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Modelling of Sea Water Intrusion

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1.0 Introduction

In many coastal areas, the development and management of fresh ground water resources are seriously constrained by the presence of sea water intrusion. Sea water intrusion is a natural phenomenon that occurs as a consequence of the density contrast between fresh and saline ground water. Normally, the denser saline water forms a deep wedge that is separated from the fresh water body by a transition zone of variable density. In some cases, this wedge can extend for many kilometers inland. Providing conditions to remain unperturbed, the saline water body will remain stationary, its position being largely defined by the fresh water potential and hydraulic gradient. However, when the aquifer is disturbed by pumping of the fresh water, sea level change or by changing recharge conditions, the saline water body will gradually move until a new equilibrium condition is achieved. Problems arise when saline water from the deep saline wedge enters pumping wells and affects the water quality. Most commonly, this occurs at individual wells where heavy pumping lowers the fresh water potential in the immediate vicinity of the well and causes saline water to be drawn upwards to the well, a phenomenon known as upconing. This type of problem is often very localized and can be rectified by distributing production amongst a group of smaller shallower wells. A similar but potentially more serious problem occurs when a coastal aquifer is overdeveloped on a regional scale. This results in lowering of the fresh water potential throughout the area and progressive and extensive invasion of the aquifer by sea water. In some heavily exploited aquifers, the inflow of sea water may represent a significant component of the aquifer's flow budget.

2.0 Ghyben - Herzberg Principle

Until fairly recently, most research on the relationship between fresh and saline ground water in coastal aquifers has been based on the analytical solutions. Ghyben (1888) and Herzberg (1901) independently developed similar formulations on sea water intrusion, widely known as the Ghyben-Herzberg principle. Their formulation was based on the hydrostatic equilibrium between fresh water and saline water (assumed immiscible) in a U-shaped tube. It states that the fresh water-saline water interface in an aquifer occurs at a depth of Z below mean sea level, as represented by

$$Z = \frac{\rho_f}{\rho_s - \rho_f} h_f \qquad \text{... (1)}$$

where, ρ_f is the density of fresh water (M/L^3), ρ_s is the density of saline water (M/L^3), and h_f is the elevation of the fresh water level above mean sea level (L).

Substitution of ρ_f (1000 kg/m^3) and ρ_s (1025 kg/m^3) in equation (1) shows that $Z = 40 h_f$. In other words, the depth to the saline water interface below mean sea level is 40 times the elevation of water table above sea level (h_f). It also follows from equation (1) that if water table in an unconfined coastal aquifer is lowered by 1 m, the fresh water-saline water interface will rise by 40 m. This simple formulation has been used widely by hydrogeologists, but it is an inadequate representation, because it describes a steady state equilibrium and does not take into account important mechanisms such as advection and dispersion.

3.0 Numerical Modelling

In practice, the spatial relationship between fresh and saline ground water in coastal and island aquifers is complex and management of the fresh water resource may be a difficult and sensitive issue. The aquifer system is rarely near equilibrium and the fresh and saline water bodies are normally separated by a transition zone created due to chemical diffusion and mechanical mixing. Under these conditions, the response of the saline water body to pumping is difficult to predict and depends on various factors including aquifer geometry and properties (intrinsic permeability, anisotropy, porosity, dispersivity); abstraction rates and depths; recharge rate; and distance of pumping wells from the coastline. Sophisticated tools are required to quantify the aquifer response to these factors. With the advent of large scale and widely available computing resources, the numerical approach to sea water intrusion analysis has moved to the forefront.

Currently, several solute transport models, suitable for the simulation of sea water intrusion and upconing of saline water beneath pumping sites, are commercially available. These include SUTRA (Voss, 1984), HST3D (Kipp, 1987) and SALTFLOW (Molson and Frind, 1994). These models provide solutions of two simultaneous, non-linear, partial differential equations that describe the conservation of mass of fluid and conservation of mass of salt in porous media. SUTRA (Saturated-Unsaturated TRAnsport) employs a two-dimensional finite-element approximation of the governing equations in space and an implicit finite-difference approximation in time and is suitable for simulation of a vertical section of an aquifer that is subject to sea water intrusion. HST3D (Heat and Solute Transport in 3 Dimensions) employs three-dimensional finite-difference approximations of the governing equations. This model is capable of simulating an aquifer with irregular geometry. SALTFLOW is also three-dimensional but utilize a finite-element approximation of the governing equations for an aquifer that is subject to the intrusion of sea water.

4.0 Saturated-Unsaturated TRAnsport Model (SUTRA)

SUTRA is a finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground water flow with energy transport or chemically-reactive single-species solute transport. SUTRA may be employed for areal and cross-sectional modelling of saturated ground water flow systems and for cross-sectional modelling of unsaturated zone flow. Solute transport simulation using SUTRA may be employed to model natural or man-induced chemical species transport including processes of solute sorption, production and decay and may be applied to analyse ground water contaminant transport problems and aquifer restoration designs. In addition, solute transport simulation with SUTRA may be used for modelling of variable density leachate movement and for cross-sectional modelling of salt water intrusion in aquifers in near-well or regional scales with either dispersed or relatively sharp transition zones between fresh water and salt water. SUTRA energy transport simulation may be employed to model thermal regimes in aquifers, subsurface heat conduction, aquifer thermal energy storage systems, geothermal reservoirs, thermal pollution of aquifers and natural hydrogeologic convection systems. Three versions of SUTRA have been released so far : Version V12842D (original version released in 1984), Version V06902D (first revision in 1990), and Version V09972D (second revision in 1997).

SUTRA is written in Fortran 77 including optional Fortran 90 statements allowing dynamic array allocation. SUTRA requires that files needed for the simulation be defined prior to execution. A Name File (SUTRA.FIL) is used for this purpose. For each file (upto six), the unit number is specified on one record followed by a record specifying the file name. Generally, the program is easily installed on most computer systems. The code has been used on a wide variety of computers, ranging from UNIX-based computers to DOS-based 386 computers with as little as 640K of RAM.

4.1 Purpose and Scope

SUTRA is a computer program which simulates fluid movement and transport of either energy or dissolved substances in a subsurface environment. The model employs a two-dimensional hybrid finite-element and integrated finite-difference method to approximate the governing equations that describe the two interdependent processes that are simulated: (1) fluid density-dependent saturated or unsaturated ground water flow, and either (2a) transport of a solute in the ground water in which the solute may be subject to equilibrium adsorption on the porous matrix and both first-order and zero-order production or decay, or (2b) transport of thermal energy in the ground water and solid matrix of the aquifer.

Simulation using SUTRA is in two dimensions, although a three-dimensional quality is provided in that the thickness of the two-dimensional region in the third direction may vary from point to point. Simulation may be done in either the areal plane or in a cross-sectional view. The spatial coordinate system may be either cartesian (x, y) or radial-cylindrical (r, z). Areal simulation is usually physically unrealistic for variable-density fluid problems.

Ground water flow is simulated through numerical solution of a fluid mass balance equation. The ground water system may be either saturated, or partly or completely unsaturated. Fluid density may be constant or vary as a function of solute concentration or fluid temperature.

SUTRA tracks the transport of either solute mass or energy in the flowing ground water through a unified equation which represents the transport of either solute or energy. Solute transport is simulated through numerical solution of a solute mass balance equation where solute concentration may affect fluid density. The single solute species may be transported conservatively or it may undergo equilibrium sorption (through linear, Freundlich or Langmuir isotherms). In addition, the solute may be produced or decay through first- or zero-order processes.

Energy transport is simulated through numerical solution of an energy balance equation. The solid grains of the aquifer matrix and fluid are locally assumed to have equal temperature, and fluid density and viscosity may be affected by the temperature.

Almost all aquifer material, flow and transport parameters may vary in value throughout the simulated region. Sources and boundary conditions of fluid, solute and energy may be specified to vary with time or may be constant. SUTRA dispersion processes include diffusion and two types of fluid velocity-dependent dispersion. The standard dispersion model for isotropic media assumes direction-independent values of longitudinal and transverse dispersivity. A velocity-dependent dispersion process for anisotropic media is also provided. This process assumes that longitudinal dispersivity varies depending on the angle between the flow direction and the principal axis of aquifer permeability when permeability is anisotropic.

4.2 Governing Equations

The simulation of sea water intrusion requires the solution of partial differential equations that describe conservation of mass of fluid and conservation of mass of solute. These are summarized below (Voss, 1984).

Conservation of mass of fluid

The fluid mass balance in a saturated porous medium can be expressed as :

$$\frac{\partial(\varepsilon\rho)}{\partial t} = -\Delta.(\varepsilon\rho V) + Q_p \qquad \text{... (2)}$$

where ε (x,y,z,t) is porosity (dimensionless); ρ (x,y,z,t) is fluid density (M/L^3); Q_p (x,y,z,t) is fluid mass source [$M/(L^3T)$]; V (x, y, z, t) is fluid velocity (L/T); x, y and z are cartesian coordinate variables (L); t is time (T); and Δ is $[(\partial/\partial x)i + (\partial/\partial y)j + (\partial/\partial z)k]$. The term on the left hand side of equation (2) expresses the change in fluid mass contained in the void space of the local volume with time. The first term on the right hand side of equation (2) represents the contribution to local fluid mass change due to excess of fluid inflows over outflows. The second term (Q_p) accounts for external additions of fluid.

The fluid mass balance (equation 2) can also be represented by:

$$(\rho S_{op})\frac{\partial p}{\partial t} + \left[\varepsilon \frac{\partial \rho}{\partial C}\right]\frac{\partial C}{\partial t} - \Delta.\left[\left(\frac{\varepsilon \rho k}{\mu}\right).(\Delta p - \rho g)\right] = Q_p \qquad \text{... (3)}$$

where $S_{op} = [(1-\varepsilon)\ \alpha + \varepsilon\ \beta]$ is specific pressure storativity (LT^2/M); α is porous matrix compressibility (LT^2/M); β is fluid compressibility (LT^2/M); C is solute mass fraction or mass of solute (M_s) per mass of fluid (M_s /M); k (x,y,z) is solid matrix permeability tensor (L^2); μ (x,y,z,t) is fluid viscosity (M/(LT)), p (x,y,z,t) is fluid pressure [$M/(LT^2)$], and g is the gravity vector (L/T^2).

Conservation of mass of solute

The solute mass balance for a single species stored in solution is expressed as :

$$\partial\frac{(\varepsilon\rho C)}{\partial t} = -\Delta.(\varepsilon\rho V C) + \Delta.\left[\varepsilon\rho(D_m I + D).\Delta C\right] + Q_p C^* \qquad \text{... (4)}$$

where D_m is apparent molecular diffusivity of solutes in solution in a porous medium (L^2/T); I is the identity tensor (dimensionless); D is the dispersion tensor (L^2/T); and C^* is the solute mass fraction of fluid sources (M_s /M). The term on the left hand side of equation (4) expresses the change in solute mass with time in a volume due to mechanisms represented by terms on the right hand side. The first term on the right hand side of equation (4), involving fluid velocity (V), represents advection of solute mass into or out of the local volume. The second term, involving molecular diffusivity of solute (D_m) and dispersivity (D), expresses the contribution of solute diffusion and dispersion to the local changes in solute mass. The diffusion contribution is based on a physical process driven by concentration gradients, and is often negligible at the field scale. The last term accounts for dissolved-species mass added by a fluid source with concentration C^*.

The mechanical dispersion tensor D is related to the velocity of ground water flow. For an isotropic porous medium in two spatial dimensions, it is expressed as follows :

$$D = \begin{bmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{bmatrix} \qquad \text{... (5)}$$

The tensor D is symmetric and its elements are :

$$D_{xx} = \frac{1}{V^2}(d_L V_x^2 + d_T V_y^2)$$

$$D_{yy} = \frac{1}{V^2}(d_T V_x^2 + d_L V_y^2)$$

$$D_{xy} = D_{yx} = \frac{1}{V^2}(d_L - d_T)(V_x V_y)$$

... (6)

where V (x,y,t) = $(V_x^2 + V_y^2)^{1/2}$ is the magnitude of fluid velocity (L/T); V_x (x,y,t) and V_y (x,y,t) are the components of velocity in the x and y directions (L/T); and d_L (x,y,t) and d_T (x,y,t) are, respectively, the longitudinal and transverse dispersion coefficients (L^2/T). The longitudinal and transverse dispersion coefficients describe dispersive fluxes along the direction of fluid flow and perpendicular to it. The coefficients d_L and d_T are velocity dependent, namely

$$d_L = \alpha_L V$$
$$d_T = \alpha_T V$$

... (7)

and α_L (x,y) and α_T (x,y) are the longitudinal and transverse dispersivity, respectively, of the solid matrix (L). Studies have shown that field observed dispersion coefficients are orders of magnitude larger than those observed in small scale laboratory tests. Similarly, field observations show that the dispersion coefficient increases with displacement distance at a given site.

4.3 Numerical Methods

SUTRA may be employed in one-dimensional or two-dimensional analyses. Flow and transport simulation may be either steady state which requires only a single solution step, or transient which requires a series of time steps in the numerical solution. Single-step steady state solutions are usually not appropriate for non-linear problems with variable density, saturation, viscosity and non-linear sorption.

SUTRA simulation is based on a hybridization of finite-element and integrated finite-difference methods employed in the framework of a method of weighted residuals. The method is robust and accurate when employed with proper spatial and temporal discretization. Standard finite-element approximations are employed only for terms in the balance equations which describe fluxes of fluid mass, solute mass and energy. All other non-flux terms are approximated with a finite-element mesh version of the integrated finite-difference methods. The hybrid method is the simplest and most economical approach which preserves the mathematical elegance and geometric flexibility of finite-element simulation while taking advantage of finite-difference efficiency.

The complex density-dependent ground water flow and mass transport models provide stable and accurate results when employed with proper spatial and temporal discretization. In general, spatial discretization requires a fine mesh in areas where either accurate results are required or where parameters vary greatly over short distances; however, the spatial discretization should also be consistent with the dispersivity parameters. Voss (1984) recommends a grid spacing of less than four times the dispersivity in each direction, whereas Daus et al. (1985) and Molson and Frind (1994) recommend more stringent criteria, in which the grid Peclet Number (ratio of the spatial discretization and the dispersion length) and the Courant Number (ratio of the advective distance during one time step to the spatial discretization) should match the following constraints:

$$P_x = \frac{\Delta x}{\alpha_L} \leq 2, \quad P_y = \frac{\Delta y}{\alpha_T} \leq 2, \quad P_z = \frac{\Delta z}{\alpha_T} \leq 2 \qquad \ldots (8)$$

$$C_x = \frac{V_x \Delta t}{\Delta x} \leq 1, \quad C_y = \frac{V_y \Delta t}{\Delta y} \leq 1, \quad C_z = \frac{V_z \Delta t}{\Delta z} \leq 1 \qquad \ldots (9)$$

where P_x, P_y and P_z are the Peclet Numbers; C_x, C_y and C_z are the Courant Numbers; Δx, Δy and Δz are the grid spacings; α_L and α_T are the longitudinal and transverse dispersivity, respectively; and Δt is the time step.

SUTRA employs a new method for calculation of fluid velocities. Fluid velocities, when calculated with standard finite-element methods for systems with variable fluid density, may display spurious numerically generated components within each element. These errors are due to fundamental numerical inconsistencies in spatial and temporal approximations for the pressure gradient and density, gravity terms which are involved in velocity calculation. Spurious velocities can significantly add to the dispersion of solute or energy. This false dispersion makes accurate simulation of all but systems with very low vertical concentration or temperature gradients impossible, even with fine vertical spatial discretization. Velocities as calculated in SUTRA, however, are based on a new, consistent, spatial and temporal discretization. The consistently evaluated velocities allow stable and accurate transport simulation (even at steady state) for systems with large vertical gradients of concentration or temperature. An example of such a system, that SUTRA successfully simulates, is a cross-sectional regional model of a coastal aquifer wherein the transition zone between horizontally flowing fresh water and deep stagnant salt water is relatively narrow.

The time discretization used in SUTRA is based on a backward finite-difference approximation for the time derivatives in the balance equations. Some non-linear coefficients are evaluated at the new time level of solution by projection while others are evaluated at the previous time level for non-iterative solutions. All coefficients are evaluated at the new time level for iterative solutions. The finite-element method allows the simulation of irregular regions with irregular internal discretization. This is made possible through use of quadrilateral elements with four corner nodes. Coefficients and properties of the system may vary in value throughout the mesh.

SUTRA includes an optional numerical method based on asymmetric finite-element weighting functions which results in "upstream weighting" of advective transport and unsaturated fluid flux terms. Although upstream weighting has typically been employed to achieve stable, non-oscillatory solutions to transport problems and unsaturated flow problems, the method is not recommended for general use, as it merely changes the physical system being simulated by increasing the magnitude of the dispersion process. A practical use of the method is, however, to provide a simulation of the sharpest concentration of temperature variations possible with a given mesh. This is obtained by specifying a simulation with absolutely no physical diffusion or dispersion and with 50% upstream weighting. The result may be interpreted as the solution with the minimum amount of dispersion possible for a stable result in the particular mesh in use.

In general simulation analyses of transport, upstream weighting is discouraged. The non-upstream methods are also provided by SUTRA and are based on symmetric weighting functions. These methods are robust and accurate when the finite-element mesh is properly designed for a particular simulation and should be used for most transport simulations.

4.4 Data Requirement

The most essential types of data required are salinity records with depth in a number of observation wells, hydro-dispersive parameters (or atleast detailed description of lithology, by which estimates of hydraulic conductivity can be made from similar type of areas), and tidal lags nd heights at various points in the region of interest. It is also necessary to have recharge information. This involves not only the knowledge of rainfall but also how much of it enters the ground water system and how much is drawn off by vegetation. Other useful information would include an accurate topographic map, a land use map, water supply data including extraction data, local knowledge and experience, and estimates of expected changes in regional rainfall patterns.

Two SUTRA data files are required: (i) SUTRA input data and (ii) initial conditions of pressure and concentration or temperature for the simulation. Re-programming of subroutines BCTIME and UNSAT is required to implement time-dependent boundary conditions and unsaturated flow functions, respectively. A graphical postprocessor, SUTRA-PLOT, developed by Souza (1987) is available for use with SUTRA. This postprocessor facilitates interpretation of the simulation results.

5.0 Conclusion

The coastal areas often contain some of the most densely populated areas in the world. The availability of flat land, communication arteries, easy sea transportation, good soils and high productivity of organic matter explains this fact. Intrusion of salt water into heavily exploited aquifers is a serious problem being faced in coastal areas. The development of ground water resources, therefore, requires careful management in coastal areas.

The application of SUTRA is very useful in those cases where a two-dimensional vertical cross-section adequately represents the ground water system. The importance of field data can not be over-emphasized. No model can replace a comprehensive field program which provides the required data. If reasonably good data is available, numerical models such as SUTRA, can be employed to provide an important means for guiding management decisions.

REFERENCES

1. Daus, T., Frind, E. O. and Sudicky, E. A. (1985), A Comparative error analysis in finite element formulation of the advection-dispersion equation, Advances in Water Resources, Vol. 8, No. 2, pp. 86-95.

2. Ghyben, W. B. (1888), Nota in verband met de voorgenomen putboring nabij Amsterdam: The Hague, Netherlands, Tijdschrift van Let Koninklijk Instituut van Ingenieurs, pp. 8-22.

3. Herzberg, A. (1901), Die Wasserversorgung einiger Nordseebader: Wasserversorgung, Vol. 44, pp. 815-819 and 842-844.

4. Kipp, K. L. (1987), HST3D - A computer code for simulation of heat and solute transport in three dimensional ground-water flow systems, U.S. Geological Survey, Water Resources Investigations Report 86-4095, 517p.

5. Kumar, C. P. (1998), The Modelling of Salt Water Intrusion, Training Report in the field of Deltaic Hydrology, UNDP Project (IND/90/003), National Institute of Hydrology, Roorkee.

6. Molson, J. W. and Frind, E. O. (1994), SALTFLOW - Density-dependent flow and mass transport model in three dimensions, User Guide, Waterloo Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, 68p.

7. Souza, W. R. (1987), Documentation of a graphical display program for the saturated-unsaturated transport (SUTRA) finite-element simulation model, U.S. Geological Survey, Water Resources Investigations Report 87-4245, 122 p.

8. Voss, Clifford I. (1984), A finite-element simulation model for saturated-unsaturated fluid-density-dependent groundwater flow with energy transport or chemically reactive single-species solute transport, U.S. Geological Survey, Water Resources Investigations Report 84-4369, 409p.