ASSESSMENT AND PREDICTION OF CONTAMINANT TRANSPORT AND MIGRATION AT A FLORIDA SUPERFUND SITE

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Abstract. An important issue in the application of mathematical models to describe or predict the fate of solutes in soil and groundwater systems is providing the necessary data to support the spatial, temporal, and hydrogeologic model parameter requirements. The larger, more complex the model and scope of application, the more likely that significant amounts of data of several types are required. A management tool is required that allows the model and the modeler to interact with various needed databases, cope with numerous database management issues, efficiently achieve model parameterization and provide visualization of model output. The three-dimensional Groundwater Modeling System (GMS) that contains a state-of-the-art flow and solute transport model and a graphical user interface for data manipulation and analysis was applied to a Superfund site in Florida to demonstrate its capabilities for predicting solute migration.

Keywords: GMS, modeling, contaminant transport and migration

1. Introduction

Numerical models provide the greatest flexibility and accuracy in representing complex environments and can be applied to to nearly all types of hydrogeologic settings. The models can also be used to predict the dynamic aspects within a Superfund site, such as changes in the size of the chemical plume resulting from natural or man-made effects. Disadvantages for this method include costs that are high relative to other methods and the need for considerable technical expertise in hydrogeology and modeling.

Exposure assessment and remedial investigation are required at Superfund sites to address groundwater contamination under the Comprehensive Environmental Response, Compenstion and Liability Act (CERCLA), as amended by the Superfund Amendments and Reauthorization Act (SARA). Prediction of spatial and temporal movement of contaminant plumes by using a three-dimensional groundwater and solute advective-dispersive-sorptive transport model is an important tool in assessing the need for remedial design at Superfund sites.

Figure 1 shows a map of the Superfund Site in Pensacola, Florida and the location of the study area referred to as Site 38. The map was produced by GIS ARC/INFO. A plume of VOC and SVOC contaminants was detected in the soil and

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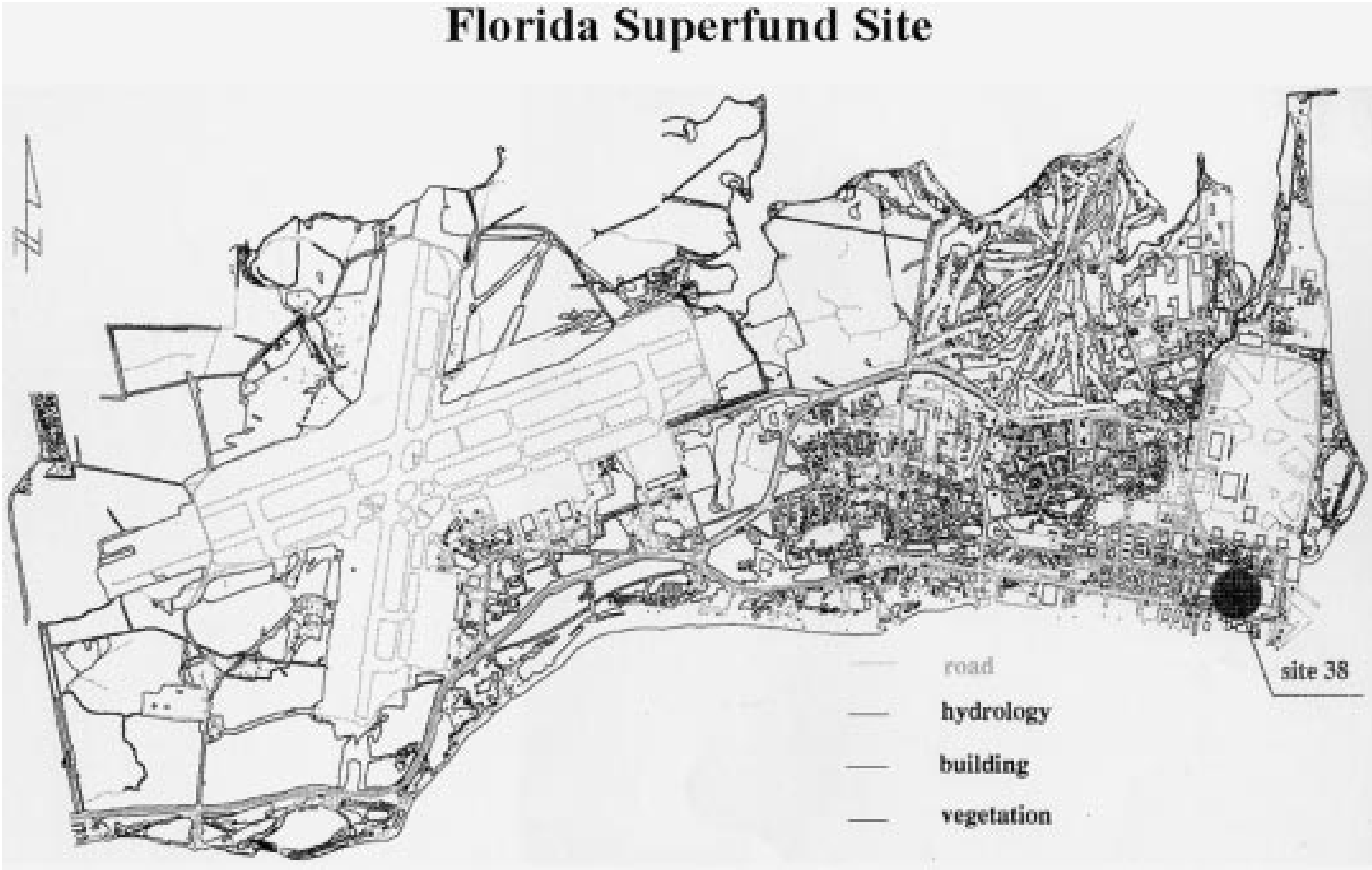

Figure 1. Site location.

groundwater centered beneath a building in Site 38 and extending into the west yard and to the seawall [1]. A chlorinated hydrocarbon plume 900 feet from the building was detected extending southward from a former underground storage tank also located in Site 38. Inorganic contaminants were detected over a broader area of the site. Current receptors are the Surficial zone and the Pensacola Bay. The objective in the present research was to use groundwater and solute transport modeling at this site to determine if the two plumes at Site 38 would merge together and migrate to the Pensacola Bay in five years. During this five year period, remedial design for the site will be completed and remedial action will begin.

Several models are capable of simulating the transport and transformation of chemicals in the soil subsurface. None of these models, however, have the flexibility to handle a wide variety of hydrogeologic parameters, soils, climate, and source type conditions. For more accurate risk analysis, a more comprehensive simulation package is required that will do more than simply provide potential exposure concentrations.

A three-dimensional finite element model of density-dependent flow and transport through saturated-unsaturated porous media FEMWATER [2] was applied to simulate the subsurface system at the Superfund site in pensacola Floride. In this research the FEMWATER model was interfaced with the Groundwater Modeling System [3] (GMS), a pre- and post-processing software program for data manipulation and analysis. Further, by using GMS which includes a Geographic Information System (GIS) link visualization of model output results was conducted in real time.

Modeling always starts with the conceptual model development and proceeds to parameter identification, mesh generation and boundary condition assignment, model calibration and sensitivity analysis, simulation, and presentation of predictive results. Initial work in this research was conducted on databases from the Florida Superfund site with the GIS software package ARC/INFO to develop the necessary data to support the conceptual model development and provide spatial, temporal and hydrogeologic input parameters. Visualization technology provided by both GIS and GMS greatly enhanced the modeling application through each modeling step.

2. Development of a Conceptual Model

The Superfund Site is located in the Gulf Coast lowlands on a peninsula bounded by the Pensacola Bay to the south and east and by the Bayou Grande to the north. Three main regional hydrogeologic units have been defines with the stratigraphy beneath the Florida, and the Floridan Aquifer System. The Surficial zone is contiguous with the land surface and contains groundwater under the water table or perched conditions. The Surficial zone is approximately 30 to 40 ft thick and is generally composed of a poorly graded quartz sand. Depth to groundwater ranges from 0 to 20 ft depending on ground surface elevation. Aquifer tests have yielded

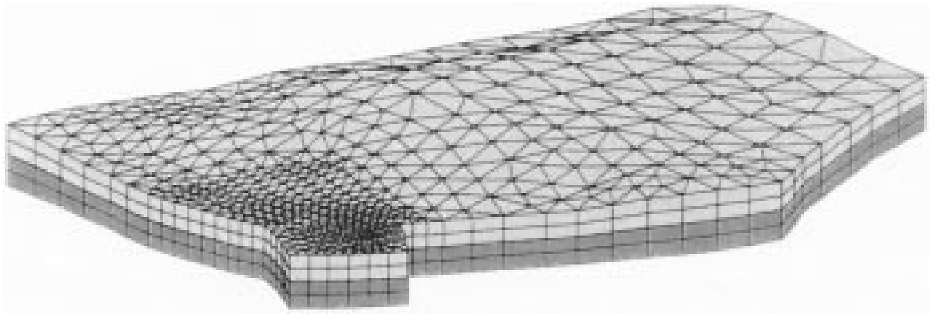

Figure 2. 3D finite element mesh.

high hydraulic conductivities, on the order to 10^1 to 10^2 ft day^{-1}. Shallow groundwater flow is generally influenced by topography, usually resulting in flow toward and discharge to, the nearest surface water body such as ditches.

A plume of VOC and SVOC contaminants was detected in the soil and groundwater centered beneath a building in Site 38 extending into the west yard and to the seawall. A chlorinated hydrocarbon plume 900 ft away was detected extending southward from a former underground storage tank. Inorganic contaminants were detected over a broader area of the site to various depths up to 20 ft. Current receptors are the Surficial zone and Pensacola bay. The risk assessment considered the Surficil/Sand-and-Gravel Aquifer as exposure media.

With the acid of GMS and GIS, the regional flow model was conceptualized as a heterogeneous, three-dimensional, isotropic unconfined aquifer. Neither the transient behavior of the groundwater flow system, nor the tidal effects were considered. The solute transport, however, is transient and the simulated period was five years. The aquifer system was represented by an irregular, finite-element mesh consisting of 4752 nodes and 7721 elements as show in Figure 2, and having four-layers – each 10 ft thick – and horizontal dimensions of about 800 m $\times$ 700 m. The model boundaries along the east and south sides were assigned constant heads (mean sea level). The northern and western boundaries were also established as constant head nodes in accordance with observed water table elevations map [1]. The impermeable bottom of the aquifer was assumed to be no flow, whereas at the top an infiltration recharge rate of 0.00354 m day^{-1} was assumed.

3. Three-Dimensional Mesh Construction

The finite-element analysis associated with the solution of partial differential equations over the simulated domain are performed using generalized numerical analysis procedures which approximate the continuous problem in terms of a discrete system. A key aspect of the finite element method is the construction of the finite element mesh used to represent the domain over which the analysis technique will be applied. Consideration of the type and distribution of finite elements in the mesh is critical since the accuracy and computational efficiency of the finite element method is dictated by the type and distribution of finite elements. The generation of the finite element mesh dominates the cost of application of the finite element method. Its construction typically represents 70–80% of the total cost. The finite element mesh is an approximate domain representation to which visualization results are fitted [4].

In the early application of the finite element method, finite element meshes were manually drawn and converted into the computer by creating input 'decks' defining each and every finite element entity. This can be particularly tedious and time-consuming in the case of an irregular three-dimensional mesh. GMS has a number of separate module interfaces such as TIN (Triangulated Irregular Network) module, solid modeling module, 3D mesh module, 3D grid module, etc. Finite element meshes can be generated in several different ways. Also, the generated meshes can be edited and renumbered. For 3D models, mesh and/or grid generation modules are the comprehensive and core part of the GMS interface.

Since the hydrogeologic stratigraphy at this site is fairly uniform, we used a very simple mesh generation technique. Steps for generating a 3D finite element mesh are: (1) important a DXF file converted from the GIS formatted file showing site extension and topography, (2) create a two-dimensional mesh covering the modeling area, (3) input a set of boreholes which define the elevations of interfaces between the stratigraphic units at scattered locations throughout the modeling domain, and (4) construct a 3D mesh by a 2D mesh and automatically interpolate surfaces using the borehole data which represent the interfaces between the stratigraphic units. Each element in the 2D mesh will be extruded into a vertical column of 3D elements. Figure 2 is a constructed 3D mesh for the simulation of groundwater and solute trasport at the site.

4. Model Calibration

Calibration is the process of adjusting model inputs until the resulting predictions give a reasonably good fit to observed data. It is an iterative and very much time-consuming process. GMS can overlay contours produced from observed water-level data onto contours generated by predicted water-level output, thus the two sets of water level contours can be compared directly on the screen. Using GMS eliminates the need for extensive printing associated with comparing hard copy results in conventional calibration techniques. This visualization capability provide rapid analyses and reduced manual manipulation of data. Figure 3 shows the results of groundwater flow calibration. The predicted head contours matched very well with the observed contours. The gradient match in the area of the plume migration between the predicted and head contours for to a certainty of greater than 95%.

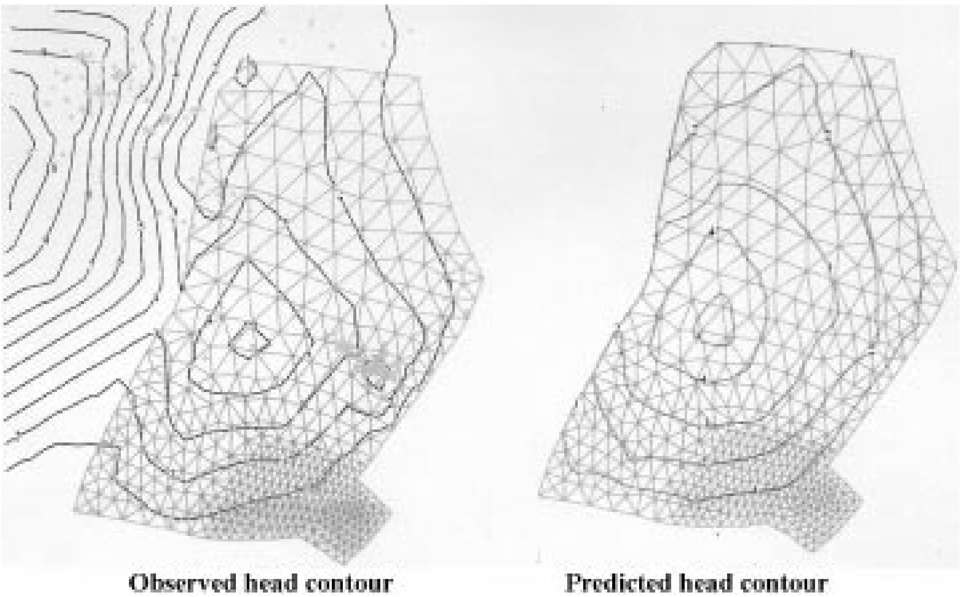

Figure 3. Model calibration.

5. Modeling Results and Input/Output Visualization

Five scenarios were calculated. Each scenario simulated advection, dispersion and retardation of one of five (5) chosen contaminants (tetrachloroethene, trichloroethene, vinyl chloride, lead, and aluminum) and assumed no source removal. A bulk density of 1.6 g cm^{-3}, effective porosity of 0.42, and retardation of 1.41 were assumed for the site. The following data were also used in the modeling calculations: (1) GIS topographical and geographical maps, which assisted in defining the region of modeling and boundary types; (2) well log, which contained the vertical distribution of geological formations, including depth, character, size of material, and structure strata; (3) hydrogeologic data such as groundwater level, permeability; (4) geochemical data to delineate the plumes of contaminants; and (5) transport parameters such as dispersivities. Results of numerous studies [1] at the Florida Superfund site yielded the following parameters:

Darcian velocity	3.8 × 10–5 cm/s
Soil type/texture	gravel 25%, sand 58%, silt/clay 17%
Hydraulic conductivity	84–340 ft day^{-1} at shallow depth
Vertical permeability	6.91 ft day^{-1}
Hydraulic gradient	0.0007 – 0.0027 ft/fr
Thickness of saturated zone	30 to 40 ft
Flow velocity	1.38–3.18 ft day^{-1}

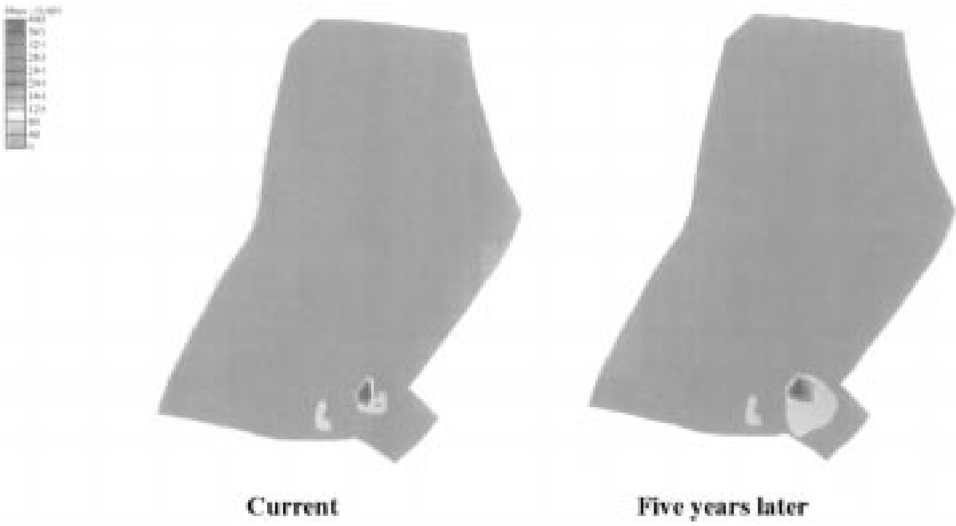

Figure 4. Development of contaminant plume.

Recharge rate	0.00354 m day^{-1}
Evapotranspiration rate	0.00066 m day^{-1}

The migration of the two contaminant plumes in Site 38 was simulated using FEMWATER, GMS and GIS with the above data to predict if they would merge together in five years. The scenarios were simulated for one contaminant at a time using six (6) month intervals starting from the present shape of the plumes and extending out to five (5) years. Figure 4 shows the comparison of the contaminant plumes for vinyl chloride as they exist the their current state and their predicted shape in five years. From the simulation in two plumes will not merge together within the five period but the main plume will move closer to the bay. The behavior of the two plumes using other contaminants was similar.

Visualization techniques, when used in conjunction with numerical modeling, provide the most meaningful means to view both the ‘input’ and ‘output’. A large number of visualization tools are provided in GMS. Highly realistic images of the Site 38 area were displayed in a 3D oblique view and rotated interactively. Contours, color fringes were iso-surfaces were generated from 3D meshes and grids. Animation sequences were generated to represent the moving contaminant plumes.

6. Modeling Enhancement by GIS

Groundwater modeling of natural phenomena is made complex and difficult by characteristics such as spatial and temporal variability and dominating mechanisms that vary with environmental circumstances. GIS technologies offer powerful tools to deal with some of these problems.

The Site 38 study map as shown in Figure 1 was produced by GIS ARC/INFO. The Pensacola GIS databases that we obtained covers a large area of about 7.35 $\times$ 5.85 square miles and contains over 400 megabytes of data on topography, well characteristics and geochemical sampling. The topographic database contains GIS files for displaying topographic contours, roads, buildings, hydrologic characteristics, and vegetation. This database was used to delineate the physiographic boundaries, estimate the groundwater divides, and to provide boundary condition assignments. The GIS software was also used in the project to support a variety of investigations and evaluations using the data query and analysis capabilities. Procedures have been developed to summarize information in a variety of forms. For example, to revise and updata interpretations of the extent and magnitude of contamination, geochemical databases was queries for data on specific contaminants, at a specific location, from a specific time period, and output the information using a table or predetermined symbology on maps that are used as a base on which interpretations are made. Data input procedures were used to upload information from GIS to GMS through converting a GIS file to DXF file format and importing a DXF file into GMS. DXF is a standard file format specified by AutoDesk's AutoCAD.

GIS applications, were used to mimic manual map-processing techniques, such as map reclassification, overlay and simple buffering around features. The new wave of applications concentrates on *data mining* employing advanced analytical operation, which uses the GIS and GMS to discover relationships among mapped variables. A variety of interpolation schemes are supported by both GIS and GMS including kriging.

We attempted to correlate vegetation parameters and recharge rate at the site. Unfortunately, there was not enough quantitative vegetation data in the GIS database for analysis. The correlation was then intuitively perceived through visual observation. However, we found that the site is almost entirely covered with concrete or asphalt and nonly a very limited vegetation area was needed to assign an infiltration/evapotranspiration rate. Secondly, we used the two-dimensional interpolation module in GMS to interpolate the concentration data from scatter points to obtain a graphical representation of the contaminant plume. In our case, the linear scheme is the preferred procedure.

7. Conclusions

The migration of two contaminant plumes at a Superfund site in Florida was simulated using FEMWATER, GMS and GIS to predict if they would merge together in five years. A similation scenario using one of the contaminants, vinyl chloride, predicted that the two plumes would not merge together in five years but that the main volume would move closer to the bay. The behavior of the two plumes using other contaminants was similar. Highly realistic images of the Site 38 area were displayed in a 3D oblique view and rotated interactively. Contours, color fringers and iso-surfaces were generated from 3D meshes and grids. Animation sequences were generated to represent the moving contaminant plumes.

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References

1. Draft Remedial Investigation Site 38', Naval Air Station, Pensacola, Florida. Prepared by Ensafe/Allen and Hoshall, Memphis, Tennessee, (1994).
2. in, H. C. and Yeh, G. T.: 1995, 'User's Manual for the FEMWATER Groundwater Computer Program: A Three-Dimensional Finite Element Model of Density-Dependent Flow and Transport through Saturated-Unsaturated Porous Media', U.S. Army Corps of Engineers Waterways Experiment Station, Vicksburg, MS.
3. righam Young University: 1994a, 'GMS, Groundwater Modeling System Reference Manual', Engineering Computer Graphic Laboratory, Provo, UT.
4. hephard, M. S. and Schroeder, W. J.: 1995, 'Analysis Data for Visualization', in R. S. Gallagher (ed.), Computer Visualization: Graphics Techniques for Scientific and Engineering Analysis, pp. 51–87.