EFFECTS OF ANISOTOPY ON A US3D FINITE ELEMENT GROUNDWATER MODEL

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Abstract

Groundwater models commonly assume that the subsurface is both homogenous and isotropic. Frequently, this is not the case. Discontinuous stratigraphic layers and scattered clay lenses are not always found in borehole data when reported from the field. This paper utilizes the finite element groundwater modeling code US3D, in order to study the effects of anisotropy on an Ethyl-Di-Bromide Plume.

Purpose and Objectives

The primary objectives of this paper are to construct a model of an Ethyl Di-Bromide (EDB) plume using the US3D code, to demonstrate the effects of anisotropy on the model, and to present these results in three-dimensions. The site in question has been modeled using other codes, therefore, existing model data is available and serves as an excellent testing ground for the development of the US3D Code.

The stratigraphy of the model area and the underlying subsurface can not be tested at every point, therefore, the geology can never be completely known. The model simulations in this paper address the issue of discontinuous layers and random distribution of clay lenses. One aspect of this research effort is to evaluate the effect that small scale stratigraphy changes have on the model. Finally, the results of this model are directly analyzed in the three-dimensional visualization software G3D. G3D is a graphical user interface designed to facilitate model development, but is primarily used here to aid in the understanding of the complex three-dimensional dynamics of the model.

Description of Parallel US3D

The US3D simulator solves for three-dimensional groundwater flow and contaminant transport. The numerical solutions of US3D which are based on finite element methods can be solved for both the saturated and the unsaturated flow conditions. A finite-element model, unlike a finite-difference model, allows the modeler to divide the grid into a mesh formed of a number of polygonal cells (Fetter, 1994). The advantage of this type of division, is that the model can better match the conditions of the site. For instance, it frequently makes sense to use a very fine grid spacing where the initial concentration values are known and don't need to be interpolated.

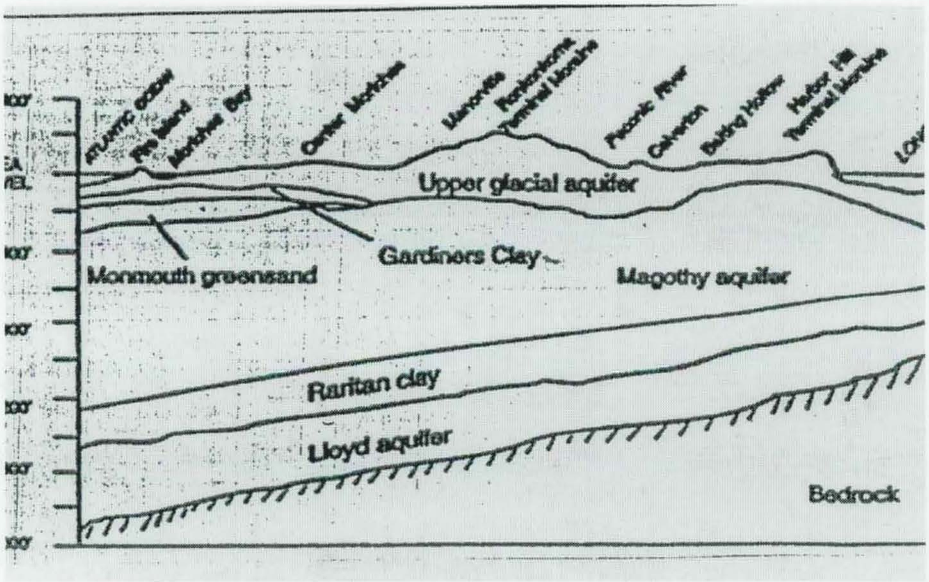

fig. 1 **Regional Long Island Stratigraphy**

The US3D code is parallelized by breaking the (logically cubic) domain into logically regular subdomains. Each subdomain is then assigned to a separate processor (Pasciak 1996). US3D's parallel processing capabilities allow for the construction of models with high resolution grids. Standard models usually have limited grid sizes because of restrictions due to single processor memory. Additionally, because US3D runs on a massively parallel processing computer, it allows for simulations of contaminant transport over very long periods of time.

Local Stratigraphy

The geological formations beneath Long Island dip gently to the south and east, a generalized cross-section throughout the Central Pine Barrens can be seen in fig. 1. The Upper Glacial aquifer is comprised of Upper Pleistocene sediments that were deposited in a glacio-fluvial environment during the Wisconsin glaciations. The Upper Glacial material near in the study area of this project consists of Outwash deposits from fluvial transport, and moraine material. Upper Glacial deposits are 100-200 ft thick (de Laguna 1963). The Upper Pleistocene (Wisconsin) deposits which comprise the Upper Glacial Aquifer are divided into two hydrogeologic units.

1. The Undifferentiated Sand and Gravel Outwash and Moraine Deposits that are characterized by crudely stratified silica-rich sands, and
2. The Unidentified Unit which is present in some locations in the southern portion of the model area is characterized by fine to medium-white to greenish-sand with interstitial clay (Geraghty & Miller 1996).

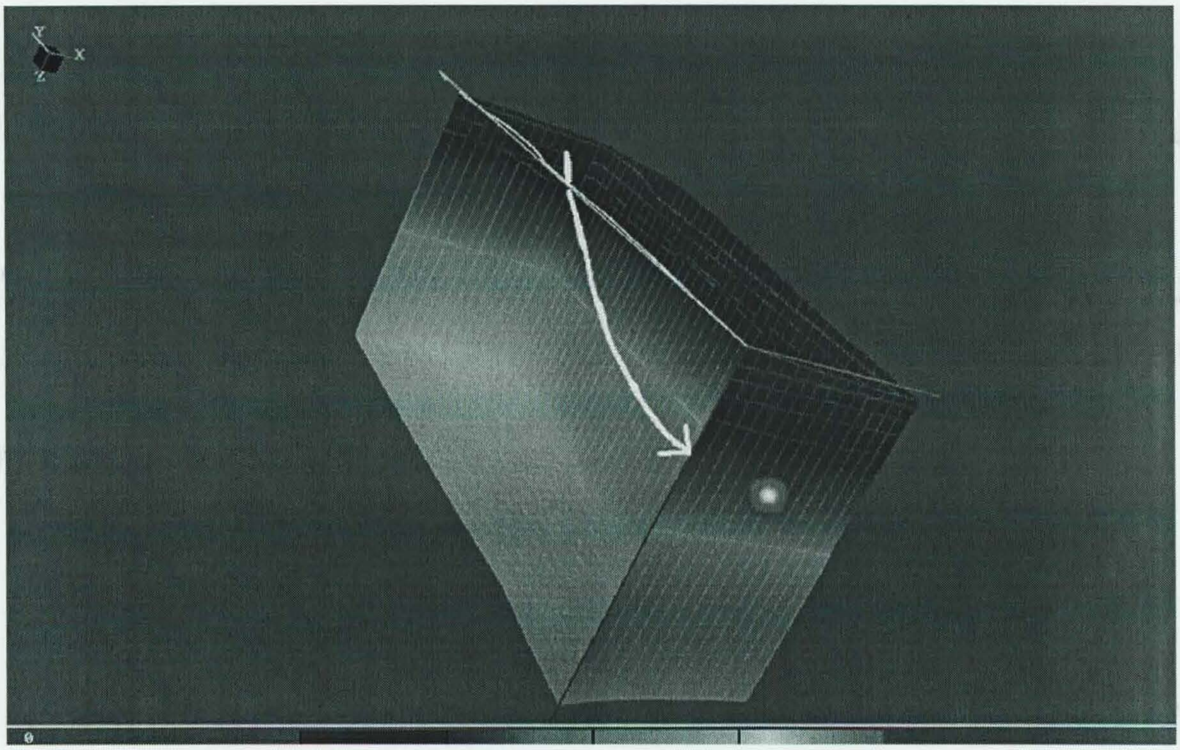

fig. 2 Hydrologic Head Values and Flow Vector

The Gardiners Clay is composed predominantly of massive green-clay, silty-sand, and gravely sediment. This unit ranges from 0 to 30 ft of thickness and is found approximately 90 to 100 ft below mean sea level (Geraghty & Miller, 1996).

The Magothy Aquifer unconformably underlies the Upper Glacial aquifer and Gardiners Clay. Where the Gardiners Clay exists, it acts as an impermeable layer between the Glacial material above, and the Magothy aquifer below. The Magothy is composed of fine sand mixed with silt and clay. Thickness ranges from 780 to 890 ft beneath the site. The lower portions of the Magothy, know as the Basal Magothy, generally have coarser material associated with it.

The Raritan Confining unit underlies the Magothy aquifer and is comprised of dark gray or black lignitic clay. It is approximately 200 ft thick, and for the purposes of this model will be assumed to be completely impermeable.

The Model

A. Initial Conditions and Boundary Conditions

The initial conditions of the model for both the flow and the transport were taken from a previous model that used the DYNTRAK and DYNFLOW codes. The original reason for using these data sets were to provide the most accurate comparison between the US3D model and the DYNFLOW/DYNTRAK model. DYNFLOW/DYNTRAK like US3D is a finite element code, however, DYNFLOW/DYNTRAK utilizes a finite element triangular mesh which is not supported by US3D. For these reasons, several PERL scripts were written to translate the vertex values of the triangular elements from the DYNFLOW/DYNTRAK model to a grid that is regular in the x, y - plane for use in US3D. One significant difference between the DYNFLOW/DYNTRAK approach to transport modeling and that of US3D, is that DYNFLOW/DYNTRAK uses a "backwards particle tracking method" to solve for concentrations at each element. By contrast, US3D solves for the finite element equations at each cell.

The initial flow conditions for the model are shown in fig. 2. The values in fig. 2 represent total hydraulic head, groundwater flows from higher head values to lower head values. The generalized groundwater flow in the model domain is from North to South and downward in the z-direction. Groundwater flow direction is indicated by the vector in fig 2.

The flow boundary condition consists of constant head nodes and constant flux elements. The top of the model corresponds to the water table, where recharge was simulated as a constant flux of 21.68 inches per year. At the bottom of the model, the boundary was simulated by zero flux elements. This is consistent with the assumption that the Raritan Clay unit is impermeable and all the groundwater circulates within the Upper Glacial and the Magothy aquifers but does not penetrate the Raritan formation (Dziedzic 1996).

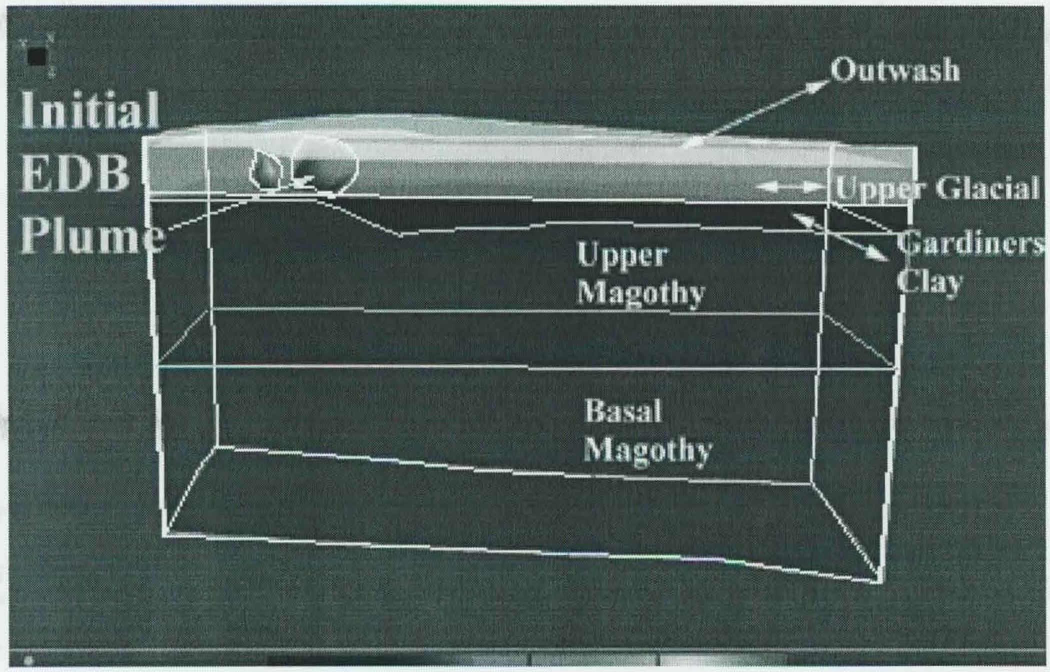

fig. 3 Stratigraphy and Initial EDB Concentrations for Model Area

The initial concentrations for EDB were assigned to elements localized within the source area. Fig. 3 shows the interpolated isosurface from these initial concentration values. The lighter shade represents a concentration of .05 ppb (drinking water standards for EDB), and the darker shade represents >.01 ppb (more than twice the drinking water standard).

B. **Grid Dimensions**

The Finite Element grid used to model the EDB plume is rectangular in the horizontal (x, y) planes, while the vertical (z) direction has non-uniform node spacing according to geological setting. Therefore, the node spacing in the z-direction follows the contours of the lithology. The origin of the model coordinate system is located in the lower right top corner of the grid.

The dimensions of the grid in feet in the x, y, z direction are (750,1550,400). The grid-cell spacing is 15x31x8 in the x, y ,z direction, and each cell is 50ft by 50ft.

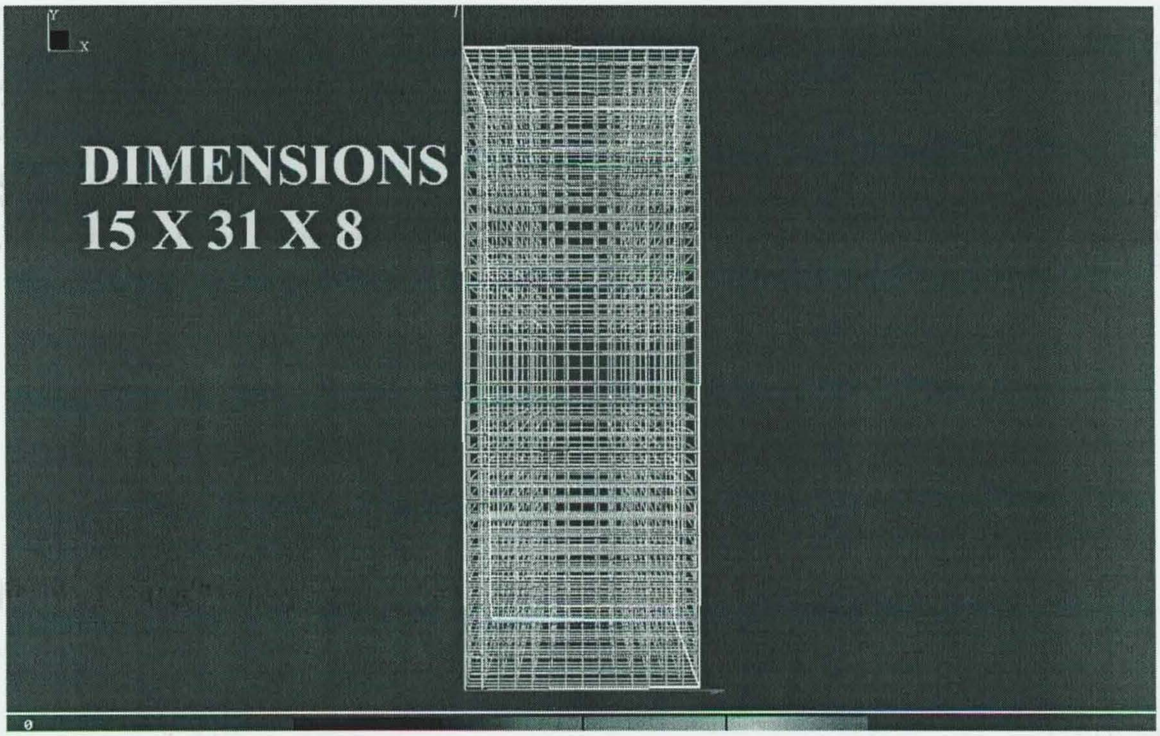

fig. 4 Model Grid Dimensions

C. Material Types and Aquifer Properties

The vertical discretization of the model for these simulations consists of one configuration which represents the following five units: an Outwash layer, an Upper Glacial Layer, a Gardiners Clay confining unit, and a Magothy aquifer which has been split into two layers. The Magothy layer consists of the Upper Magothy and a Basal Magothy unit which have approximately uniform thickness around 200ft. The stratigraphic divisions are shown in fig. 3. The following hydraulic parameters for each grid element are contained in the governing equation for flow and transport and are needed for US3D to run:

1) Hydraulic Conductivity (K) A coefficient of proportionality describing the rate at which water can move through a permeable medium (Fetter, 1994).
2) Specific Storativity (S_s) -The amount of water per unit volume of a saturated formation that is stored or expelled from sediment, owing to compressibility of the pore water per unit of change in head. Essentially, the specific storativity defines the amount of water that sediment can hold.
3) Dispersivity (D_x, D_y, D_z) or (d*l*, d*t*, d_v) - Describes the phenomenon by which a solute or contaminant flowing in groundwater mixes with uncontaminated water and becomes reduced in concentration.

4) Porosity (f) - Refers to the amount of pore space in sediment. It is defined as being the ratio of the volume of pore space in sediment of the total volume of the sediment (Fetter, 1994).

Hydrologic Unit	**K_x (ft/day)**	**K_y (ft/day)**	**K_z (ft/day)**	**(ϕ)**	**S_s (1/ft)**
Outwash	250	250	25	0.24	0.2
Upper Glacial	175	175	1.75	0.24	0.1
Gardiners Clay	1	1	0.05	0.1	0.0048
Upper Magothy	65	65	0.60	0.15	0.0048
Basal Magothy	75	75	0.75	0.24	0.0048

Table 1.

These six parameters, K, S_s, D_x, D_y, D_z, and ϕ are responsible for the properties of groundwater flow and the extent and duration that a pollutant will remain in the system. In this Model, five different material types were used.

Table 1 summarizes the hydraulic parameters of the particular material types. The same dispersivities and diffusion coefficients were assigned for each material. The longitudinal dispersivity $dl = 30$ft, horizontal transverse dispersivity $dt = 3$ ft, vertical transverse dispersivity $d_v = 0.3$ ft, and the diffusion coefficient $d_f = 0$. These values were taken from the CDM 1995 Groundwater Modeling Report in order to assess the effects of contaminant adsorption onto the solid matrix of the aquifer, the retardation factor was specified as 1.3 (CDM, 1995).

Model Simulations

The groundwater flow and transport model US3D was run with the values from Table 1. Three variations on the basic model were conducted. The primary purpose for creating these simulated differences is to test the effects of anisotropy on the model. In all three simulations the hydrologic properties in Table 1 were used. The three simulations are as follows:

1. Conservative Simulation
2. Discontinuous Gardiners Clay
3. Clay Lenses in the Upper Glacial

The US3D Model has been calibrated with the existing DYNTRAK/DYNFLOW model for the area and produces similar results. In the simulations discussed, Retardation (R) was taken to be 1.3, unless stated otherwise. In all three simulations, the contaminant, EDB, falls below the

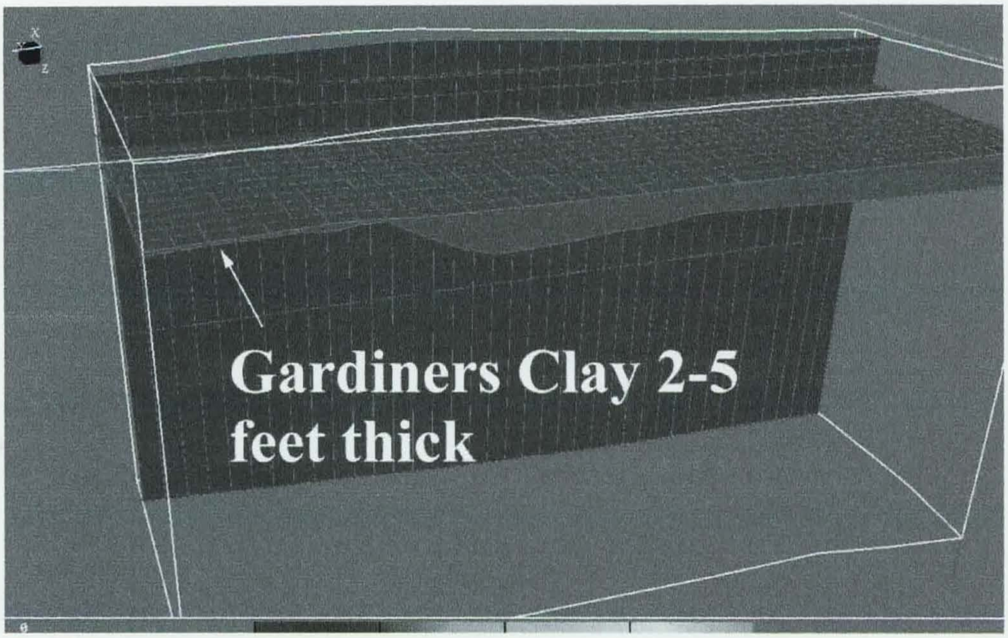

fig. 5 Isolation of the Gardiners Clay Layer (the left hands side shows that the Gardiners Clay is only about 3-8 feet thick)

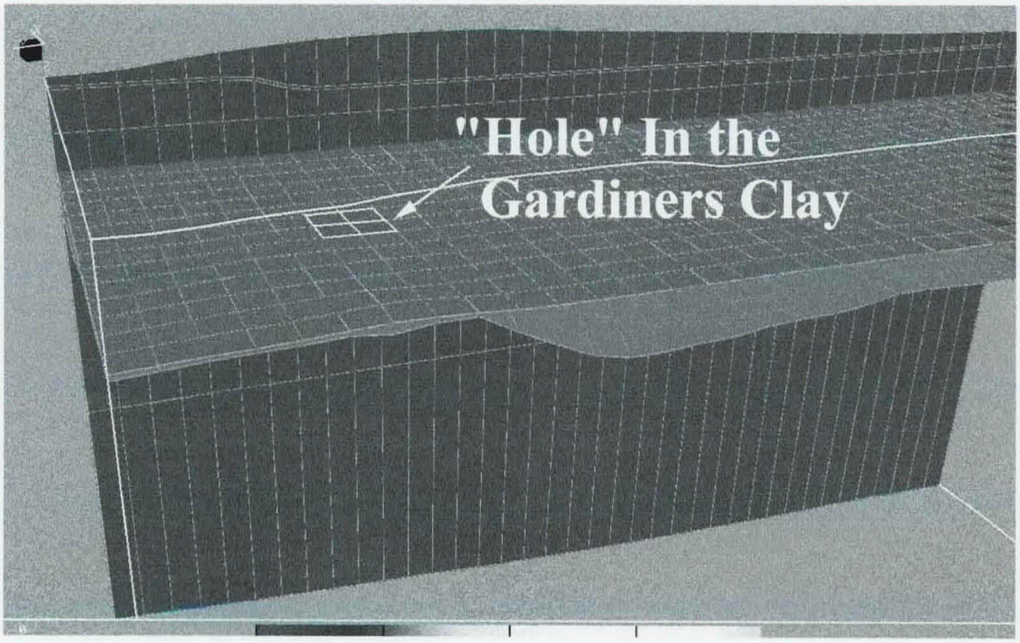

fig. 6 Simulated "Hole" in the Gardiners Clay

drinking water standard of .05 ppb at some time in the future. This time varies with each simulation.

1. **The Conservative Model** - The conservative model run simulates conditions where no chemical reactions take place. Primarily, no retardation factor has been added, so the EDB plume is dictated solely by advection and dispersion. Sorption is no longer a factor. Its extent is indicated in Fig. 9.

2. **Discontinuous Clay** - The Discontinuous Clay scenario was run to simulate a few holes in the Gardiners Clay. The justification for this is that the Gardiners Clay becomes extremely thin in the northern section of the model area, and although there is no proof that these "holes" exist, if they did, there is a high likelihood that they would be in this region of glacially scoured sediment. The thin section of the Gardiners Clay can be seen in fig. 5 on the left hand side. Additionally, the simulated "hole" can be seen in fig. 6. In the previous simulation, the EDB isosurface does not penetrate the Gardiners Clay. However, due to the removal of some of the sections of the Gardiners Clay (fig. 6), the EDB plume penetrates the Gardiners Clay entering the Magothy and can be seen at its maximum extent in fig. 7. Subtraction of a portion of the Gardiners Clay has the effect of slowing down the overall plume migration to the south. It's furthest extent is shown in fig. 9.

3. **Clay Lenses** - This simulation attempts to look at the case where the Upper Glacial Unit has a random distribution of clay. Clearly, well logs for this area and for many other locations on Long Island indicate that small discontinuous clay lenses exist. Therefore, this simulation attempts to look at how the existence of a few lenses would effect EDB transport. These clay lenses which show up as cubes can be seen above the Gardiners Clay in fig. 8. The effect of these clay lenses act to break up the plume and limit its southern extent as indicated in fig. 9.

Conclusions

Three different groundwater model simulations using the US3D finite element code were conducted to study the effects of anisotropy on a model. The three simulations all resulted in different outcomes and are summarized in Table 2. The model results clearly showed differences due to the changes in the materials file. However, the discontinuous Gardiners Clay

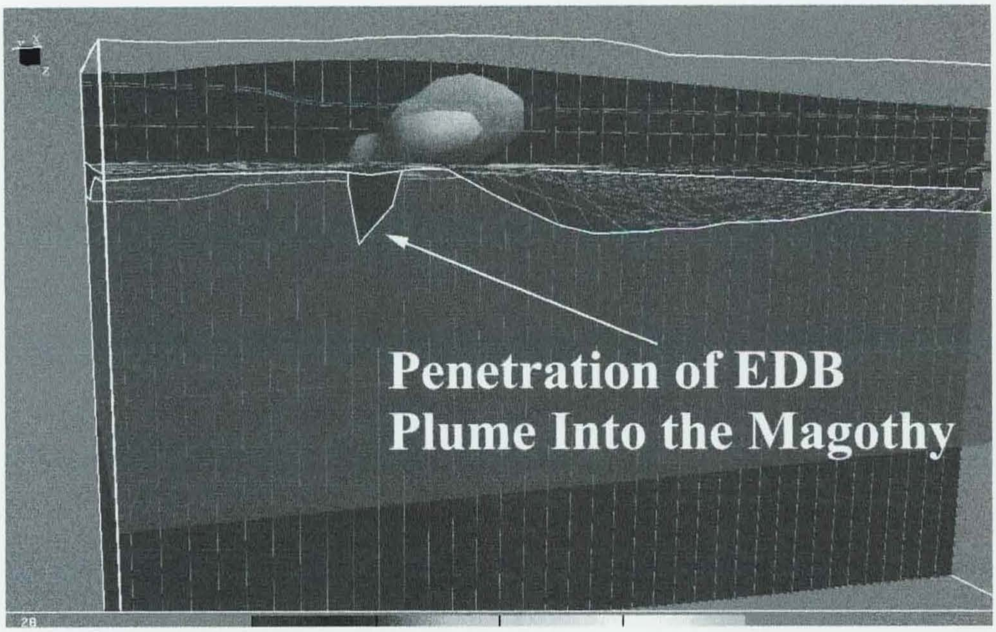

fig. 7 **Marks the Furthest Extent that the EDB Plume Enters the Magothy Aquifer**

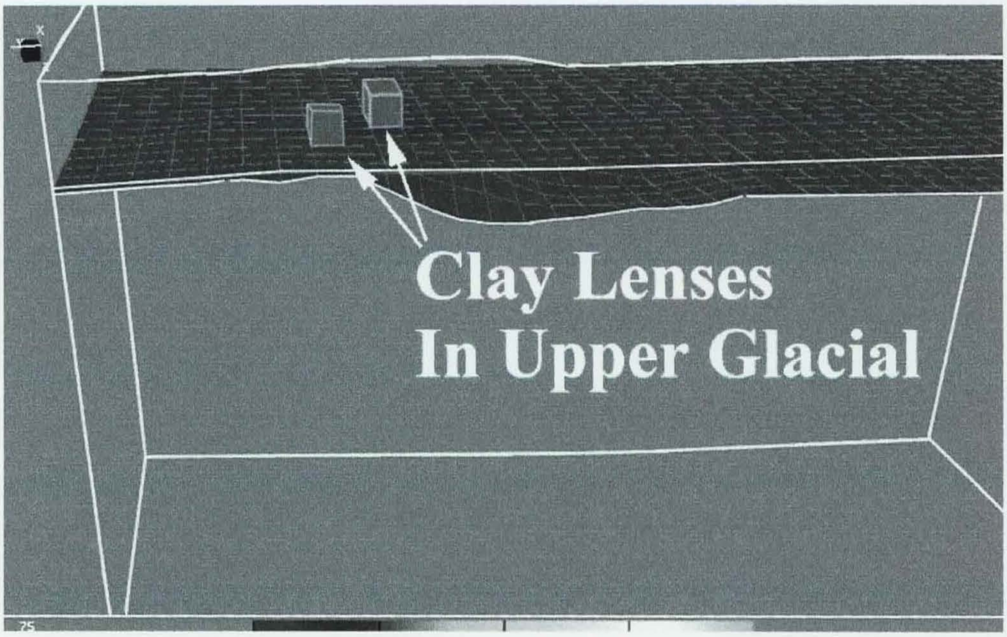

fig. 8 **Two Simulated Clay Lenses**

resulted in the longest time for attenuation to occur, one would have expected the conservative simulation to take the longest because there is no absorption taking place.

	Simulation Name	Approx Time to Attenuation Below Drinking Water Standard	Approx Distance Traveled Before Attenuation Below Drinking Water Standard
1.	Conservative Simulation	50	587
2.	Discontinuous Gardiners Clay	71	575
3.	Clay Lenses in the Upper Glacial	66	586

Table 2

Acknowledgments

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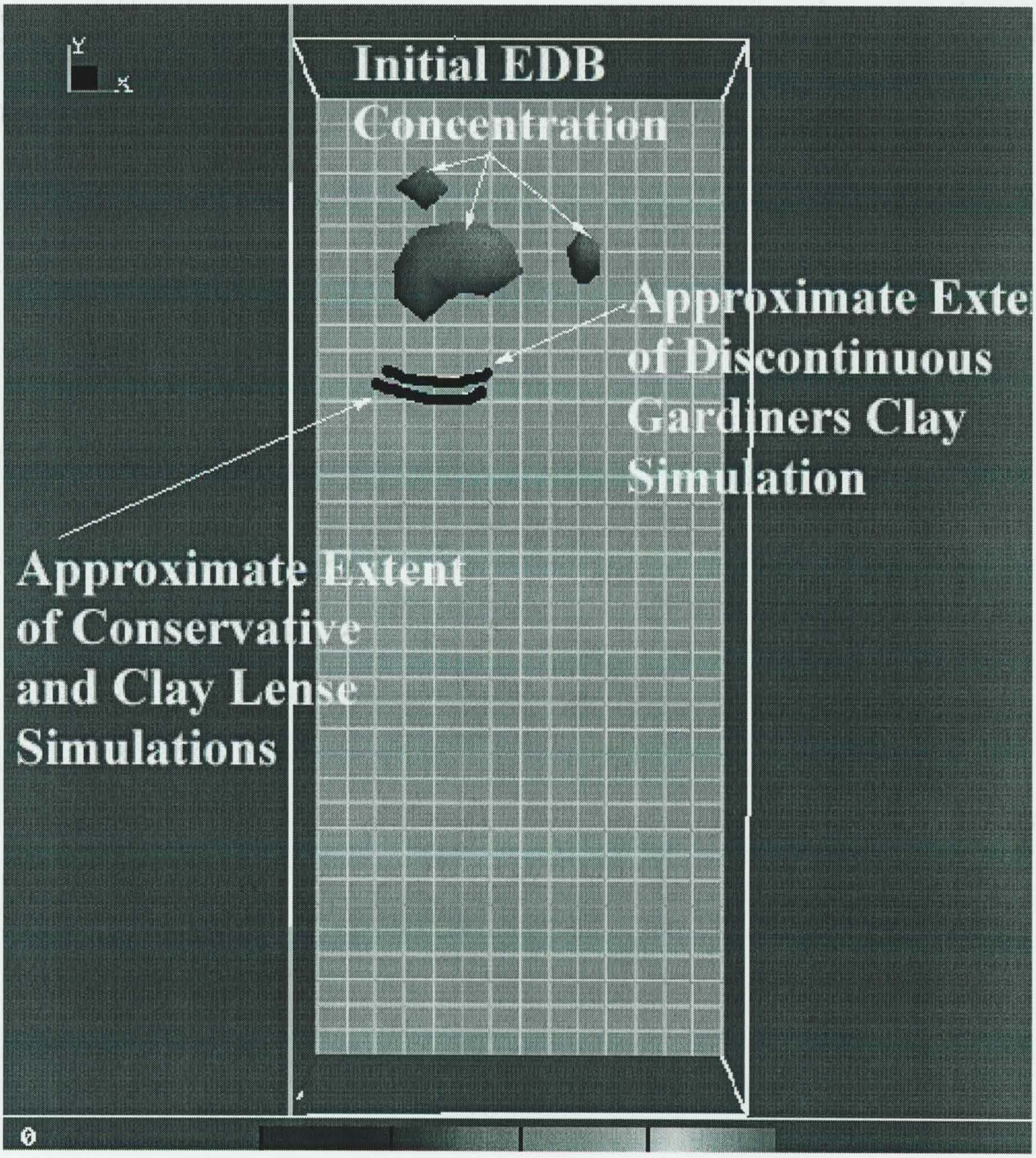
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