometry and boundary conditions (derived primarily from hydrogeologic mapping), (3) aquifer stresses, such as well pumpage, recharge rates, and chemical concentrations in fluid sources (estimated from direct or indirect field measurements whenever possible), and (4) spatial and temporal variations in dependent variables, such as hydraulic head and chemical concentration, which provide initial conditions and calibration criteria (derived from systematic hydraulic and chemical monitoring).

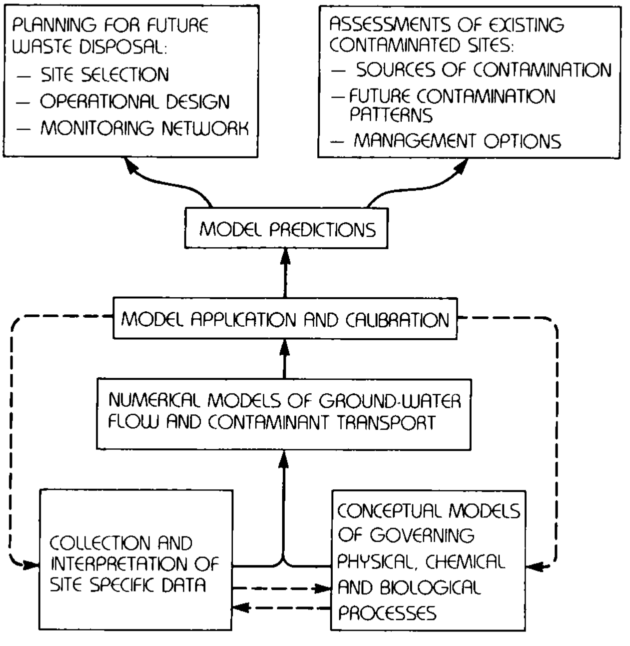

Fig. 1. Schematic overview of the role of simulation models in evaluating ground-water contamination problems.

Perhaps the most common type of problem is analyzing sites contaminated at present. Typically, the need for analyzing such a site has arisen because contaminants have been detected where they were not expected. In these cases, a numerical simulation model can help to assess the hazards or consequences of continued spreading of contaminants, either if no action is taken or if some particular management option is implemented. The predictive capabilities of a simulation model can also provide valuable input to planning future waste-disposal operations, so that any consequent ground-water contamination will be expected, tolerable, minimal, and detectable. The model analysis can help to meet these constraints of planning through (1) predictions of contaminant spreading patterns for alternative sites being considered, (2) comparisons of alternative design specifications and operational options for specific sites, and (3) by optimizing requirements for spatial and temporal sampling densities for a monitoring network.

A major difference between evaluating existing sites and new sites is that for the former, if the contaminant source can be reasonably well defined, the history of contamination itself can, in effect, serve as a surrogate long-term tracer test that provides critical information on velocity and dispersion at a regional scale. At new sites, historical data are commonly not available to provide a basis for model calibration and to serve as a control on the accuracy of predictions. As indicated in Fig. 1, there should be allowances for feedback from the stage of interpreting model output both to the data collection and analysis phase and to the conceptualization and mathematical definition of the relevant governing processes.

SOLUTE-TRANSPORT MODELS

Governing equations

The purpose of a model that simulates solute transport in ground water is to compute the concentration of a dissolved chemical species in an aquifer at any specified place and time. Because convective transport and hydrodynamic dispersion depend on the velocity of ground-water flow, the mathematical simulation model must solve at least two simultaneous partial differential equations. One is the equation of flow, from which ground-water velocities are obtained, and the second is the solute-transport equation, describing the chemical concentration in ground water.

The theory and development of the equations describing ground-water flow and solute transport have been well documented in the literature. The equation describing transient flow of a homogeneous slightly compressible fluid through a nonhomogeneous anisotropic aquifer may be written in Cartesian tensor notation as:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right) = S_s\frac{\partial h}{\partial t} + W^* \qquad (1)$$

where K_{ij} is the hydraulic conductivity tensor, LT^{-1}; h is hydraulic head, L; S_s is specific storage, L^{-1}; $W^* = W^*(x,y,z,t)$ is volume flux per unit volume (positive sign for outflow), T^{-1}; x_i, x_j are the Cartesian coordinates, (x,y,and z), L; and t is time, T. An expression for the average seepage velocity of ground water can be derived from Darcy's law and can be written in Cartesian tensor notation as:

$$V_i = \frac{-K_{ij}}{\varepsilon} \frac{\partial h}{\partial x_j} \tag{2}$$

where ε is the effective porosity. In cases where fluid properties, such as density or viscosity, vary significantly in time or space because of changes in pressure, temperature, or chemical composition, the fluid is nonhomogeneous, and the relations among water levels, heads, pressures, and fluid velocities are less straightforward. Calculations of flow rates and directions then require pressure, density, and elevation data, instead of just head measurements.

A generalized form of the solute-transport equation was presented by Grove (1976), in which terms are incorporated to represent chemical reactions and solute concentrations both in the pore fluid and on the solid surface, as follows:

$$\varepsilon\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon c V_i) - \frac{\partial}{\partial x_i}(\varepsilon D_{ij}\frac{\partial c}{\partial x_j}) + C'W^* = CHEM \tag{3}$$

where CHEM equals

$-\rho_b \frac{\partial \bar{c}}{\partial t}$ for linear equilibrium controlled ion-exchange reactions,

$\sum_{k=1}^{s} R_k$ for s chemical rate controlled reactions,

$-\lambda(\varepsilon c+\rho_b\bar{c})$ for decay,

and where c is concentration of the solute, ML^{-3}; D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2T^{-1}; C' is concentration of the solute in the source or sink fluid, ML^{-3}; ρ_b is bulk density of the solid, ML^{-3}; $\bar{c}$ is concentration of the species adsorbed on the solid; R_k is the rate of production of the solute in reaction k of s different reactions, $ML^{-3}T^{-1}$; and λ is the decay constant (equal to ln 2/half life), T^{-1}.

Much of the recently published work on solute-transport has focused on the nature of dispersion phenomena in ground-water systems and whether or not equation 3 accurately represents the processes causing changes in concentration in an aquifer, even for nonreactive solute species. For example, in discussing the development and derivation of the solute-transport equation, Bear (1979, p. 232) states, "As a working hypothesis, we shall assume that the dispersive flux can be expressed as a Fickian type law." The third term of equation 3, therefore, represents the dispersion process as one in which the concentration gradient is the driving force for the dispersive flux. This, in effect, is a practical engineering approximation for the dispersion process that proves adequate for some field problems. But, because it incorrectly represents the actual physical processes causing observed dispersion at the scale of many field problems, which is commonly called macrodispersion, it is inadequate for many other situations. Smith and Schwartz (1980) conclude that macroscopic dispersion results from large-scale spatial variations in hydraulic conductivity and that the use of relatively large values of dispersivity with uniform hydraulic conductivity fields is an inappropriate basis for describing transport in geologic systems. Both Gelhar et al. (1979) and Matheron and de Marsily (1980) examined flow and transport in a stratified porous medium and concluded that transport may be non-Fickian in nature. Gelhar et al. (1979) indicate that the mean transport process becomes Fickian for large time and that the value of dispersivity increases asymptotically to a constant value. On the other hand, Matheron and de Marsily (1980) argue that if flow is parallel to the bedding, solute transport will generally be non-Fickian, even for large times.

In the conventional formulation of equation 3, the dispersion coefficient itself is a function both of the intrinsic properties of the aquifer (such as heterogeneities in hydraulic conductivity) and of the fluid flow. This relationship was expressed by Scheidegger (1961) as:

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} \tag{4}$$

where α_{ijmn} is the dispersivity or characteristic length of the porous medium (a fourth-order tensor), L; V_m and V_n are the components of the flow velocity of the fluid in the m and n directions, respectively, LT^{-1}; and $|V|$ is the magnitude of the velocity vector, LT^{-1}. Both Scheidegger (1961) and Bear (1979) show that the dispersivity of an isotropic porous medium can be defined by two constants. These are the longitudinal dispersivity of the medium, α_L, and the transverse dispersivity of the medium, α_T. Most applications of transport models to ground-water contamination problems in the United States that have been documented to date have been based on this conventional formulation.

Numerical methods

Perhaps the most important technical advancement in the analysis of ground-water contamination problems during the past 10 years has been the development of deterministic numerical simulation models that efficiently solve the governing flow and transport equations for the properties and boundaries of a specific field situation. However, no single model is available yet that is equally suitable for the entire spectrum of possible problems. Particularly difficult numerical problems arise if the chemical reaction terms are highly nonlinear or if the concentration of the solute of interest is strongly dependent on the concentration of numerous other chemical constituents.

Three types of numerical methods are usually used to solve the solute-transport equation: finite-difference methods, finite-element methods, and the method of characteristics. Each has some advantages, disadvantages, and special limitations for applications to field problems. Each method also requires that the area of interest be subdivided by a grid into a number of smaller subareas.

The method of characteristics was originally developed to solve hyperbolic equations. When solute-transport is dominated by convective transport, as is common in field problems, then equation 3 closely approximates a hyperbolic equation and is highly compatible with the method of characteristics. The development and application of this technique to problems of flow through porous media have been presented by Garder et al. (1964), Reddell and Sunada (1970), and Bredehoeft and Pinder (1973), and a general computer program is documented by Konikow and Bredehoeft (1978).

Finite-difference methods solve an equation that approximates the partial differential equation. Although problems of numerical dispersion, overshoot, and undershoot may induce significant errors for some problems, these methods can efficiently provide accurate answers, particularly when dispersive transport is large compared to convective transport. In general, the finite-difference methods are the simplest mathematically and the easiest to program for a digital computer. A three-dimensional, transient, finite-difference model that simultaneously solves the pressure, energy-transport, and mass-transport equations for nonhomogeneous fluids is described by INTERA (1979).

Finite-element methods use assumed functions of the dependent variables and parameters to evaluate equivalent integral formulations of the partial differential equations. Pinder (1973) and Grove (1977), among others, have indicated that Galerkin's procedure is well suited to solve solute-transport problems. Pinder and Gray (1977) present a comprehensive analysis and review of the application of finite-element methods to ground-water flow and transport problems. These methods generally require the use of more sophisticated mathematics than the previous two methods, but for many problems may be more accurate numerically and more efficient computationally. Grove (1977) demonstrates for one-dimensional problems that numerical dispersion and oscillations can be minimized in the Galerkin method by using higher-order basis functions, but that computational costs using cubic basis functions increased by a factor of 10 compared to linear basis functions. A major advantage of the finite-element methods is the flexibility of the finite-element grid, which allows a close spatial approximation to irregular boundaries of parameter zones.

MODEL CALIBRATION

For sound interpretations based on model output, it must be demonstrated that the model accurately solves the governing equations and accurately represents the real system. There are several sources of error in model output to be recognized. Some errors may be introduced by inappropriate approximations inherent in the assumed governing equations because of inadequacies of the conceptual model. Other errors in the solution are introduced by the numerical algorithm used to solve the governing equations (this is rarely a problem for the solution to the flow equation, but may sometimes be significant for the solute-transport equation). However, in most model applications to field problems, the dominant cause of errors in model output is the presence of errors or uncertainty in the input data, which reflect our inability to accurately and quantitatively describe the aquifer properties, stresses, and boundaries.

To demonstrate that a deterministic ground-water simulation model is realistic, field observations of aquifer responses are compared to corresponding values obtained from the model. The objective of this calibration procedure is to minimize differences between the observed data and the computed values. In effect, the model is calibrated by reproducing a set of historical data with some acceptable level of accuracy.

Matalas and Maddock (1976) argue that model calibration is synonymous with parameter estimation. The calibration of a deterministic ground-water model is often accomplished through a trial-and-error adjustment of the model's input data (aquifer properties, sources and sinks, and boundary and initial conditions) to modify the model's output. Because a large number of interrelated factors affect the output, this may become a highly subjective procedure. Recent advances in parameter identification procedures, such as described by Cooley (1979), Neuman (1980), and Umari et al. (1979), help to eliminate some of the subjectivity inherent in model calibration. However, the hydrologic experience and judgement of the modeler will always be an important factor in calibrating a model both accurately and efficiently. The modeler should be familiar with the specific field area being studied to know that both the data base and the numerical model adequately represent prevailing field conditions. The modeler must also recognize that the uncertainty in the specification of sources, sinks, and boundary and initial conditions should be evaluated during the calibration procedure in the same manner as the uncertainty in aquifer properties.

In general it is more difficult to calibrate a solute-transport model of an aquifer than it is to calibrate a ground-water flow model. Fewer parameters need to be defined to compute the head distribution with a flow model than are required to compute concentration changes with a solute-transport model. Because the ground-water seepage velocity is determined from the head distribution, and because both convective transport and hydrodynamic dispersion are functions of the seepage velocity, a model of ground-water flow is usually calibrated before an adequate and reliable solute-transport model can be developed.

One of the objectives of model calibration is to improve the conceptual model of the aquifer. The conceptual model consists of our understanding of the physical and functional nature of the aquifer. Because the simulation model numerically integrates the effects of the many factors that affect ground-water flow or solute transport, the computed results should be internally consistent with all input data, and we can determine if any element of the conceptual model must be revised. In fact, previous concepts or interpretations of aquifer parameters or variables, such as represented by potentiometric maps or the specification of boundary conditions, may be revised during calibration as a result of feedback from the model's output. In a sense, any adjustment of input data constitutes a modification of the conceptual model.

In most field problems there are some inadequate data, so the values for some parameters have to be estimated. A common approach is to first assume the best estimates of values for parameters and then adjust the values until a best fit is achieved between observed and computed dependent variables. Although this can probably be accomplished most efficiently with a parameter-estimation model, the trial-and-error method is currently most commonly used. In order to maintain the value of the process-oriented structure of a deterministic model, the degree of allowable adjustment of any parameter is generally directly proportional to the uncertainty of its value or specification and limited to its range of expected values or confidence interval. As parameter adjustment produces a change in model output, the responses should be evaluated quantitatively to provide a measure of progress in model calibration and to guide the determination of direction and magnitude of subsequent changes in model input. This requires an evaluation of successive changes in the goodness of fit between observed data and model output.

Another objective of the calibration procedure is to determine the sensitivity of the model to factors that affect ground-water flow or solute transport. Evaluating the importance of each factor helps determine which data must be defined most accurately and which data are already adequate or require only minimal definition. If additional data cannot be collected, then the sensitivity tests help to assess the reliability of the model by demonstrating the effect of a given range of uncertainty or error in the input data on the output of the model. The relative sensitivities of the parameters that affect flow and solute transport vary from problem to problem. Thus, a sensitivity analysis is vital during the early stages of a model study.

A calibrated simulation model can be used to predict future system responses. The model's predictions can be utilized to help evaluate the impact of alternative decisions or policies regarding problems of water planning, water management, and water-quality control, or to study the effects of an extreme hydrologic event such as a flood or a drought.

EXAMPLE OF MODEL APPLICATION

The Rocky Mountain Arsenal has been operating near Denver, Colorado, since 1942. Its operations have produced liquid wastes that contain complex organic and inorganic chemicals, including a characteristically high chloride concentration, apparently as high as 5,000 mg/L. From 1943 to 1956 the high-chloride wastes were discharged to several unlined disposal ponds, a, b, c, d, and e, shown in Fig. 2. Figure 2 also shows that after about 14 years the definable high-chloride plume had extended to nearly 10 km. Interpretation of the hydraulic, chemical, and geologic data indicates that liquid wastes seeped out of the unlined disposal ponds, infiltrated into the underlying alluvial aquifer, and migrated downgradient toward the South Platte River (Konikow, 1977).

The solute-transport model described by Konikow and Bredehoeft (1978) was used to simulate the movement of chloride through the alluvial aquifer in an effort to reproduce the 30-year history of contamination and to evaluate possible management alternatives. The stringent data requirements for applying the solute-transport model pointed out deficiencies in the data base available at the start of the study. Specifically, it was found that the velocity distribution determined from the water-table configuration mapped in 1956 (see Petri and Smith, 1956) was in part inconsistent with the observed pattern of spreading, which separated into one main plume and a smaller secondary plume. The subsequent quantitative analysis and reinterpretation of available hydrogeologic data led to a revised conceptual model of the aquifer properties and boundaries that strongly influenced solute transport.

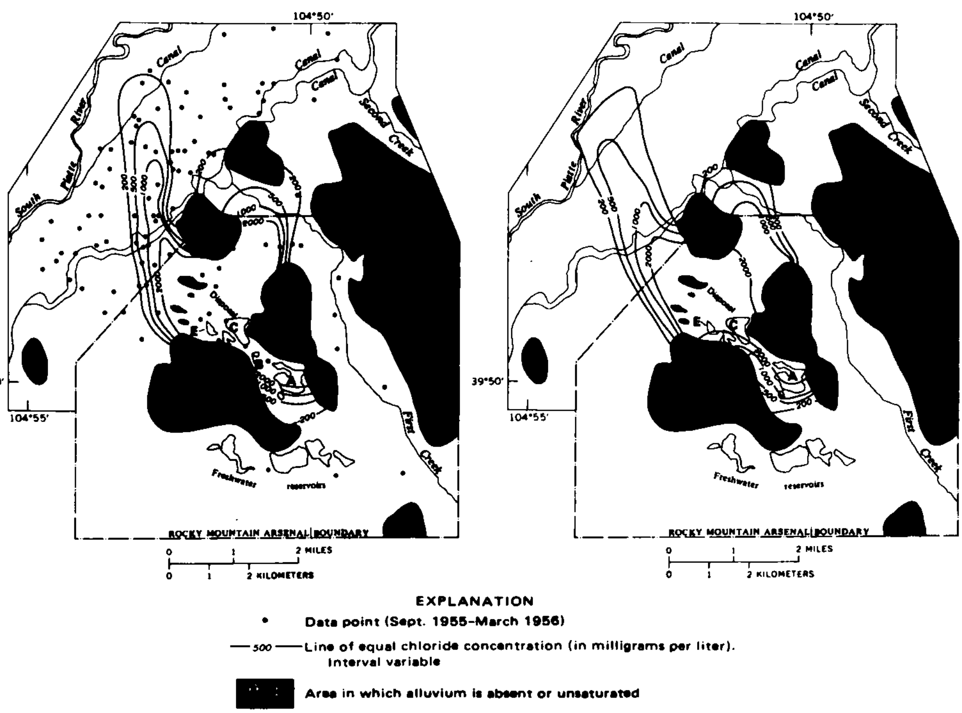

Fig. 2. Observed (left) and computed (right) chloride concentrations, 1956 (Konikow, 1977).

The reinterpretations indicate that the alluvial aquifer is nonuniform in thickness, sloping, discontinuous, and heterogeneous (Konikow, 1975). Areas in which alluvium is either absent or unsaturated most of the time form internal barriers that significantly affect rates and directions of ground-water flow within the alluvial aquifer, as reflected by the water-table configuration shown in Fig. 3, and, hence, significantly influence solute transport.

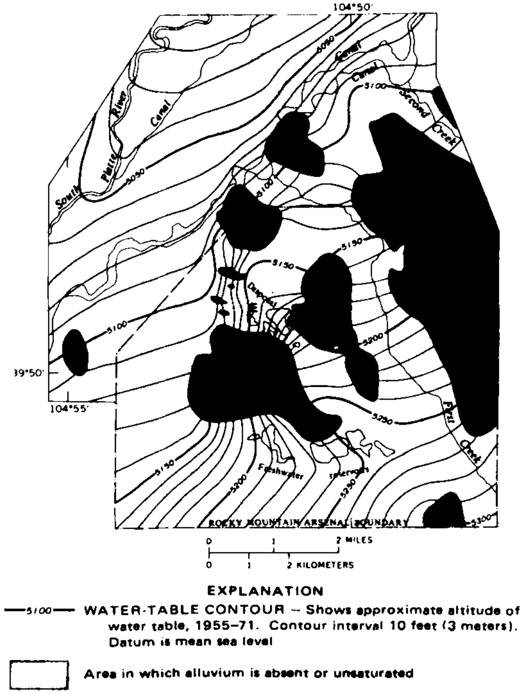

Fig. 3. General water-table configuration in the alluvial aquifer, 1955-1971 (Konikow, 1977).

In calibrating the flow and transport models for the alluvial aquifer, the water-table configuration served as the basis for evaluating goodness of fit with respect to adjustments of transmissivity, net recharge in irrigated areas, and some boundary conditions. Initial estimates of net recharge were used in a preliminary calibration of the model. Next, transmissivity values and boundary conditions in the model were adjusted between successive simulations with an objective of minimizing the differences between observed and computed water-table altitudes in the irrigated area. As shown in Fig. 4, the standard error of estimate generally decreased as successive simulation tests were made. After about seven tests, additional adjustments produced only small improvements in the fit between the observed and computed water tables. A final estimate of recharge in irrigated areas was made using the set of values for other parameters that minimized the

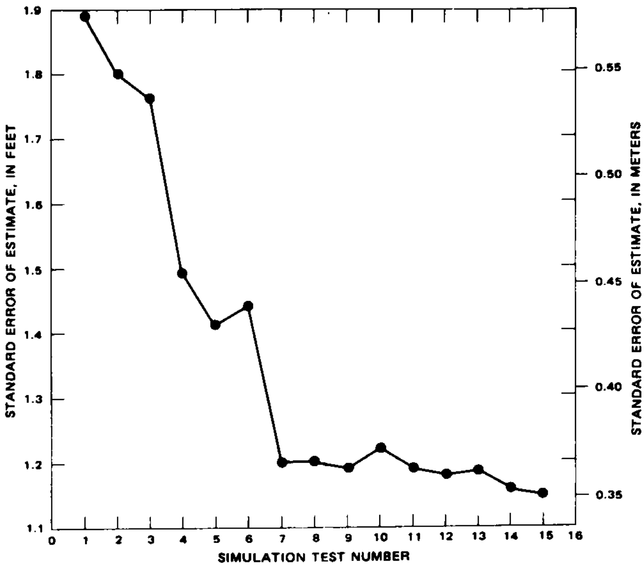

Fig. 4. Change in standard error of estimate of water-table altitudes for successive simulation tests (Konikow, 1977).

standard error of estimate. The mean of the differences between observed and computed heads at all nodes in the irrigated area was then minimized when a net recharge rate of approximately 0.47 m/yr was assumed.

Figure 2 shows that the computed chloride concentration pattern for 1956 agrees closely with the observed pattern. Since 1956, disposal has been into an asphalt-lined reservoir, thereby contributing to a subsequent decrease in the extent and magnitude of ground-water contamination. Figure 5 illustrates that by 1972 chloride concentrations greater than 1,000 mg/L had become limited to just two small parts of the main area of contamination. Both are areas of relatively low hydraulic conductivity. The pattern of contamination computed for 1972, also shown in Fig. 5, agrees fairly well with the observed pattern, although the former shows somewhat longer plumes. After the 30-year simulation period, the model identifies (1) the two areas of high chloride concentrations, (2) the reduction in size and strength of the plume since 1956, and (3) changes in water-table elevations in response to changes in water input to unlined ponds.

Other simulations predicted the effects of implementing several possible aquifer reclamation plans and of the option of no action. Results of these analyses indicate that it would take decades for this aquifer to recover naturally to its original chloride concentrations, but that carefully planned and engineered water management could reduce this restoration time to the order of only years.

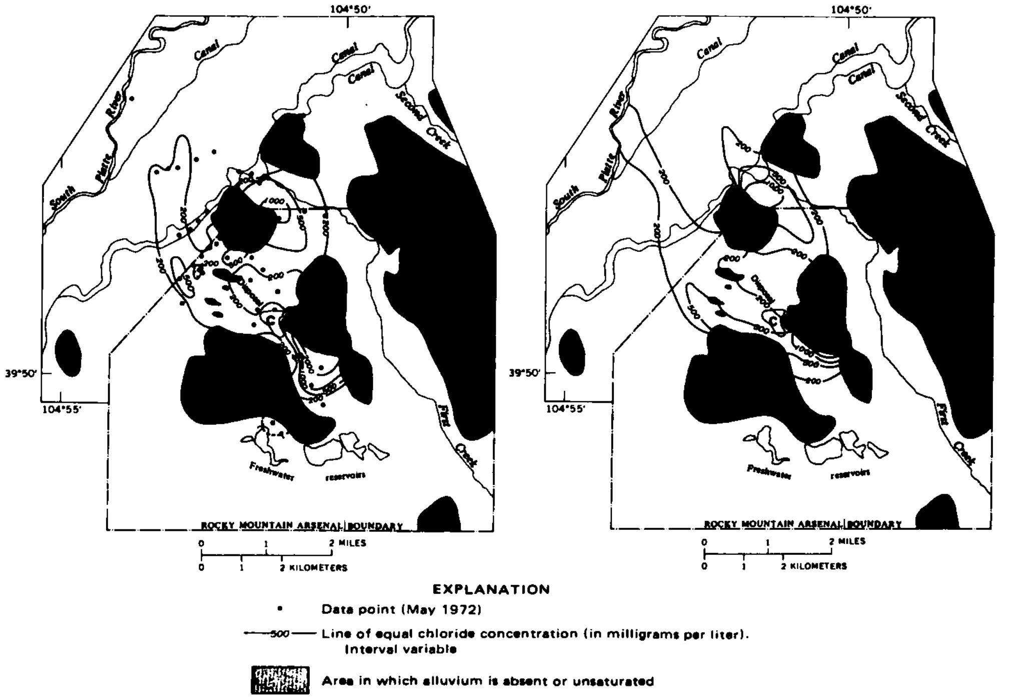

Fig. 5. Observed (left) and computed (right) chloride concentrations, 1972 (Konikow, 1977).

CONCLUSIONS

Although every ground-water contamination problem is in many ways unique, the solute-transport principles and investigative approaches are general and transferable; they are linked by the universal nature of the physical and chemical laws governing fluid flow, transport processes, and chemical solubility. Comprehensive investigations of ground-water contamination problems are greatly aided by the application of solute-transport models, which provides a disciplined format for assessing the consistency within and between (1) concepts of the governing processes and (2) data describing the relevant coefficients. Feedback from preliminary models not only helps the investigator to set improved priorities for the collection of additional data, but also helps test hypotheses concerning governing processes in order to develop an improved conceptual model of the problem. The resulting simulator enables predictions and evaluations to be made of effects on quality and quantity of ground water and surface water that would ensue from implementing a new land-or water-management policy.

The predictive capability of a solute-transport model also aids in designing a monitoring network by indicating the most and least probable areas of future contamination and rates of spreading. Rational choices for sampling locations and frequencies are then available. This is vital because proper evaluation of ground-water pollution problems is most limited by inadequacies in field data.

The results of applying a solute-transport model at the Rocky Mountain Arsenal indicate that a simulation model can adequately and quantitatively integrate the effects of the major factors that control changes in solute concentration in a 30-year history of chloride contamination. This example illustrates the value of a model as an investigative tool to help understand the processes and parameters controlling the movement and fate of contaminants in ground-water systems.

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