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PREFACE

This document, funded as an IDA Central Research Project, has been prepared to examine the use of newly developed models to study how contamination is transported. Standard use of streamlines and particle tracking methods have limitations. However, recent developments in numerical simulations of oil, water, and gas flow in petroleum reservoirs have provided the opportunity to improve the speed and accuracy of current approaches.

This document summarizes research on streamlines at Stanford University and commercial development of streamline-based simulators by StreamSim Technologies for the potential aid they may provide in environmental cleanup. Further investigation of such methods may provide enhanced information regarding how these techniques can best be applied to contaminant transport problems.

This document was researched and written by Martin Blunt and Martha Crane of the Department of Petroleum Engineering at Stanford University; Rebecca R. Rubin of the Institute for Defense Analyses was the project leader. The authors wish to thank Dr. Robert L. Hirsch of Advanced Power Technologies, Inc., for his review and helpful suggestions.

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THE USE OF STREAMLINE-BASED METHODS TO MODEL CONTAMINANT TRANSPORT IN THE SUBSURFACE

A. SUMMARY

The use of streamlines—lines that follow the instantaneous flow field—are standard in hydrology to map capture zones of wells and to visualize flow patterns. Particle tracking methods, where contaminant mass is transported along streamlines, are also widely used. These methods model contaminant transport free from numerical artifacts, but their application is limited to simple single-phase flow problems. When the flow field changes with time, when non-aqueous phase liquids and air are also present, or where there are complex non-linear geochemical or radioactive interactions between chemical species, particle tracking methods have severe limitations. For such cases, conventional finite difference or finite element numerical models are used. But these suffer from numerical errors and grid orientation effects and tend to be very slow.

Recent developments in the numerical simulation of the flow of oil, water, and gas in petroleum reservoirs have extended the use of streamline-based methods to complex, non-linear problems that are mathematically similar to those encountered in contaminant transport. This offers the opportunity to develop streamline-based methods in hydrology and environmental engineering, resulting in a significant improvement in speed and accuracy compared with current simulation approaches.

In this report, we first give a brief summary of research on streamlines at Stanford University and the commercial development of streamline-based simulators by StreamSim Technologies. We then provide a review of streamline methods and particle tracking in the hydrology literature, describe new ideas in a streamline-based approach to simulating contaminant transport, and outline its potential applications.

B. RESEARCH AT STANFORD AND COMMERCIAL DEVELOPMENT

Much of the recent research on streamline-based simulation for predicting oil recovery in petroleum reservoirs has been performed at Stanford University in the Department of Petroleum Engineering by Rod Batycky, Marco Thiele, and Martin Blunt. Current research at Stanford, performed by Martha Crane, is exploring the use of streamline-based methods to model contaminant transport. This work is being performed in collaboration with Andy Tompson and co-workers at Lawrence Livermore National Laboratory with the aim of applying the method to study the movement and fate of radionuclides at the Nevada Test Site.

In the oil industry, there is considerable interest in commercial applications of streamline-based reservoir simulation. StreamSim Technologies was founded in 1997 by Rod Batycky, Martin Blunt, and Marco Thiele to develop a streamline-based reservoir simulator based on research conducted at Stanford University from 1991 to 1996. The development effort is supported by a consortium of major oil companies. The primary application of the simulator will be to predict oil recovery from detailed geological models of the reservoir using significantly less computer time than traditional finite-difference approaches. The technology is particularly suitable to analyze "what if" scenarios, such as multiple geological models, infill drilling benefits, pattern conversions, and enhanced recovery options. In the future, we anticipate that a commercial contaminant transport simulator could be developed using the same ideas and that could be used to predict the fate and movement of contaminants in the subsurface and aid in the design of optimal remediation and containment strategies.

1. Introduction

Modeling of contaminant transport has been the focus of much attention over the past few decades because the ability to make quantitative predictions about flow and transport in the subsurface is needed to properly utilize ground-water resources and to restore polluted ground water. The ability to do realistic ground-water flow simulation requires a quantitative description of the hydrogeological setting, which often requires transforming more qualitative geological data into single or multiple realizations of the hydraulic properties. Although there is uncertainty in the assignment of hydraulic properties throughout the flow field, there is a consensus that ground-water flow modeling

has been fairly successful at determining an accurate pressure distribution and velocity field. For example, models which solve the ground-water flow equation numerically using either finite difference or finite element techniques have yielded good results.

When the migration of dissolved constituents by ground-water flow is considered, the difficulty of simulation is greatly increased because of the complexity of the transport process. The transport of solutes in ground water is effected by a large number of processes, including advection, dispersion, diffusion, chemical processes, and biochemical processes. Because of this wide range of chemical and physical processes, scientists from many disciplines have contributed to the understanding of contaminant transport in the subsurface. In fact, solute transport modeling is now recognized as an interdisciplinary challenge (Abriola, 1987). The mathematical statement of the transport of a non-reactive solute is the advection-dispersion equation:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - \nabla \cdot (vC) \qquad (1)$$

where C is solute concentration, v is the Darcy velocity of the ground water, and D is a dispersion coefficient. Many numerical methods for solving the advection-dispersion equation have been explored by ground-water hydrologists.

This report will provide an overview of the methods most commonly used in modeling the transport of solutes in ground water. Such models consider advective, dispersive, and reactive transport. Particular attention will be given to the ground-water literature concerning advection-dominated transport because it is generally agreed that for heterogeneous porous media, especially if there are strong sources and sinks, considering advective forces only provides an adequate approximation (Schafer-Perini and Wilson, 1991). In fact, in field cases, macroscopic dispersion is believed to be controlled by the heterogeneity of hydraulic properties (Smith and Schwartz, 1980). Therefore, if the spatial variability of properties such as hydraulic conductivity is sufficiently described, ignoring dispersive transport is a reasonable approximation. Finally, streamline methods developed in the petroleum literature will be described and compared with the particle tracking approach in order to consider future directions for contaminant transport modeling.

2. Numerical Methods for Modeling Solute Transport

In the ground-water literature, transport models are categorized as Eulerian, Lagrangian, or mixed Eulerian-Lagrangian. In the Eulerian approach, the transport equation is solved on a fixed spatial grid, so concentrations are associated with fixed

points or volume elements in space (Bear, 1972). Both finite difference and finite element methods are examples of this method. Because of their wide use and success in flow simulations, these methods were among the first used in transport modeling. It is now recognized that these methods handle dispersion-dominated transport accurately and efficiently; but, in advection-dominated transport problems, Eulerian methods suffer from numerical dispersion and artificial oscillations, especially in the region of sharp concentration fronts (Kinzelbach, 1986; Bear and Verruijt, 1987). In order to minimize numerical errors, small discretization in time and space is needed, which requires enormous and sometimes prohibitive computational effort especially when considering field scale problems. Since many field situations are advection dominated, an alternative to Eulerian methods was needed to handle field scale solute migration in heterogeneous porous media.

In Lagrangian methods, concentration is associated with fluid elements or particles that move with the prevailing velocity field (Bear and Verruijt, 1987; Zheng and Bennett, 1995). This method avoids directly solving the advection-dispersion equation by representing the solute mass by a large number of particles which move with the ground-water velocity. The Lagrangian formulation of the advective transport equation is presented in detail in Zheng and Bennett (1995), but the final result can be given as: $DC/Dt=0$, where C is the concentration of a particular fluid element. This equation reflects the notion that, as a fluid particle moves along its pathline, its concentration, provided the transport is purely advective, does not change. Therefore, the solution to the advective transport problem is reduced to defining pathlines. Lagrangian methods are free of numerical dispersion and are accurate and efficient for modeling advection-dominated transport. These methods have been quite successful in representing the movement of steep concentration fronts (Moltyaner et al., 1993). Because of the success of the Lagrangian approach for solving the advective transport equation, these methods are widely used for modeling field scale advective transport (e.g., Bair et al., 1990; Guven et al., 1992).

When dispersive transport must be considered, mixed Eulerian-Lagrangian methods (such as the method of characteristics approach in Konikow and Bredehoft's (1978) widely used two-dimensional solute transport model) have attempted to combine the strengths of the two previous methods. The Lagrangian approach is used to solve the advection term of the transport equation, and the Eulerian approach is used for the dispersive term. In formulating a solution, first the advective transport is solved using a

Lagrangian approach in which each particle is assigned an initial concentration value. Particles are moved along pathlines for one time step and placed in a gridblock on the underlying Cartesian grid. After an advective step, each cell node is assigned a concentration by averaging the concentration of all particles within that cell. Changes in concentration due to dispersive transport are then calculated using a finite difference method on the rectangular grid. After this step, the particle concentration values are updated to reflect the changes in grid concentration values. Then another advective step is taken. Zheng (1993) extended the method of characteristics to model three-dimensional solute transport.

Moltyaner et al. (1993) compared the different methods for numerical simulation of tracer transport in a field scale experiment at the Twin-Lake site. The results indicated that while the finite element model chosen for this study could successfully describe the pressure field, the transport solution suffered from numerical dispersion. For both the method of characteristics approach and a Lagrangian method, the random walk particle method (Prickett, 1981), superior results in the transport simulation were obtained. The final assessment in this paper was that the best results were achieved by the random walk particle method; and the subsequent studies of tracer flow at the site used this approach only.

a. Modeling Advective Transport

In many field cases, or as a first approximation, transport is considered to be dominated by advection (Bear and Verruijt, 1987; Zheng and Bennett, 1995). For this reason, many studies of solute migration have focused on purely advective transport (Guven et al., 1992; Bair et al., 1990). When dispersion is neglected, ground-water flow paths coincide with the paths of contaminant solutes. These pathways have typically been determined using particle tracking. An alternative to particle tracking for defining pathlines is stream functions. Stream functions have been used in two-dimensions to assess the travel time of contaminants (Nelson, 1978; Javadel et al., 1984; Fogg and Senger, 1985; Frind and Matanga, 1985). Approximating streamlines in three-dimensions by using stream functions has also been attempted, but the mathematics are difficult (Strack, 1984).

Particle tracking is a simple concept. Many small fluid particles are placed in the flow field, and their position is monitored as they move through the flow domain over a series of time steps. A concentration value is assigned to each fluid particle. For

contaminant transport modeling, non-contaminant particles receive a concentration of zero; contaminant particles receive a finite concentration so that the entire solute mass is represented. Clearly the mass assigned to each particle is determined by the number of particles chosen to represent the solute species. The contaminant particles are distributed either randomly or uniformly in the source region (Zheng and Bennett, 1995). The particles are then advanced through the region of interest along path lines calculated from the flow field. The description of the flow field can be analytical in which case the velocity is known everywhere; but, more commonly, the velocities are defined on a grid used to solve the discretized flow equations. When the values of velocity are known only at the interfaces of gridblocks, an interpolation scheme is necessary to evaluate the velocity at any point in the domain.

One major difference in the particle tracking methods described in the ground-water literature involves the choice of interpolation schemes. The most commonly used velocity interpolation schemes for particle tracking are simple linear interpolation or multilinear interpolation. In linear interpolation, each component of the velocity vector varies linearly in its own coordinate direction. Therefore changes in the x-velocity component are independent of changes in the y and z directions (Pollock, 1988). Multilinear interpolation considers each component of the velocity vector to be a linear function of all the coordinate directions. For example, in bilinear interpolation, which is used for two-dimensional models, the x-component of the velocity is formulated as a linear function of both the x and y positions (Anderson and Woessner, 1992). These two interpolation schemes give somewhat different representations of the flow field. In essence, linear velocity interpolation satisfies a cell-by-cell mass balance but gives a discontinuous velocity field, and the multilinear schemes give a completely continuous velocity field but fails to satisfy mass balance. Other velocity interpolation schemes, such as bicubic interpolation, have been used as well but are not common (Zheng and Bennett, 1995). The choice of a velocity interpolation scheme hinges on the numerical method used to solve the flow problem. If a finite difference method is used to solve for the velocity field, only a simple linear interpolation scheme is consistent with this formulation and will therefore conserve mass locally within each finite difference cell (Pollock, 1988). Pollock's method has been extended and applied to finite element representation of the velocity field (Cordes and Kinzelbach, 1992).

Choosing a velocity interpolation method is the first step in particle tracking. The next and final step involves choosing a tracking scheme. Particles are tracked along pathlines by solving the equations:

$$dx/dt=v_x, \tag{2}$$

$$dy/dt= v_y, \tag{3}$$

$$dz/dt= v_z \tag{4}$$

The methods that are typically used to solve these equations include semianalytical, Euler, and Runge-Kutta (Anderson, 1992). The semianalytical solution is outlined in Pollock (1988) and is possible only if a linear velocity interpolation scheme is used. Euler's method involves the simple numerical integration (e.g., in the x-direction):

$$x_{n+1} = x_n + v_x(x_n,y_n,z_n)dt. \tag{5}$$

This was the tracking approach used in some of the early particle tracking literature (Konikow and Bredehoft, 1978; Prickett, 1981). Since the value of velocity at the starting point is extrapolated over the entire interval, the time step must be sufficiently small to make accurate predictions about the particles' movement; for this reason, it may take several time steps to advance a particle through one gridblock. Euler's method is only a first order approximation of the integral, so the accuracy has been improved by using higher order numerical integration methods such as the fourth-order Runge-Kutta method (Zheng, 1989). Euler's and Runge-Kutta methods can be used with any velocity interpolation scheme. However, since a linear interpolation scheme is consistent with a finite-difference approximation of the velocity field, and the semianalytical tracking method introduces no numerical error, Pollock's method for pathline computation is the best for using with finite-difference flow models.

b. Semianalytical Pathlines

Because Pollock's method for pathline generation is most commonly used because of its appropriateness for interpolating a finite-difference generated velocity field, the details of this tracking procedure are included. As mentioned before, the pathline each individual fluid particle follows is determined from knowledge of the velocity field and an underlying assumption that the velocity field varies linearly in each coordinate direction and is independent of the velocities in the other directions. The velocity in the x direction is defined as

$$V_x = V_{x,o} + m_x\left(x - x_o\right) \tag{6}$$

where m_x is the velocity gradient defined as

$$m_x = \frac{V_{x,\Delta x} - V_{x,o}}{\Delta x} \tag{7}$$

Knowing that $v_x = dx/dt$, Equation 6 can be integrated to find the time required to reach the x exit face $\Delta t_{e,x}$,

$$\Delta t_{e,x} = \frac{1}{m_x}\left[\frac{V_{x,o} + m_x(x_e - x_o)}{V_{x,o} + m_x(x_i - x_o)}\right] \tag{8}$$

The time to exit the other faces is derived in similar fashion. The pathline will exit the face with the smallest exit time value (Δt_e). Finally, the exit position is computed by substituting Δt_e into Equation 8 and solving for x_e,

$$x_e = \frac{1}{m_x}\left[V_{x,i}\exp(m_x \Delta t_e) - V_{x,o}\right]. \tag{9}$$

When a pathline is traced, the inlet and exit position in each gridblock as well as the time to cross each gridblock ($\Delta t_{e,i}$) is recorded. The gridblock k containing the particle traveling on a particular pathline at time t is then calculated by summing the time it takes the pathline to cross each gridblock until the time of interest is reached:

$$\sum_{i=0}^{i=k} \Delta t_{e,i} \le t \le \sum_{i=0}^{i=k+1} \Delta t_{e,i} \tag{10}$$

It is important to point out what information emerges from a particle tracking approach. The main results of particle tracking methods are mass arrival time, arrival position, and concentration. Because these are the data required by many environmental agencies, particle tracking is commonly used to model regulatory problems involving ground-water contamination (Anderson, 1995).

Particle tracking has been used to study the pattern and rate of ground-water movement and contaminant transport. In particular, it has been used to delineate regional flow systems as well as recharge and discharge area for the ground-water system of Long Island, New York (Buxton et al., 1991). The results from this study indicated that particle tracking yields results that are consistent with the conceptual understanding of the system. Particle tracking has also been used to delineate the capture zone of wells (Shafer, 1987; Bair et al., 1990; Schafer-Perini and Wilson, 1991). In general, capture zones of wells are delineated through reverse particle tracking where particles are started at the well and traced backward to a source region. Schafer-Perini and Wilson (1991) also suggested a

method for dynamically allocating particles in order to best capture the migration of the contaminant front. Bair et al. (1990) used particle tracking to predict the pathways of contaminants from hypothetical release points along a highway. Guven et al. (1992) used particle tracking to model a two-well tracer test. Their model considered only advection when describing the transport of tracer between an injection and production well. The results of this study indicated that purely advective models were successful when sufficient knowledge of the spatial distribution of hydraulic conductivity. In recent years, some of the more interesting applications of particle tracking involve coupling with other models to explore the effects of such mechanisms as dispersion (Prickett, 1981) and geochemistry (Fabriol et al., 1993).

c. Modeling Other Transport Processes

One major limitation of particle tracking is that it simulates only advective transport. Some work has been done to incorporate particle tracking into more complete transport models. Most importantly, the effects of dispersion on contaminant transport were introduced in the "random walk" model (Prickett, 1981). The random walk method uses the particle tracking technique of associating a mass of solute with each particle, and then the effect of dispersion is included by adding a random displacement to the particle location after each advective time step. Basically, dispersion can be incorporated in a particle tracking method by adding a random motion to the motion along pathlines. For the spreading of solute by dispersion, the random dispersive displacement can be described by a normal distribution. Since Prickett first introduced the use of random walk to model the advection-dispersion equation, numerous other researchers have used the method to look at transport in porous media (e.g., Uffink, 1988; Gelhar, 1990; LaBolle et al., 1996). Dispersion is an important mechanism to model in solute transport because a dispersed plume is more widespread than a plume moving by advection alone; also the concentration of solute in the plume is reduced by the dispersive process (Mercer and Waddell, 1993). In addition, the arrival of the first contaminant particles at a point of interest is often controlled by dispersion.

Simple chemical reactions have also been included in particle tracking codes. For example, adsorption has been modeled by adding a retardation factor to the mass transport equation (Wen and Kung, 1995). The process of adsorption reduces the rate at which the contaminant front is moving because of reactions between the solid matrix and the solute which cause some of the solute to bond to the solid surface. If this reaction is fast (relative to the physical transport), reversible, and modeled by a linear isotherm, the effect can be

represented by a retardation factor. The retardation factor allows the transport equation to be expressed in a purely advective form by replacing the Darcy velocity with a retarded velocity given by:

$$v_{retarded} = \frac{v}{R}$$, where R is a retardation factor.

This is an important mechanism to understand because adsorption makes it more difficult to remove the solute at a given site. Another process, which has been included in particle tracking codes, is radioactive decay (Wen and Kung, 1995). Obviously, this is an important phenomenon to consider at sites polluted with nuclear wastes. If the half-life is of the same order or less than the residence time in the ground-water system, then radioactive decay can be an important mechanism for attenuation. Also, the daughter products of the radioactive species add to the complexity of the system (Mercer and Waddell, 1993). Radioactive decay is included in particle tracking analysis through the addition of a decay constant (l) to the mass-transport equation. (Kinzelbach, 1986). Essentially, the mass associated with each particle changes over time according to the relation:

$$M_{particle}^{n+1} = M_{particle}^{n} e^{-\lambda \Delta t}$$, where M is the mass of the particle.

Goode and Konikow (1989) modified the method of characteristics code to account for decay as well as equilibrium controlled sorption.

d. Assessment of the Particle Tracking Approach

Clearly, the Lagrangian approach has many advantages for modeling contaminant transport. The problem of numerical dispersion is eliminated. Some of the key transport processes can be included in a straightforward and intuitive way. But, there are drawbacks to the method as well. The concentration field is computed by evaluating the location and mass of the particles. The accuracy of this method depends completely on the number of particles chosen to represent the contaminant mass. Representing more than one solute species requires a huge number of particles; and the method loses its computational efficiency. Because of these difficulties, modeling multi-species transport and considering interactions or coupling between species is not possible. Since most contaminants are composed of many components that interact with each other, particle tracking is somewhat limited in its application to practical problems.

It has become clear that for solute transport modeling to be a predictive tool, the reactive processes that affect the movement of contaminant plumes must be incorporated.

Most of the processes that have been modeled using the Lagrangian approach are straightforward processes such as linear sorption and decay, which can be handled in a particle analysis by adjusting the velocity and mass of the particles. More complex and coupled interactions can be approached through sequentially solving advective and reactive transport equations. There are examples in the ground-water literature of coupled transport and geochemical models (e.g., Gerla, 1992; Fabriol, 1993; Garcia-Delgado and Koussis, 1997). Streamline methods recently used for modeling a variety of transport phenomenon in petroleum reservoirs provide an intuitive approach to coupling more complete reactive transport models with ground-water flow models to provide new insight into reactive transport.

e. Streamline Methods

A streamline method for flow in porous media is a computational technique that approximates the transport of fluid constituents using a collection of one-dimensional mass conservation equations. These mass conservation equations correspond in a one-to-one fashion with the number of streamlines in the model. The path each streamline will follow is computed in the same way as the tracing of pathlines described by Pollock (1988) and discussed earlier. Therefore, the streamline method requires the solution to the ground-water flow equation as input. Additionally, the formulation of a streamline method requires that the appropriate mass conservation equation be transformed from its three-dimensional form to a one-dimensional form along a streamline This transformation is summarized below for the case of single-phase, multicomponent, incompressible flow (after Thiele et al., 1997). In this case, the multidimensional form of the mass conservation equation can be expressed as

$$\phi \frac{\partial C_i}{\partial t} + \vec{u}_t \cdot \nabla F_i = 0, \quad \text{for } i = 1, \ldots, \text{number of components}, \tag{11}$$

where C_i is the concentration of component i and F_i is the convective flux of component i. By defining a time-of-flight coordinate along a streamline as

$$\tau = \int_o^{\zeta} \frac{\phi}{|u_t|} d s, \tag{12}$$

where s is the streamline direction, the divergence operator can be rewritten according to

$$|u_t| \frac{\partial}{\partial s} \equiv \vec{u}_t \cdot \nabla = \phi \frac{\partial}{\partial \tau}. \tag{13}$$

Substitution in Equation 11 transforms the conservation equation to a one-dimensional formulation for each component

$$\frac{\partial C_i}{\partial t} + \frac{\partial F_i}{\partial \tau} = 0, \quad \text{for } i = 1,..., \text{number of components.} \tag{14}$$

A one-dimensional numerical solver is used to solve Equation 14. This method can be extended to any equation that describes the physics of interest in one dimension.

A streamline method for transport in porous media is better suited than particle tracking for looking at the complexities of reactive transport. Once streamlines are traced through a three-dimensional flow field, each streamline is treated as a one-dimensional system along which mass is transported by a model that appropriately captures the physics of flow. Current reactive transport models that embody the most complete and rigorous representation of chemical processes are generally limited to one- and two-dimensional saturated flow systems. Full three-dimensional reactive transport simulations are typically very coarsely resolved (Johnson et al., 1997). For example, Fabriol et al. (1993) used coupled reactive transport simulator with a five-by-five grid to predict the composition of water that percolated through sandstone. Clearly, a fully coupled reactive transport simulator could not be used to solve field-scale contaminant transport model unless an extremely coarse grid is used. The trend in modeling complex transport processes has been toward decoupled or sequential solutions, which are conceptually intuitive. These solutions involve coupling together flow, advective, dispersive, and reactive transport models.

The streamline approach has already been used to model numerous single- and two-phase transport problems in heterogeneous petroleum reservoirs (Batycky et al., 1997). Most of the mass transport in particle tracking considers the movement of a single component through the flow field. If many components are to be considered, the accounting issues become overwhelming. Since the streamline method moves compositions instead of mass, dealing with multicomponent systems is computationally more efficient. In addition, particle tracking is not well suited to looking at coupling between the components in the system. Most pollutants in ground water contain multiple components, which react with one another and the porous media. These components are coupled together through processes such as radioactive decay or competition for sorption sites. Equations such as those describing the migration of a radionuclide decay chain can easily be formulated as a set of coupled one-dimensional equations (Gureghian and

Jansen, 1985). This set of equations can be solved along each streamline, thereby capturing the evolution of the solute over time.

It seems clear that the field of solute transport modeling is moving toward a more complete description of the many processes that influence the development of contaminant plumes. This process necessarily involves looking at full three-dimensional representations of the flow field and solute mass. But the most complete reactive transport models are one-dimensional. Since streamlines are one-dimensional pathways, the reactive transport models can be applied to each streamline in the system. Because the intersection of the streamlines with an underlying three-dimensional grid is also known, these one-dimensional reactive transport solutions can be placed in a three-dimensional setting. This could greatly enhance the ability to model field-scale contaminant transport problems.

3. Conclusions

Streamline-based methods recently developed to simulate multiphase transport in petroleum reservoirs may be extended to model contaminant transport. This method overcomes the limitations of particle tracking techniques, and the errors and poor performance of conventional grid-based methods. Using streamline methods, there is the potential to enhance considerably the ability to model complex nonlinear transport phenomena in heterogeneous aquifers.

REFERENCES

1. Abriola, Linda M. 1987. "Modeling Contaminant Transport in the Subsurface: An Interdisciplinary Challenge." *Reviews of Geophysics*, 25 (2), 125-134.

2. Anderson, M.P. 1995. "Ground-water Modeling in the 21st Century." *Ground-water Models for Resources Analysis and Management.* A.I. El-Kadi (ed), 79-93.

3. Anderson, M.P. and W.W. Woessner. 1992. *Applied Ground-water Modeling: Simulation of Flow and Advecive Transport.* Academic Press Inc., San Diego, 381 pp.

4. Bair, E.S., R.A. Sheets, S.M. Eberts. 1990. "Particle Tracking Analysis of Flow Paths and Travel Times from Hypothetical Spill Sites Within the Capture Area of a Wellfield." *Ground Water.* 28(6), 884-892.

5. Batycky, R.P., M.J. Blunt, and M.R. Thiele, 1997. "A 3D Field Scale Streamline-Based Simulator." *SPE Reservoir Engineering*, 12, November 246-254.

6. Bear, J. and A. Verruijt. 1987. *Modeling Ground-water Flow and Pollution.* D. Reidel Publishing Company, Dordrecht, Holland, 414 pp.

7. Bear, J. 1972. *Dynamics of Fluids in Porous Media.* Elsevier Science Publishers, New York, 764pp.

8. Buxton, H.T., T.E. Reilly, D.W. Pollock, D.A. Smolensky. 1991. "Particle Tracking Analysis of Recharge Areas on Long Island, New York." *Ground Water.* 29(1), 63-71.

9. Fabriol, R. J-P.Sauty, and G. Ouzounian. 1993. "Coupling Geochemistry with a Particle Tracking Transport Model." *Journal of Contaminant Hydrology.* 13, 117-129.

10. Fogg, G.E., and R.K. Senger, 1985. "Automatic Generation of Flow Nets with Conventional Ground-water Modeling Algorithms." *Ground Water.* 23(3), 336-344.

11. Frind, E.O. and G.B. Matanga, 1985. "The Dual Formulation of Flow for Contaminant Transport Modeling, 1: Review of Theory and Accuracy Aspects." *Water Resources Research.* 21(2), 159-169.

12. Garcia-Delgado, R.A. and A.D. Koussis, 1997. "Ground-Water Solute Transport with Hydrogeochemical Reactions." *Ground Water*. 35(2), 243-249.

13. Gerla, P. 1992. "Pathline and Geochemical Evolution of Ground Water in a Regional Discharge Area, Red River Valley, North Dakota." *Ground Water*. 30 (5), 743-753.

14. Goode, D.J. and L.F. Konikow. 1989. "Modification of a Method of Characteristics Solute-Transport Model to Incorporate Decay and Equilibrium Controlled Sorption or Ion Exchange." *U.S.G.S. Water Resources Investigations Report 89-4030.* 65 pp.

15. Gureghian, A.B. and G. Jansen, 1985. "One-Dimensional Analytical Solutions for the Migration of A Three-Member Radionuclide Decay Chain in a Multilayered Geologic Medium." *Water Resources Research.* 21(5), 733-742.

16. Guven, O, F.J. Molz, J.G. Melville, S. El Didy, and G.K. Boman. 1992. "Three-Dimensional Modeling of a Two-Well Tracer Test." *Ground Water.* 30(6), 945-957

17. Javandel, I., C. Doughty, and C.F. Tsang, 1984. *Ground-water Transport: Handbook of Mathematical Models.* Water Resources Monogram 10, A.G.U., Washington, D.C.

18. Johnson, J.W., A.F.B. Tompson, R.D. Hornung, R.D. Aines and K.J. Jackson, 1997. "Development of Advanced GET Reactive Transport Capabilities to Address Critical Problems Associated with Nuclear Materials Disposal and Environmental Safety." Lawrence Livermore National Laboratory, Livermore, CA.

19. Kinzelbach, W. 1986. *Ground-water Modelling an Introduction with Sample Programs in BASIC.* Elsevier Science Publishers, New York, 333 pp.

20. Kinzelbach, W. 1988. "The Random Walk Method in Pollutant Transport Simulation." *Ground-water Flow and Quality Modelling,* E. Custodio, A. Gurgui, and J.P. Ferreira (ed), 227-246.

21. Konikow, L.F. and J.D. Bredehoft. 1978. "Computer Model of Two-dimensional Solute Transport and Dispersion in Ground Water." *U.S.G.S. Water Resources Investigation Book 7, Chapter C2,* 90 pp.

22. LaBolle, E.M., G.E. Fogg and A.F.B. Tompson, 1996. "Random-walk Simulation in Heterogeneous Porous Media: Local mass-conservation problems and Implementation Methods." *Water Resources Research.* 32(3), 583-593.

23. Mercer, J.W. and R.K. Waddell. 1993, "Contaminant Transport in Groundwater." *Handbook of Hydrology.* D.R. Maidment (ed), Chapter 16.

24. Moltyaner, G.L, M.H. Klukas, C.A. Wills, and R.W.D. Killey. 1993. "Numerical Simulations of Twin Lake Natural-Gradient Tracer Tests: A Comparison of Methods." *Water Resources Research.* 29 (10), 3433-3452.

25. Nelson, R.W. 1978. "Evaluating the Environmental Consequences of Ground-water Contamination," Parts 1-4. *Water Resources Research.* 14(3), 409-450.

26. Pollock, D.W. 1998. "Semi-analytical Computation of Pathlines for Finite-Difference Models." *Ground Water.* 26(6), 743-750.

27. Prickett, T.A., T.G. Naymik, and C.G. Lonnquist. 1981. "A Random-Walk Solute Transport Model for Selected Ground-water Quality Evaluations." *Illinois State Water Survey,* Bulletin 65, 103 pp.

28. Schafer-Perini A.L. and J.L. Wilson. 1991. "Efficient and Accurate Front Tracking for Two-Dimensional Ground-water Flow Models." *Water Resources Research.* 27(7), 1471-1485.

29. Shafer, J.M. 1987. "Reverse Pathline Calculation of Time Related Capture Zones in Nonuniform Flow." *Ground Water.* 25, 283-289.

30. Smith, L. and F.W. Schwartz. 1988. "Mass Transport 3: Role of Hydraulic Conductivity in Prediction." *Water Resources Research.* 17(5), 1463-1479.

31. Strack, O.D.L. 1984. "Three-Dimensional Streamlines in Dupuit-Forchheimer Models." *Water Resources Research.* 20(7), 812-822.

32. Thiele, M.R., R.P. Batycky, and M.J. Blunt, 1997. "A Streamline-Based 3D Field Scale Compositional Reservoir Simulator," *SPE paper 38889 in the Proceedings of the 1997 SPE Annual Technical Conference and Exhibition*, San Antonio, TX, October.

33. Tompson, A.F.B. and L.W. Gelhar, 1990. "Numerical Simulation of Solute Transport in Three-Dimensional Randomly Heterogeneous Porous Media." *Water Resources Research.* 26(10), 2541-2562.

34. Uffink, G. 1988. "Modeling of Solute Transport with the Random Walk Method." *Ground-water Flow and Quality Modelling,* E. Custodio, A. Gurgui, and J.P. Ferreira (ed), 247-265.

35. Wen, X-H and C-S Kung. 1995. "A Q-Basic Program for Modeling Advective Mass Transport with Retardation and Radioactive Decay by Particle Tracking." *Computers & Geosciences.* 21(4), 463-480.

36. Zheng, C., G.D. Bennett, and C.B. Andrews. 1991. *Concepts, Strategy, and Software for Practical Three-dimensional Contaminant Transport Modeling.*

37. Zheng, C. 1993. "Extension of the Method of Characteristics for Simluation of Solute Transport in Three Dimensions." *Ground Water.* 31(3), 456-465.

38. Zheng, C. and G.D. Bennett. 1995. *Applied Contaminant Transport Modeling: Theory and Practice.* International Thomson Publishing Inc, New York, 440 pp.

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13. ABSTRACT *(Maximum 200 words)*

Estimates of future environmental and health risk, assessment of environmental cleanup cost, and liability decisions often depend on numerical modeling of the subsurface movement of ground water and of ground-water contamination. There are two main approaches, grid point methods (for example, finite element analyses) and flow methods (for example, particle tracking and streamline calculation). Each approach has its strengths and weaknesses; for example, grid point methods are better at calculating dispersion and flow methods are better at calculating the advective movement of sharp fronts of contaminant concentration. A major drawback of grid point methods is that greater accuracy requires both smaller grid spacing and shorter time steps, resulting in unsupportable computational burdens. Streamline calculations are much faster but have been restricted to single-phase systems. Recent advances in numerical technique, motivated by petroleum recovery problems, have expanded the application of streamline methods to complex, nonlinear mutli-phase flow and allow very rapid calculation and numerical solution. This paper outlines the approach and considers how these same techniques could be applied to environmental contaminant transport problems and concludes that useful potential applications exist.

14. SUBJECT TERMS

Environment, ground water, subsurface, contamination, contaminant, transport, numerical modeling, streamline, hydrology, particle tracking, flow.

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