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Three-Dimensional Computer Simulations of Bioremediation and Vapor Extraction

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Abstract

Numerical simulations of two remediation strategies are presented. These calculations are significant in that they will play a major role in the actual field implementation of two very different techniques. The first set of calculations simulates the actual spill event of nearly 60000 gallons of No. 2 diesel fuel oil and its subsequent flow toward the water table for 13 years. Hydrogen peroxide saturated water flooding is then performed and the bioremediation of the organic material is then calculated. The second set of calculations describes the vacuum extraction of organic vapors and indicates the sensitivity to various assumed formation properties and boundary conditions.

Numerical Simulation of Bioremediation

This report summarizes a preliminary set of three-dimensional calculations we have carried out of the diesel fuel spill at Sandia National Laboratories, Livermore. Previous 2-D simulations (Travis and Trent, 1991) indicated that the infiltration of rainfall is a very important factor. It has since been established in laboratory experiments that water is the wetting fluid. Hence any rainfall will tend to displace oil downward towards the water table, and the amount of water that infiltrates is indeed, therefore, an important factor.

We are attempting to achieve a reasonable comparison with observed fuel oil subsurface migration as our primary goal, and to examine sensitivity to factors such as infiltration of rainfall. Our ultimate goal is to optimize bioremediation at this site. This will provide a field validation of our model. To simulate a bioremediation experiment successfully, we must first have a good estimate of the subsurface 3-D distribution of water and fuel oil.

Setting up the TRACR3D Calculations

All Los Alamos simulations were performed with the TRACR3D computer code (Travis and Birdsell, 1991; Travis, 1984). TRACR3D solves the equations describing unsaturated/saturated flow and multi-component transport in 1-D, 2-D or 3-D heterogeneous porous media. Transport mechanisms include advection (in both phases - air and liquid), diffusion, dispersion and sorption. TRACR3D also treats migration of volatile organics. A version of our model called TRAMP (Bentley and Travis, 1991) simulates biological activity using Monod kinetic and inhibition equations; this version will be used for analyzing bioremediation tests at the site. All versions are based on a mass-conserving finite difference numerically implicit algorithm.

Our computational mesh consists of a regular array of 30 cells in each horizontal direction and 32 cells in the vertical (28,800 cells in all). The horizontal extent of the mesh is 50 meters on each side and is 32 meters deep, and encloses the trench and the area in which the bulk of the contaminant was observed. This mesh geometry was used for both TRACR3D simulations discussed in this report.

The three-dimensional geometry used here is not just an extension into the third (horizontal) direction of the 2-D geometry used previously. A coarse interpolation of lithologic units was made, based on the various cross-sections of the site (Remedial Investigation Report, 1990). The resulting soil distribution is truly 3-D; however a better interpolation of units between the cross-sections will be done for future studies, after the laboratory determination of hydrologic properties becomes available. Figure 1a shows the computational block used in the simulations; each soil type is color-coded. The block is shown with a large cut-out so that the interior structure can be viewed. The trench is visible on the surface as the orange-red line lying diagonally, about in the center. The fuel leak occurred at that end of the trench which is not in the large green-coded soil region. Fig. 1b shows the same block from the reverse side, also with a large cut-out for viewing the interior structure. The soils are obviously varying in all three dimensions. The water table lies at the bottom of the block.

Next the baseline material properties for the nine soils identified at the site are listed in Table 1.

Table 1. Properties of Formation Materials at SNLL Fuel Oil Spill Site

Mat #	Prm. (darcy)	Por	Ave. Part. Size (cm)	Irr. H2O Saturatn.	Van Gen. exp.	Bub. Prs. (cm)	Matrix. Density. (gm/cc)	color in Fig. 1
1	0.1	0.35	0.01	0.22857	.375	-25	2.5	purple
2	0.5	0.35	0.01	0.22857	.375	-25	2.5	dk. blue
3	1.0	0.35	0.01	0.22857	.375	-25	2.5	lt. blue
4	5.0	0.35	0.01	0.22857	.375	-25	2.5	white
5	10.	0.35	0.01	0.22857	.375	-25	2.5	turquoise
6	50.	0.35	0.01	0.22857	.375	-25	2.5	green
7	100.	0.35	0.01	0.22857	.375	-25	2.5	yellow
8	500.	0.35	0.01	0.22857	.375	-25	2.5	tan
9	1000.	0.35	0.01	0.22857	.375	-25	2.5	orange

All the soils are assumed to have the same characteristic curves. This is probably far from correct, but will have to do until laboratory measurements are released. The Van Genuchten formulation was used for the matrix potential and relative permeability fields. Average dry soil density is 1.82 g/cc.

All the fuel oil (162 m^3) was injected at a uniform rate at a point near, but not in, one end of the trench over a ten day period. The point source is a single computational mesh cell centered at a depth of 1.5 feet (0.5 m). The trench (orange-red line on the surface in Fig. 1) was represented as a material with a very high permeability (1000 darcys). Here, as in the actual field event, the diesel fuel will percolate laterally toward the trench and begin to flood the trench while at the same time the fuel oil moves downward from the point source. The left and right sides and bottom boundary were held to no-flow conditions; the front and back were also no-flow boundaries except at the bottom layer. This allows water to flow through the saturated zone in the approximate direction of the local groundwater flux, and permits rainwater filtering down to exit the domain without accumulating at the bottom.

A separate transport equation is solved for the diesel fuel. The influx at the top is pure diesel fuel, and the initial fluid saturation (0.356) in the subsurface is only water. We assume that the diesel fuel has the same density and viscosity as water. This constraint can be removed later when data are available on the particular oil components involved in the SNLL spill.

Results From the TRACR3D Calculations

Rainfall Effects in 3-D

In the low infiltration case, twenty percent of the annual rainfall was assumed to infiltrate through the surface. During the first five years, the rainfall rate was 38 cm/yr. Subsequently, a long drought period settled in, lasting for the next 8 years. Rainfall during the drought was assumed to be 3.8 cm/yr, i.e., just 10 % of normal. We are also assuming a steady influx of rainwater throughout the entire simulation, even though the rainfall is episodic, occurring primarily in the winter. The average effect is all we are after at this point. The actual rainfall histories can be included in future simulations, if desired.

Figures 2a to 2c show the 3-D distribution of fuel oil concentrations after 0.5, 5 and 13 years, respectively. In these figures, concentration is color-coded. Red is the highest concentration representing values greater than 10,000 mg/kg. Dark blue is the lowest, corresponding to a value of 250 mg/kg. The background purple color does not represent any concentration (nor does it correspond to any soil type). The oil moves a considerable distance downward in the first half-year; for example the 1,000 mg/kg level has just reached to the 70 foot depth at one very localized spot. By five years, the 10,000 mg/kg concentration has just arrived at that depth, but there is still nothing at the water table level. The deepest fuel oil is moving laterally along the high permeability layer at about 65 -70 feet depth which lies just above a very low permeability zone. The permeability variations are channeling the transport along the paths of least resistance--sometimes that path is horizontal, sometimes vertical. (Lower concentration levels will be present even deeper but we arbitrarily chose 250 mg/kg as the smallest contour level to plot.) The distribution of oil is very non-uniform. At five years (Fig. 2b), the general distribution is very similar to that seen at 0.5 years; the major difference is that more oil is present around the 65 foot depth level and less is present near the surface.

From five to 13 years, there is little further migration because of the low infiltration rate and the low rainfall (drought conditions). There is still a residual saturation near the surface, especially below the original leak point. Most of the fuel oil is at intermediate depths; only very little has reached the top of the water table. The bulk of the fuel oil is trapped in the low resistance layer at 65 feet depth by the underlying low permeability lens. The 10,000 mg/kg concentration level reaches about 70 feet, and the 1,000 mg/kg concentration level just reaches to the 90 feet depth mark.

In the high infiltration case, eighty percent of the rainfall was assumed to infiltrate the surface. Influx then for the first five years = (0.80) * (38 cm/yr) / (3.15 e7 sec/yr) = 1.0 e-6 cm/sec and then the drought conditions were 10 percent of that (i.e., 1.0 e-7 cm/sec) for the following eight years. The concentration surfaces computed for this case are shown in Figs. 3a to 3c for years 0.5, 5 and 6.5, respectively. These correspond to the view of Fig. 1a. Figs. 4a to 4c show the concentration distributions at 0.5, 5 and 6.5 years for the view perspective of Fig. 1b. As in the previous case, the oil quickly flows into the trench; this is followed by a fairly rapid infiltration of oil. The plume migration slows considerably during the next few years. By 6.5 years, the oil has spread out over the high permeability layer at 65 feet depth, and has continued on to the water table region and is beginning to exit the calculational domain (Fig. 4c). There appears to be a discontinuity in the concentration of oil at depth in Figs. 4b and 4c -- this is only apparent. Oil is flowing around a low permeability zone and getting into the high permeability layer near the bottom through the back part of the domain, which can't be seen in this view, but is apparent from the reverse side (Figs. 3b and 3c). We have not continued this simulation further in time. Since we do not have the true material properties, these simulations serve as sensitivity and scoping studies primarily. After five years, however, the influence of the additional rainfall has pushed the contamination plume down to the assumed water table (no flow boundary at a depth of 32 m). This simulation looks very much like the low infiltration case but with an accelerated time scale.

The actual diesel fuel distribution was measured in 10-20 feet depth intervals approximately 13 years after the spill occurred. (A summary of the results are shown in Figs. 1.9 to 1.16 in the Remediation report [DOE, 1989].) Figs. 5a-5c compare measured with calculated concentrations on one plane layer centered at a depth of about 40 feet. Fig. 5a shows concentration contours on this plane (at 40 feet) at 13 years for the low infiltration case and Fig. 5b shows contours from the high infiltration case taken at 6.5 years. Fig. 5c shows the measured concentrations on that same plane. Both simulations show a small region with a peak concentration over 1,000 mg/kg (upper right area of Figs. 5a,b,c), and a larger area of concentration in the region which is directly below the original leak point (lower left area of Figs.5a,b,c). Measured concentrations reached about 17,000 mg/kg in the center of this area; simulated values were close, with both cases showing a core region of over 10,000 mg/kg. Measured and simulated peak concentrations in the smaller zone were in the range of 1,000 to 2,000 mg/kg. Even though we are not yet in a position to match the observed concentrations (since we still need to perform the simulations with laboratory measurements of material properties rather than estimates based on soil types), the comparison shown in Fig. 5 is very encouraging. The general shape and concentration levels are comparable (at this level and other levels not shown).

In both simulations, there are clearly three phases to the oil flow -- an initial gravity flow driven mainly by the weight of the oil (first 6 months); a second phase in which oil movement is driven primarily by infiltrating rainfall which displaces the oil; and a third phase, characterized by slow migration (capillary drive and diffusion) of the fuel oil after the "rain drive" is effectively eliminated by the drought. These simulations also clearly show that the three-dimensional nature of the source, boundary conditions and formation properties are strongly reflected in the resulting three-dimensional flow and transport.

Areas of Uncertainty

(1) We need to know how much rainfall infiltrates the ground, typically, vs. runoff. Also, it would be useful to know how many rainstorms on average deliver the rainfall.
(2) We need to know properties of the diesel fuel, e.g., density, viscosity, and wettability of the soils vs. water.
(3) The actual saturated permeabilities, porosities and characteristic curves are needed for each material.

Simulation of Bioremediation

The bioremediation submodel of TRACR3D calculates bacterial growth and decay in the presence of organics in porous media. It solves five nonlinear coupled time-dependent 3-D transport equations, one each for oxygen, nitrogen, two substrates and microbes. Anaerobic to aerobic conditions are included. Monod kinetics are assumed. This coupled system is solved by an iterative finite-difference algorithm. The biological activity model (Bentley and Travis, 1991) is similar to others published in the literature (e.g. Widdowson, et al., 1988). The model requires a number of coefficients for the kinetics governing consumption of substrates and oxygen and nitrogen. These must necessarily be provided on the basis of laboratory experiments.

The TRACR3D model also has the capability of performing sensitivity analyses using the differential adjoint sensitivity (DAS) theory. DAS was used to estimate the sensitivity of the oil distribution to uncertainties in soil properties such as the location of lithologic unit boundaries. Based upon the results of this analysis, the unit boundaries were modified somewhat to be fully consistent with both the stratigraphic logs and the oil distribution measurements.

Finally, 3-D simulations of a bioremediation strategy were conducted to estimate the time course and spatial extent of bacterial action on the diesel fuel and sensitivity to location and duration of oxygen injection. Keeping in mind the limitations and assumptions underlying present models of biological activity in complex environments, it appears that bioremediation can be an effective means of removing subsurface organics, and the action of bacteria can be controlled to some degree through careful monitoring of injected oxygen and nutrients.

Numerical Simulation of Vapor Extraction

For several decades, Area L has served as a disposal site for many different organic liquids (IT Corporation, 1987). These have included ethylbenzene, bromobenzene, toluene, chlorobenzene, tetrachloroethene, mix-xylenes, carbon tetrachloride, chloroform, benzene, 111-trichloroethene, trichloroethene, o-xylene and 124-trimethylbenzene. Most of the fluids were placed in shafts, approximately 10 meters deep, and spaced horizontally a few meters apart from each other. Detailed records of what was placed in each shaft are not available for the early years so an accurate description of the source term is not possible. An extensive monitoring program has been in place since 1988 to determine the location and nature of the plume of organic vapors which has been migrating from the initial disposal shafts through the unsaturated geologic media.

As a result of this unrestrained movement, a vapor extraction program has been proposed in order pull the plume back to within a certain region. Numerical modeling has been performed in order to evaluate the effectiveness of such a plan and to determine the optimum locations of the wells and anticipated power requirements. All the simulations were performed with the TRACR3D computer code (Travis and Birdsell, 1991; Travis, 1984). TRACR3D solves the equations describing unsaturated and/or saturated flow and multi-component transport in 1-D, 2-D or 3-D in heterogeneous, anisotropic porous and/or fractured media. Transport mechanisms include advection (in both phases - air and liquid), diffusion, dispersion and sorption, and also treats volatilization, biological activity and radioactive decay and decay chains. It employs a mass-conserving finite-difference implicit algorithm. It is very stable and robust.

In order to characterize the extent of the plume and to establish initial conditions for the model, a data base was developed which provides access to contaminant concentrations of each of the thirteen chemical species, in nearly thirty monitoring wells, with up to ten sampling depths per well. Monitoring has taken place on seven different occasions, resulting in over 20,000 concentration readings. Three-dimensional volume-rendering graphics are employed to visualize the different contaminant fronts at different times.

The TRACR3D code can be used to solve the inverse problem of estimating the unknown permeability field and/or flow paths, given the known, time-dependent distribution of contaminant concentrations. The known stratigraphy at specific locations (from borehole logs) was used as an initial estimate and the code modified the three-dimensional permeabilities to be more consistent with the observed vapor concentrations. TRACR3D also indicated the optimum locations for additional monitor wells as part of the inverse solution. This is quite helpful since resources for drilling are limited and the best locations are difficult to determine a priori.

The permeability and initial concentration fields were then used to set up a series of vapor extraction numerical experiments. Several vacuum wells were incorporated and the influence of a wall of positive pressure wells was studied to determined its effect on pushing contamination toward the vacuum wells and on stopping the advance of the vapor plume. Oscillatory flow scenarios were modeled to determine how fractures might influence the decontamination of the less permeable matrix material. Finally, an adjoint sensitivity analysis was performed to determine the optimum location, diameters and power requirements of the production wells used to draw the volatile organic plume within the desired boundaries.

The use of the TRACR3D code to help determine the monitor well and production well locations and characteristics represents a significant advance in the use of numerical tools for environmental remediation. Given the limitations and assumptions inherent to numerical models of this type, the calculations have shown that vacuum vapor extraction would be an effective means of controlling the extent of the volatile organic vapor plume at Area L. Furthermore, the TRACR3D model has provided a quantitative estimate of field requirements, such as the the cyclic period of oscillatory extraction, given the in-situ fracture spacing and permeability.

Acknowledgments

Sandy Leo at Sandia National Laboratories, Livermore and John Krueger at Los Alamos National Laboratory are gratefully acknowledged for their support of the bioremediation and vapor extraction work, respectively. This work was performed under the auspices of the U.S. Department of Energy.

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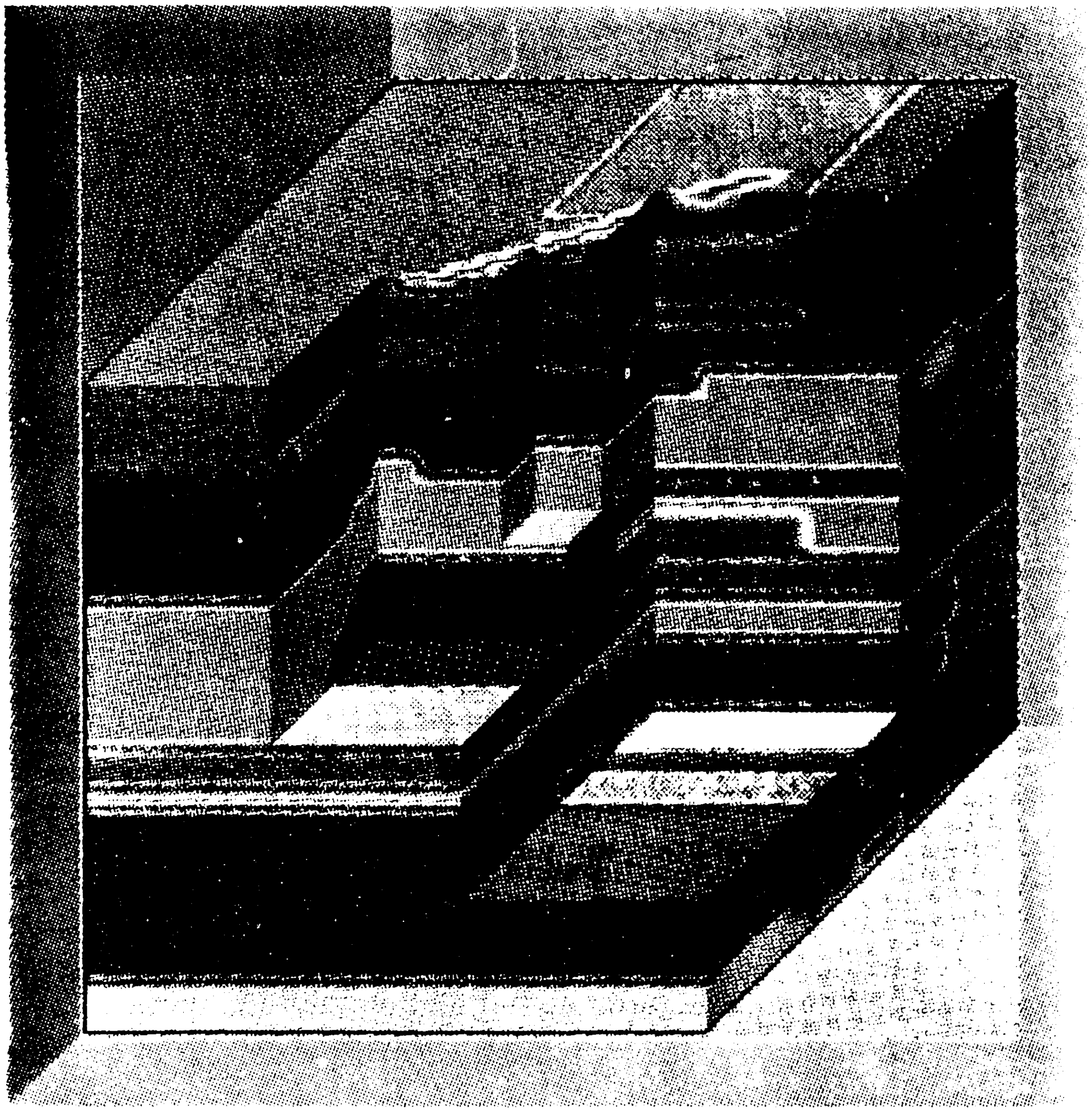

Fig. 1a Distribution of soil types--Perspective A. Cut-out allows viewing of subsurface structure. Soil types are color-coded. Domain shown is 50 m in each horizontal dimension and 30 m deep.

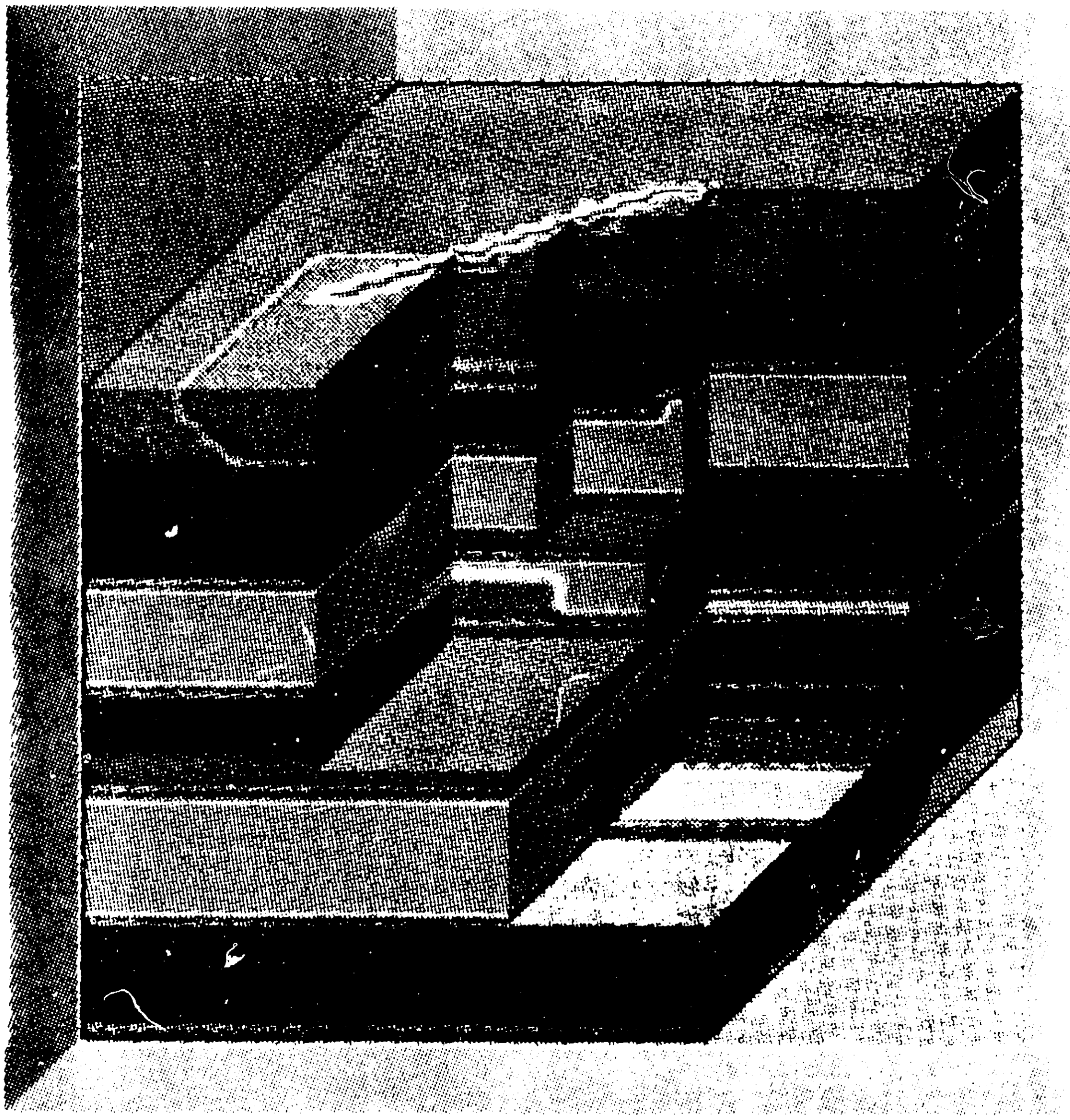

Fig. 1b Distribution of soil types--Perspective B (180° rotation of Perspective A.) Cut-out allows viewing of subsurface structure. Soil types are color-coded. Domain shown is 50 m in each horizontal dimension and 30 m deep.

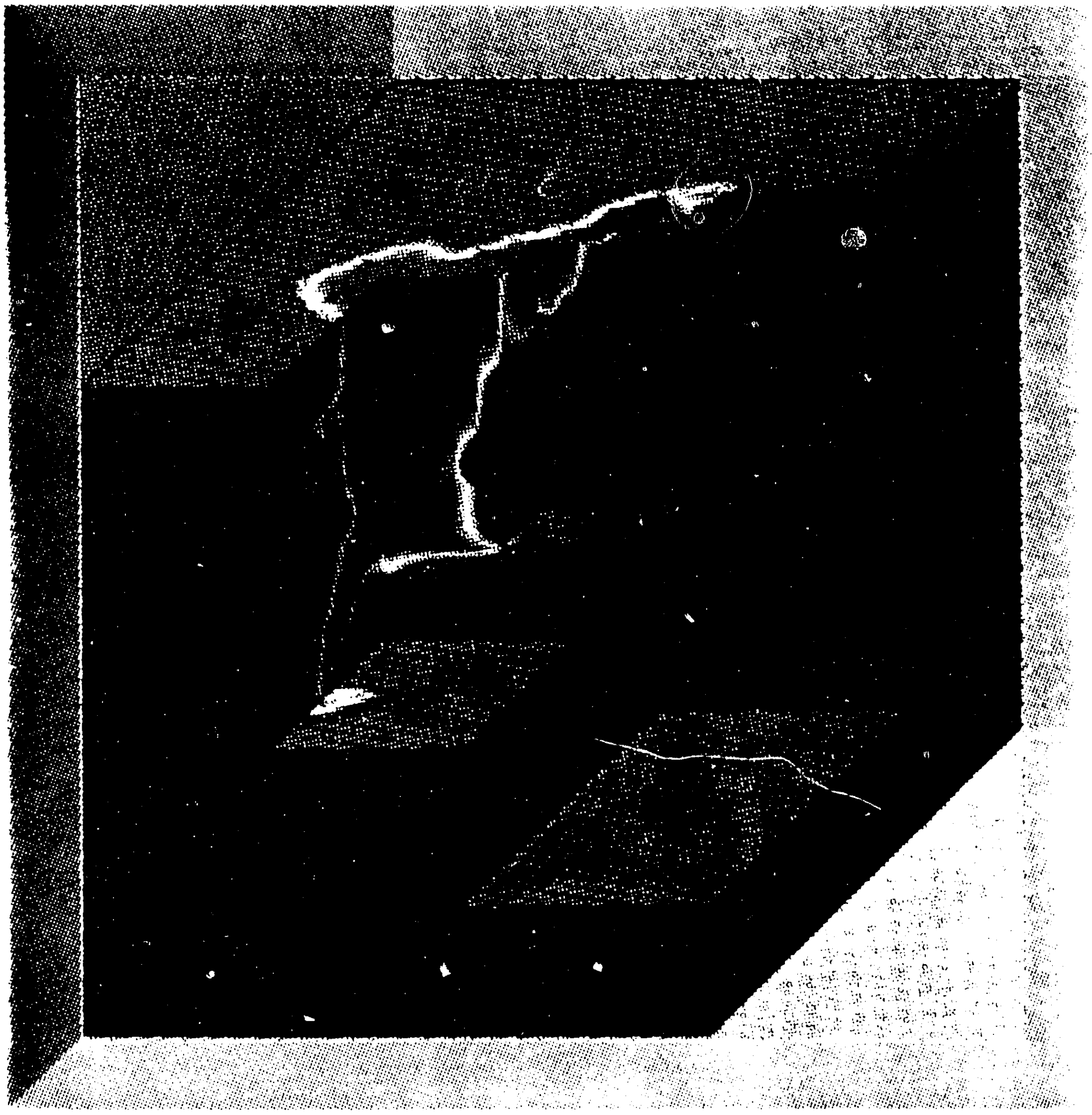

Fig. 2a Subsurface distribution of fuel oil at 0.5 years for low infiltration case. Concentration is color-coded. Perspective A.

Fig. 2b Subsurface distribution of fuel oil at 5.0 years for low infiltration case. Concentration is color-coded. Perspective A.

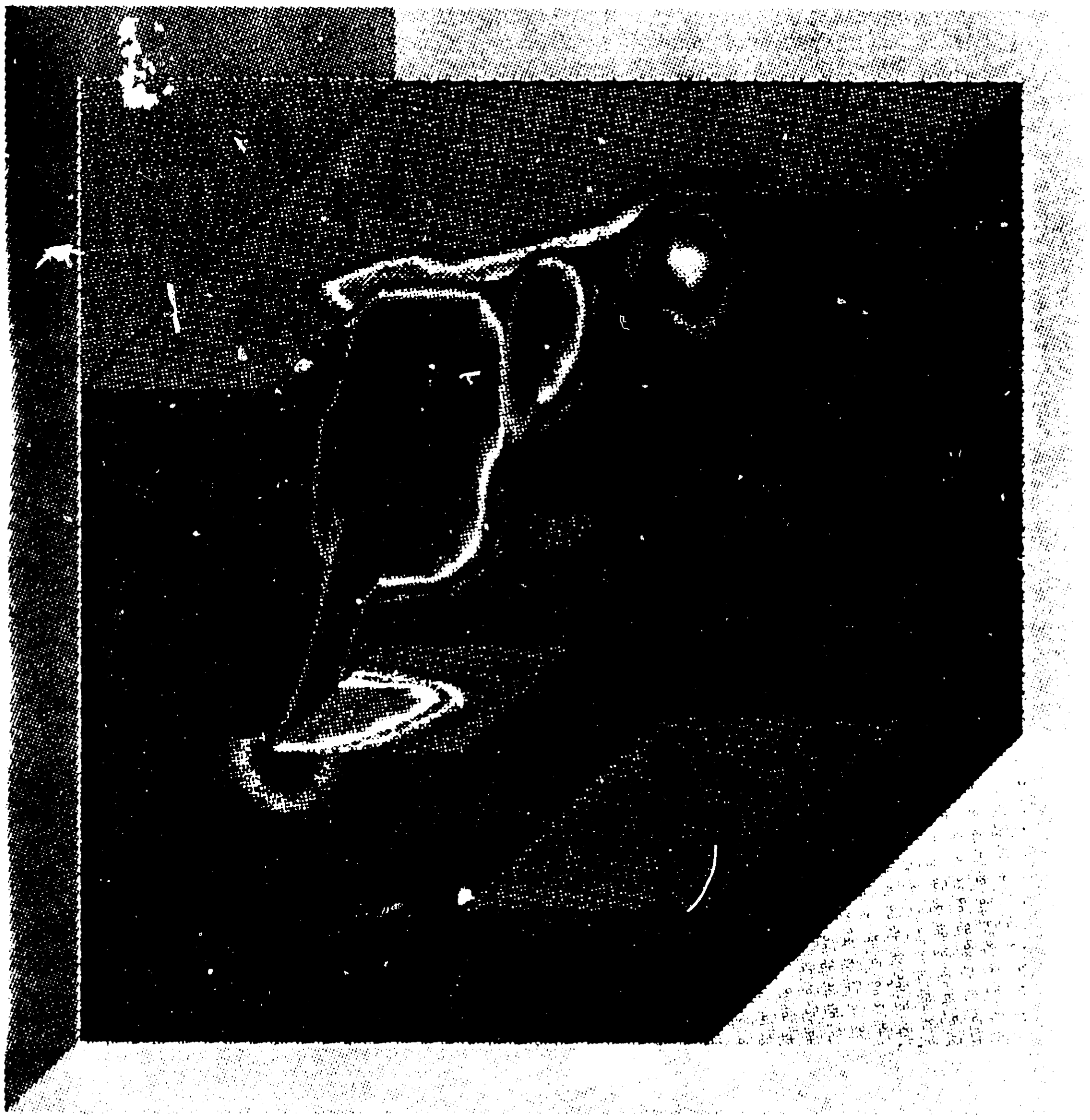

Fig. 2c Subsurface distribution of fuel oil at 13. years for low infiltration case. Concentration is color-coded. Perspective A.

Fig. 3a Subsurface distribution of fuel oil at 0.5 years for high infiltration case. Concentration is color-coded. Perspective A.

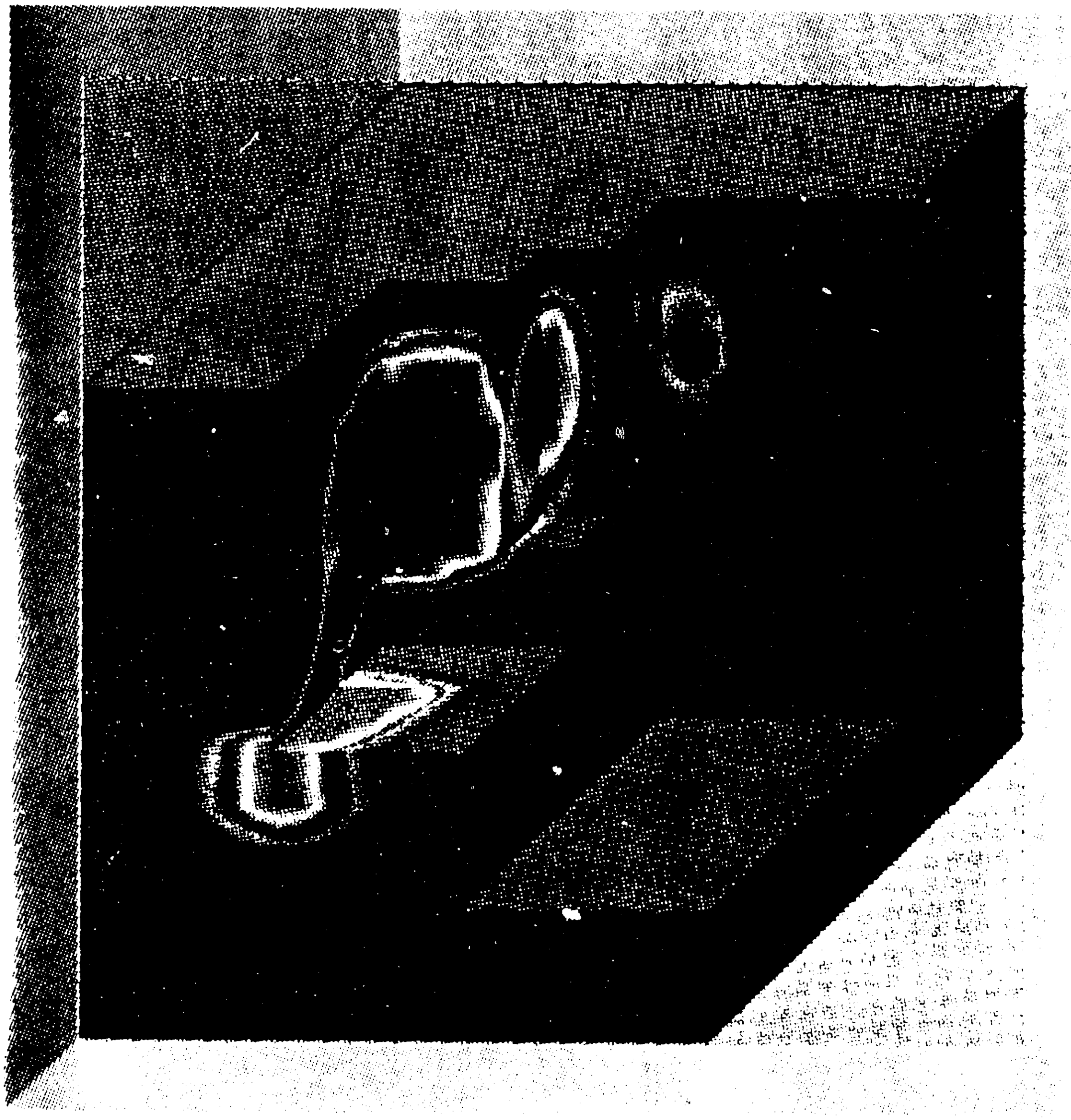

Fig. 3b Subsurface distribution of fuel oil at 5.0 years for high infiltration case. Concentration is color-coded. Perspective A.

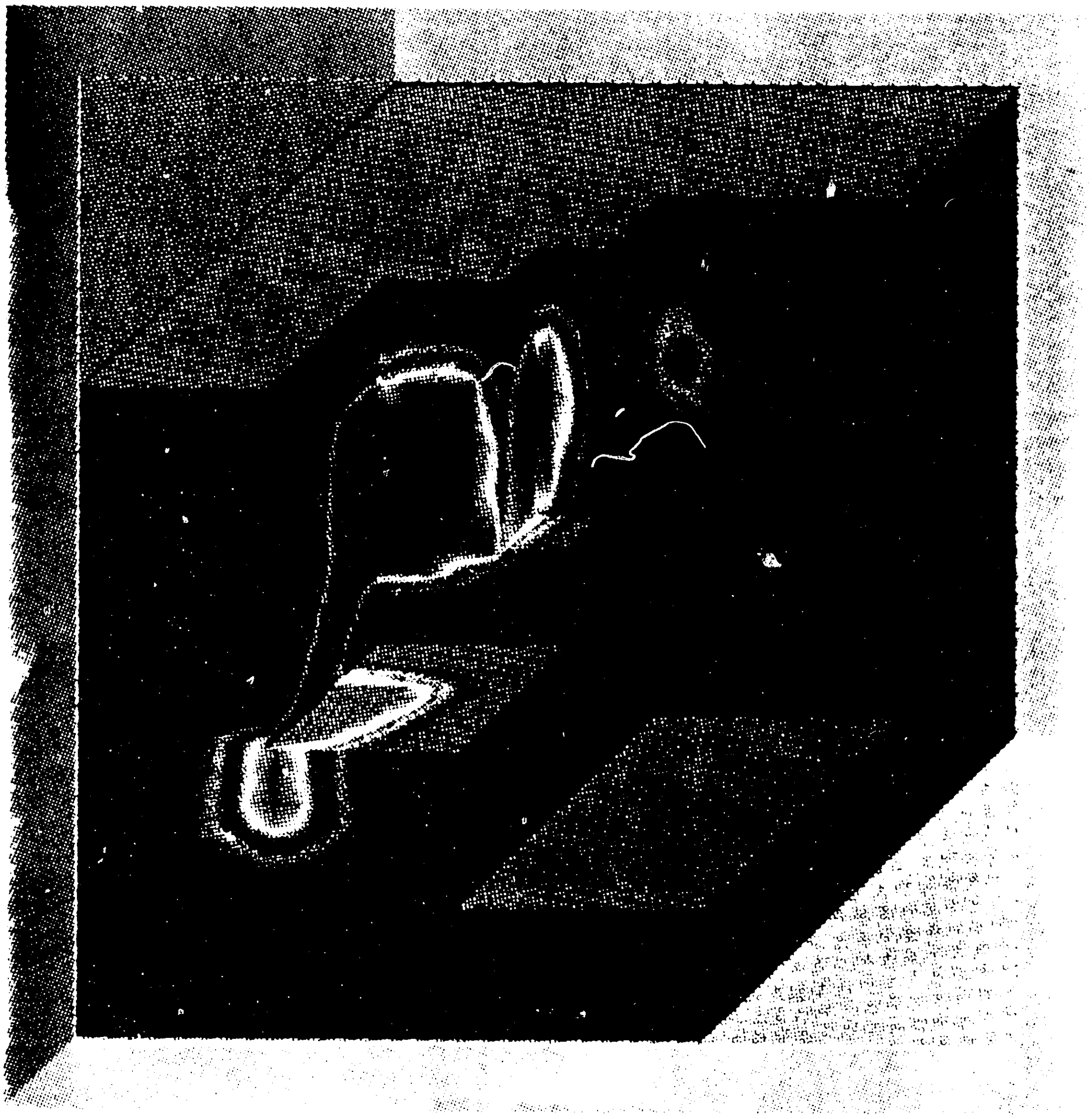

Fig. 3c Subsurface distribution of fuel oil at 6.5 years for high infiltration case. Concentration is color-coded. Perspective A.

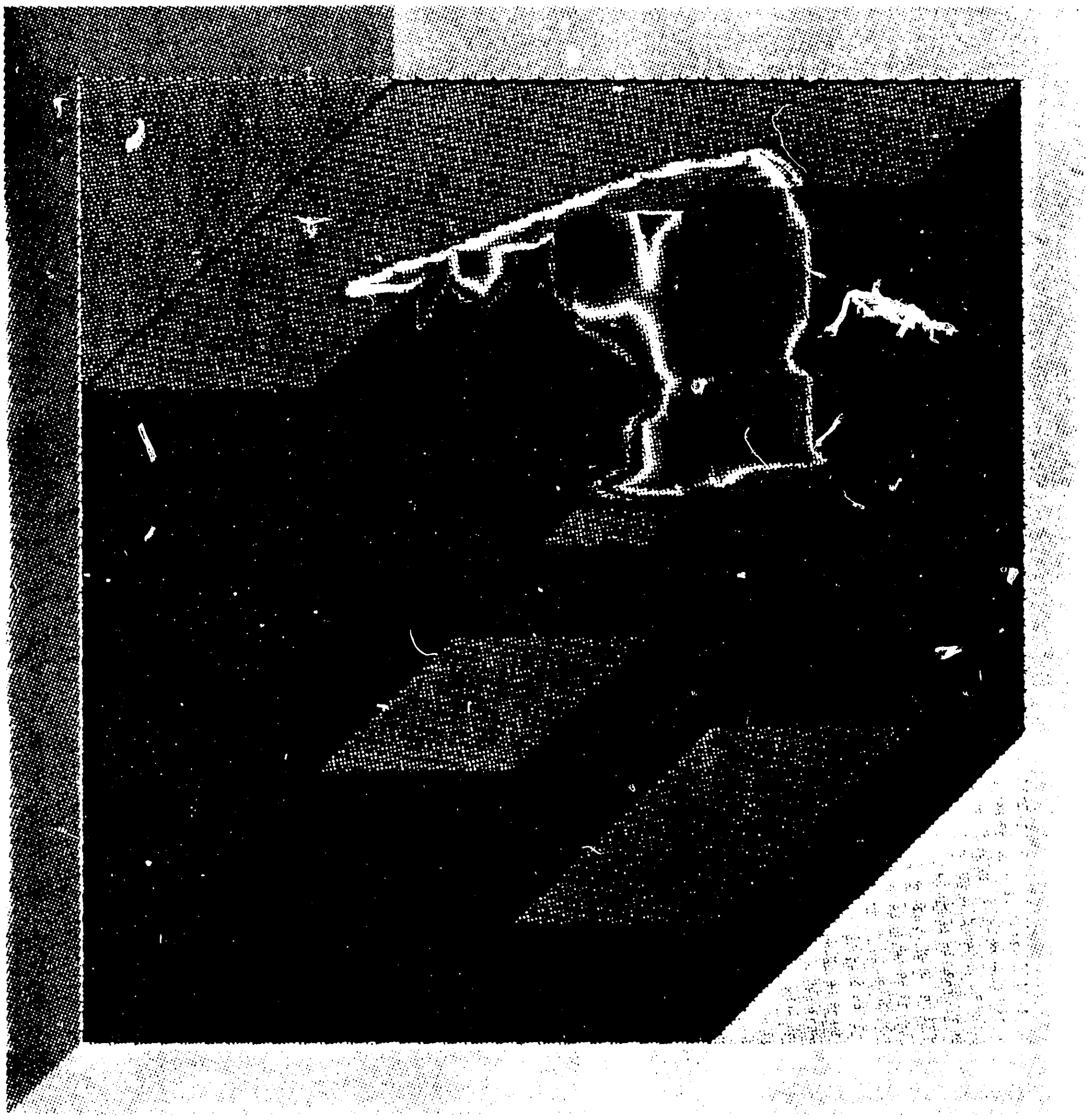

Fig. 4a Subsurface distribution of fuel oil at 0.5 years for high infiltration case. Concentration is color-coded. Perspective B.

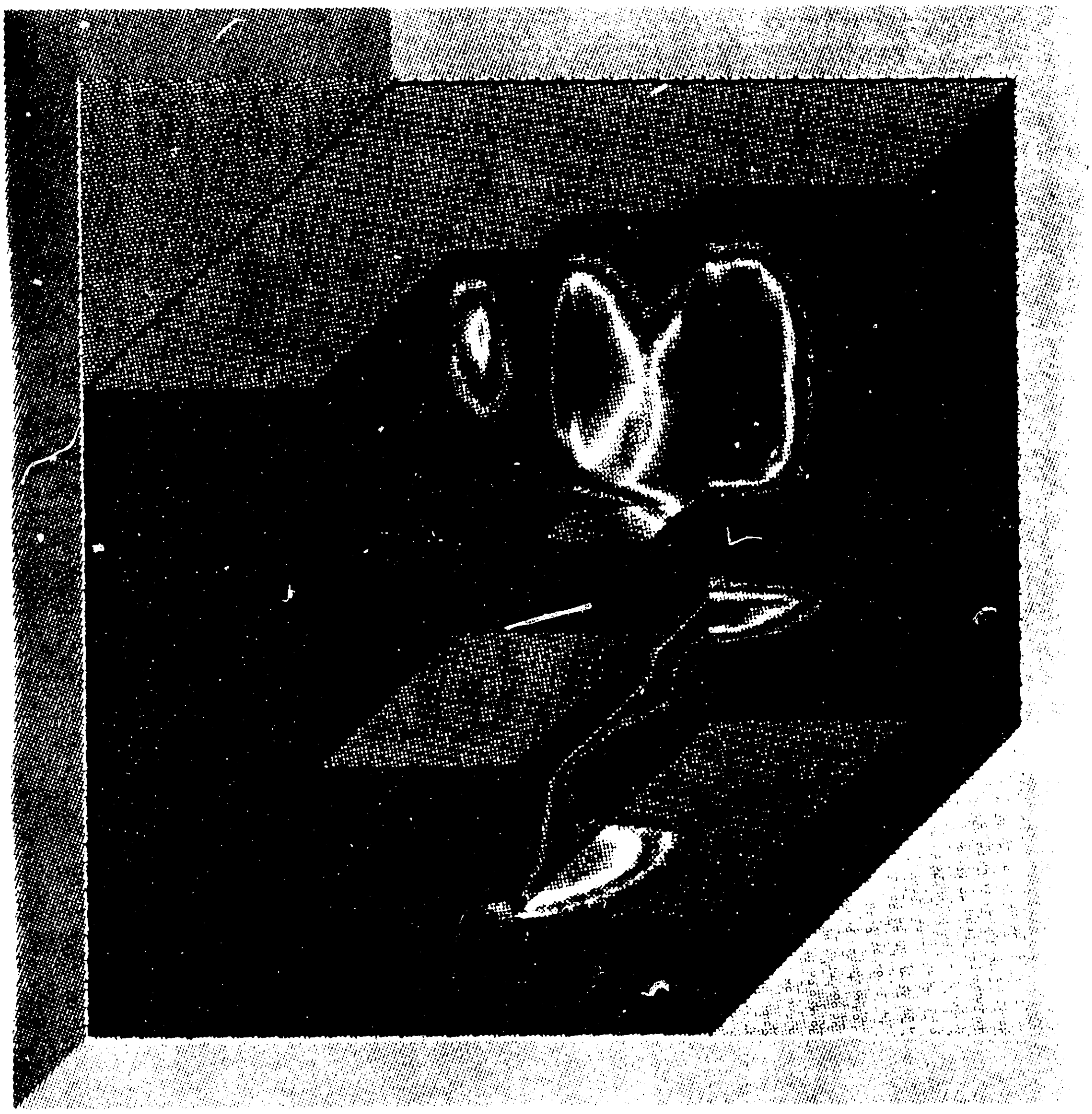

Fig. 4b Subsurface distribution of fuel oil at 5.0 years for high infiltration case. Concentration is color-coded. Perspective B.

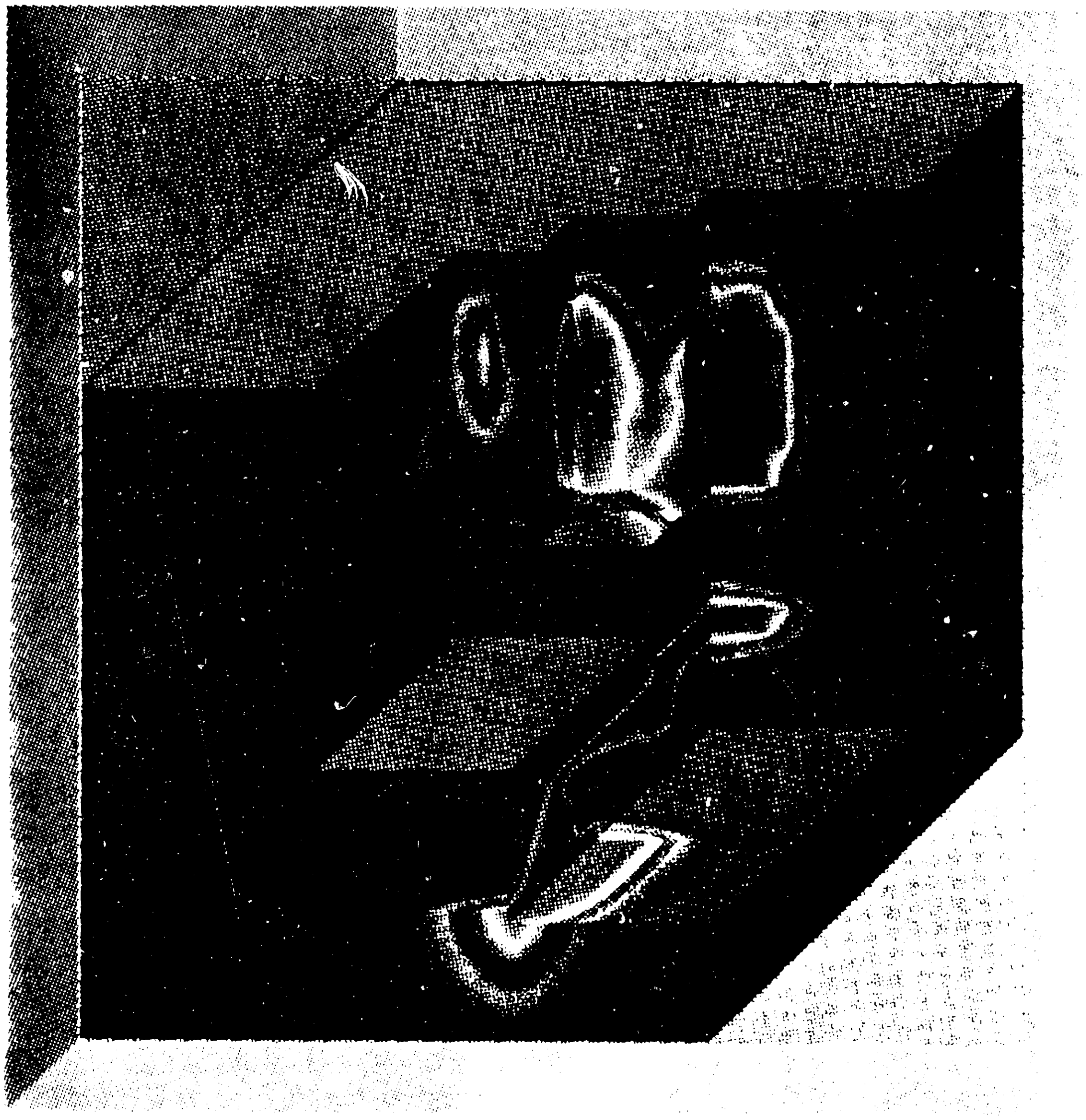

Fig. 4c Subsurface distribution of fuel oil at 6.5 years for high infiltration case. Concentration is color-coded. Perspective B.

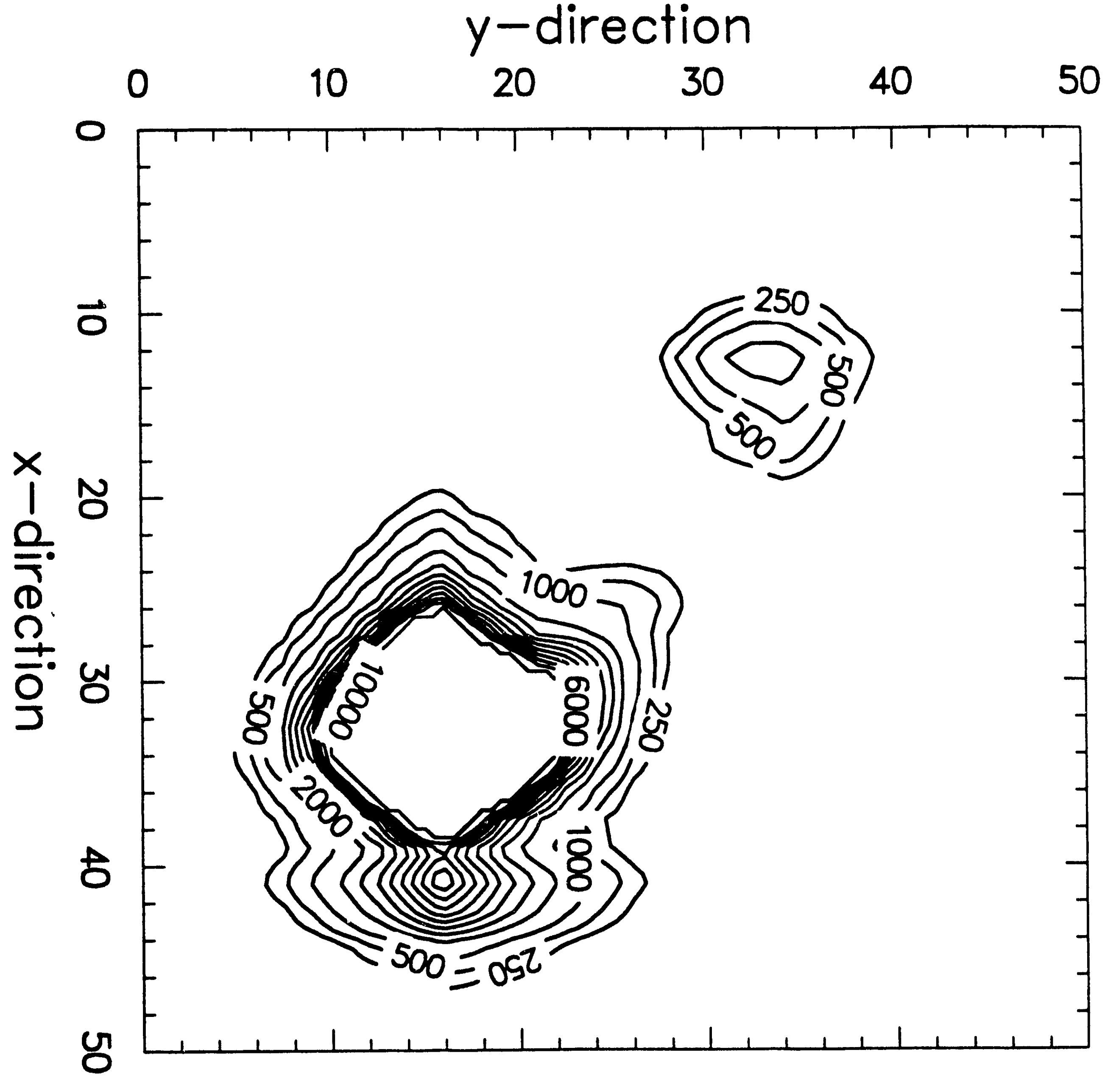

Fig. 5a Concentration contours (mg/kg) of fuel oil on a horizontal plane at a depth of 40 feet at 13 years, for low infiltration case. X and Y length scales are in meters.

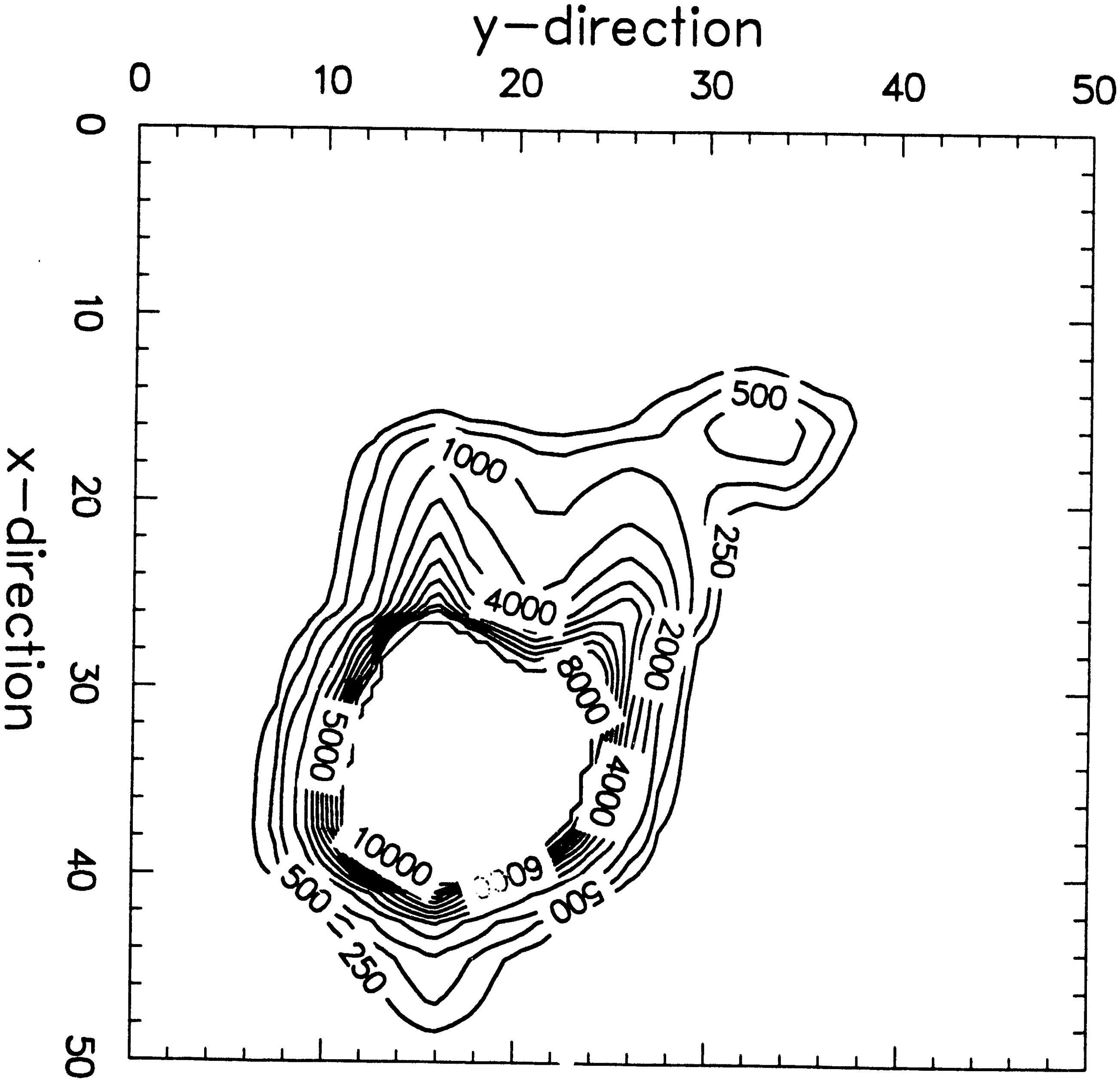

Fig. 5b Concentration contours (mg/kg) of fuel oil on a horizontal plane at a depth of 40 feet at 6.5 years, for high infiltration case. X and Y length scales are in meters.

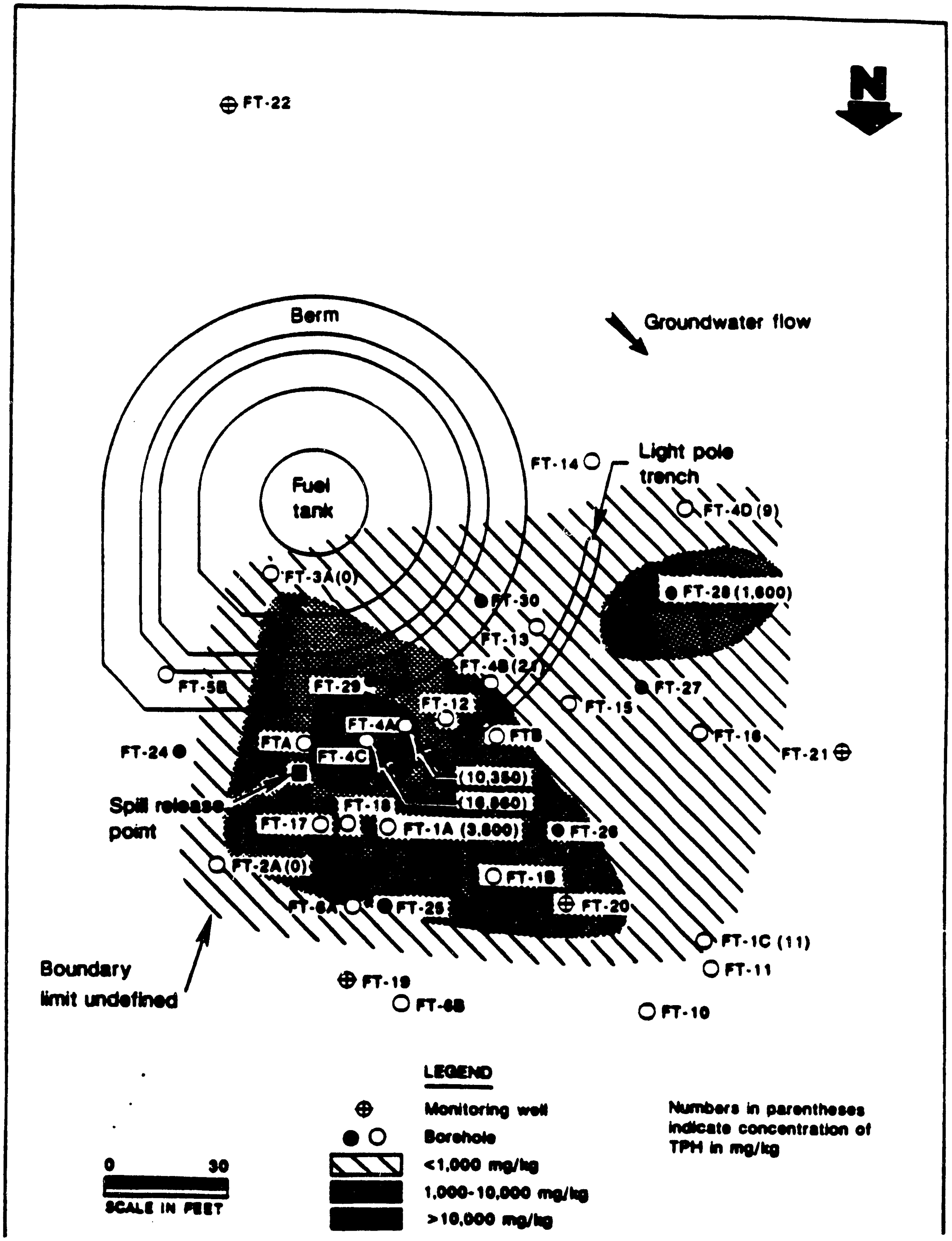

Fig. 5c Measured concentration contours (mg/kg) of fuel oil on a horizontal plane for the depth interval of 30 to 50 feet, at 13 years. (From DOE, 1989.)

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