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Preliminary Analysis of NAPL Behavior in Soil-Heated Vapor Extraction for *In-Situ* Environmental Restoration

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Simulations of soil-heated vapor extraction have been performed to evaluate the NAPL removal performance as a function of borehole vacuum. The possibility of loss of NAPL containment, or NAPL migration into the unheated soil, is also evaluated in the simulations. A practical warning sign indicating migration of NAPL into the unheated zone is discussed.

Soil-heated vapor extraction is proposed as a process to remove solvents and chemicals from contaminated soils. In this process, the ground is heated electrically, and borehole(s) within the heated zone are maintained at a vacuum to draw air and evaporated contaminants into the borehole and a subsequent treatment facility. Sandia National Laboratories has designed a field demonstration of the process at the Chemical Waste Landfill at Sandia, designated TEVES (Thermal Enhanced Vapor Extraction System), which is currently underway. Additional details are given in [1] and [2].

As part of the evaluation process, detailed two-phase fluid flow and heat transfer simulations have been performed using the single-component NAPL version of the TOUGH2 computer code. The behavior of liquid water and contaminants will be influenced by a number of factors including soil heating rate and local temperature gradients, evaporation rate of the liquid water and contaminants, air flow rate, and borehole (vapor extraction) location(s). If the air flow rate is too small, the heating and evaporation processes may drive the contaminant vapors out of the heated zone and into the cooler unheated soil where they may condense, and contaminant migration into previously uncontaminated areas would occur. Figure 1 shows the general TEVES process setup. In this process, the ground is electrically heated, and borehole(s) within the heated zone are maintained at a vacuum to draw air and evaporated contaminants into the borehole and a subsequent treatment facility. The ground above the heated zone and beyond is insulated to minimize heat loss to the ambient environment. A vapor barrier is used over a yet larger area to provide for a more complete air sweep of the contaminated soil.

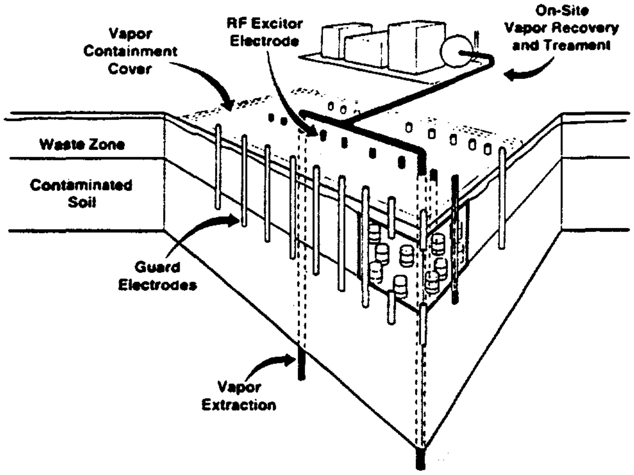


Fig 1 Soil-Heated Vapor Extraction Configuration (TEVES)

MODEL DEVELOPMENT

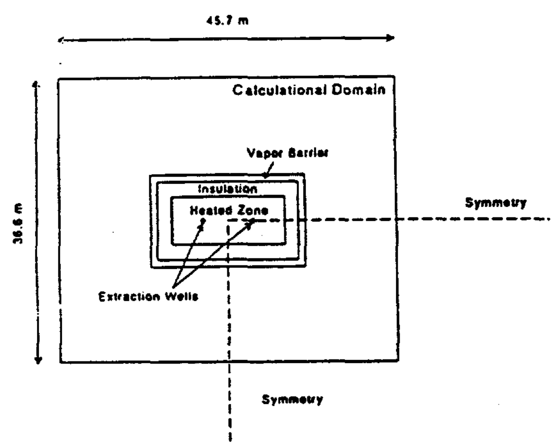
Simulations of soil-heated vapor extraction have been performed using a modified version of the TOUGH2 computer code [3]. TOUGH2 simulates fluid flow and heat transport in porous and fractured media including unsaturated conditions. The original TOUGH2 program considers fluid flow and heat transport for water and air. Recent modifications to the code include the capability to simulate a single-component NAPL in addition to the water and air components already present [4], and the addition of a conjugate gradient solver package to improve the numerical performance

DISCLAIMER

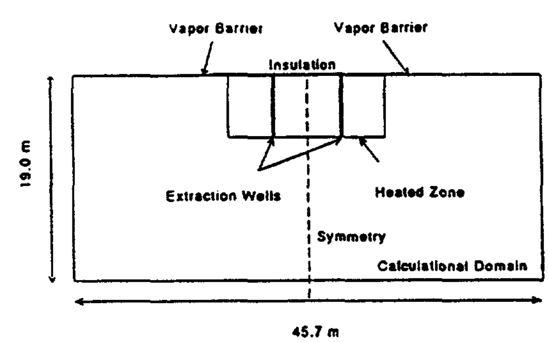
[5]. Test versions of these modifications were provided to the author for testing and evaluation. The assistance and cooperation of Lawrence Berkeley Laboratory in providing these versions is gratefully acknowledged.

The single-component NAPL capability in TOUGH2 is based on the work of Falta, et al. [6,7] and the STMVOC computer program [8]. The formulation is restricted in that the gas and liquid phases can not completely disappear; this effect is noted in the present results. More recently, further improvements have been made in the NAPL simulation capability in the M²NOTS code [9] which is an extension of the TOUGH2 code. The multi-component NAPL formulation is planned to be used in future analyses to address multi-component issues.

Figure 2 shows the conceptual model of TEVES used for the analysis. A three-dimensional TOUGH2 model with over 2200 elements is employed using quarter symmetry to simplify the model; the nodalization is shown in Figures 3. Vapor extraction occurs through two vapor extraction wells located near the center of the heated zone. The nominal borehole vacuum is 2.5 kPa (10 inches of water). The borehole is modeled as a constant pressure and temperature boundary with no heat transfer between the soil and the borehole. The borehole vacuum is an important parameter, because if the air sweep into the borehole is not sufficient, water vapor and VOCs generated by the heating process could migrate from the heated zone into the unheated soil resulting in a loss of containment.

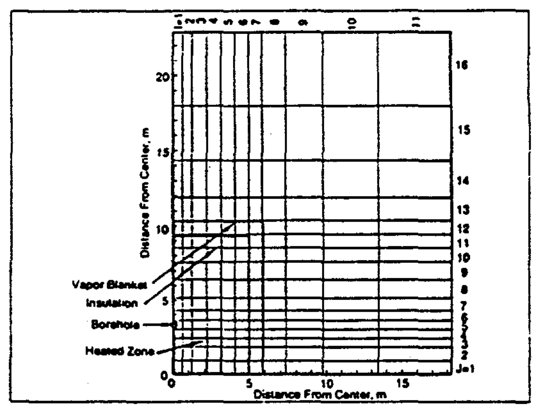


(a) Top View



(b) Side View

Fig 2 Conceptual Model



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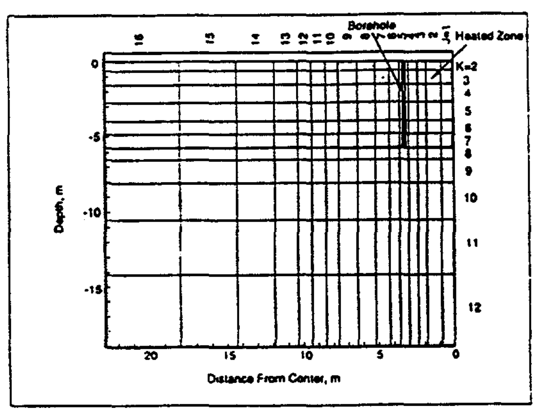


(b) Side View

Fig 3 Computer Model Nodalization

Heat is added uniformly to the heated zone at the rate of 100 kW, or a volumetric heating rate of 190 W/m^3. If all the heat is assumed to go into evaporation of the initial water in the soil, approximately 0.044 kg/s of water vapor would be generated. The vapor barrier is assumed impermeable to flow. The permeability of the soil is assumed to be 50 darcies with a porosity of 0.333 and an initial liquid water saturation of 0.20, less than the liquid residual saturation. An initial o-xylene saturation of 0.05 in the entire heated zone is assumed to simulate an initial NAPL inventory. No NAPL is initially present in the unheated zone.

The soil is initially at ambient conditions, and heating and the venting occur simultaneously. As time proceeds, the soil heats up, and liquid water and NAPL are vaporized and generally transported toward the borehole. At 60 days, heating is stopped but venting continues. The soil cools down due to heat losses to the unheated soil and to the atmosphere.

The Parker et al. three-phase characteristic curves [10] have been used, although both liquid phases are initially immobile because the liquid residual saturation is greater than the initial value. Liquid transport only occurs due to evaporation and condensation phenomena, not due to transport of the liquid phase unless evaporation and condensation processes increase the local saturation sufficiently to mobilize the liquid.

The borehole vacuum was decreased from the nominal value of 2.5 kPa until NAPL migrated into the unheated soil surrounding the heated zone, which occurred at a borehole vacuum of 0.5 kPa. Webb[2] presents the results for borehole vacuums of 2.5 kPa and 1.0 kPa. For 0.5 kPa vacuum, the NAPL migration percentage was small compared to the total inventory, and the NAPL quickly re-evaporated and was transported to the vapor extraction location as time went on. Nevertheless, migration into the unheated zone represents a loss of containment of the NAPL within the heated zone.

SIMULATION RESULTS

The time variation of the soil temperature in the heated zone out to 60 days is shown in Figure 4 for a 0.5 kPa borehole vacuum; the time variation is very similar to other borehole vacuum cases. After 60 days, the heated zone average temperature is about 264°C with a range of 137 to 375 °C; these values are only about 15-20°C higher than for 2.5 kPa vacuum [2] indicating minor heat losses to the air flow through the soil. Top and side-view temperature contours at 60 days are shown in Figure 5.

Figure 6a gives the time variation of the water and NAPL liquid masses in the heated zone. The NAPL mass in the heated zone is mostly gone within about 12 days; for a higher borehole vacuum of 2.5 kPa, the time

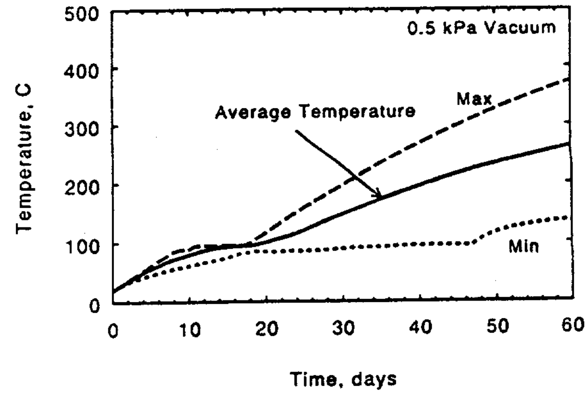
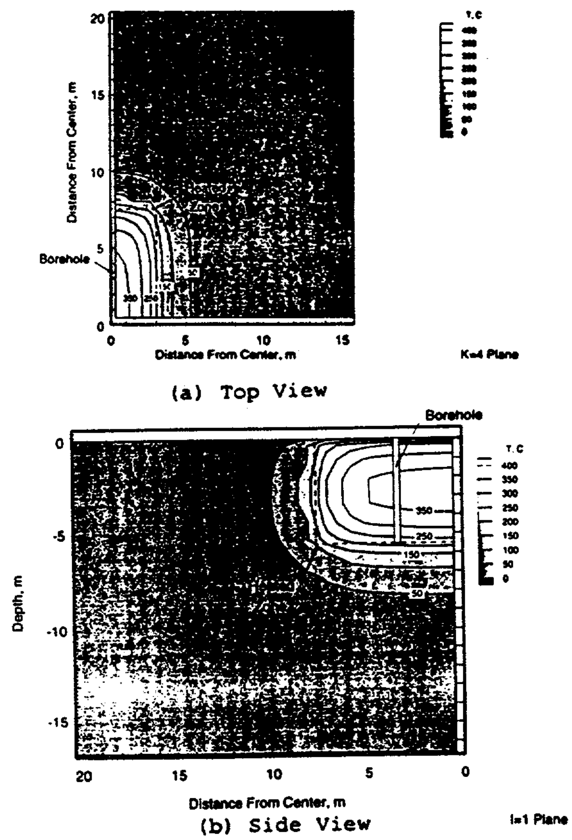


Fig 4 Heated Zone Temperatures



(a) Top View

(b) Side View

Fig 5 Temperature Contours at 60 Days

is about 7 days. The increased time for the lower vacuum is due to the lower air flow rate through the soil. Figure 6b shows the NAPL masses in the heated and unheated soil. At about 14 days, just before the last of the NAPL in the heated zone disappears, NAPL starts to migrate to the unheated soil. The NAPL in the unheated soil continues to increase until about 20 days. After this time, NAPL migration from the heated zone stops, and NAPL in the unheated soil starts to decrease as the unheated soil temperature increases and NAPL evaporates into the air

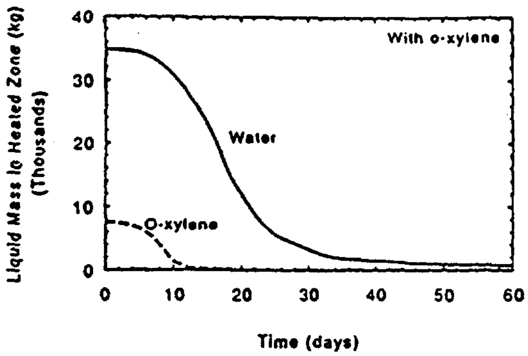


Fig 6a Heated Zone Water and NAPL Masses

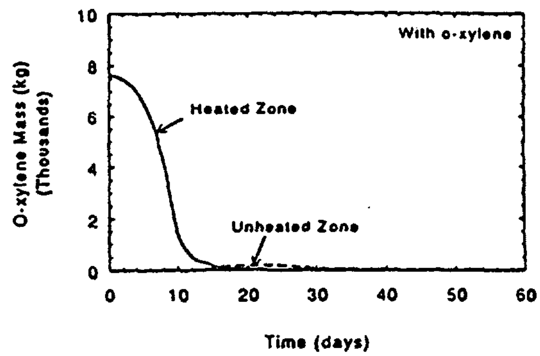
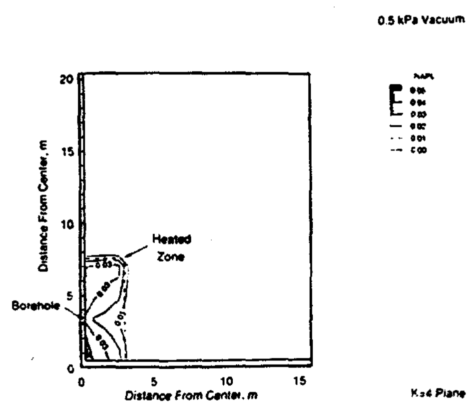


Fig 6b Heated and Unheated Zone NAPL Masses

flowing through the soil toward the extraction borehole. The maximum NAPL mass in the unheated soil is about 200 kg compared to an initial mass of almost 8000 kg in the heated zone, or less than 3% of the initial mass. While this migrated NAPL is eventually evaporated and transported to the borehole, the migration into the unheated soil represents undesirable contaminant migration caused by insufficient air sweep.

NAPL contours at 8 and 11.6 days are given in Figures 7 and 8, respectively. The saturation contours show a zone of NAPL which is left behind on the edges of the heated zone. Transport into the unheated zone is due to evaporation in the heated zone, flow into the unheated soil, and condensation in the cooler unheated soil. Liquid water saturation contours at 30 days, which are not shown, also indicate an insufficient air sweep. Water evaporates in the heated zone and is subsequently transported and condensed in the unheated soil as indicated by liquid saturations higher initial saturations along some of the edges of the heated zone.



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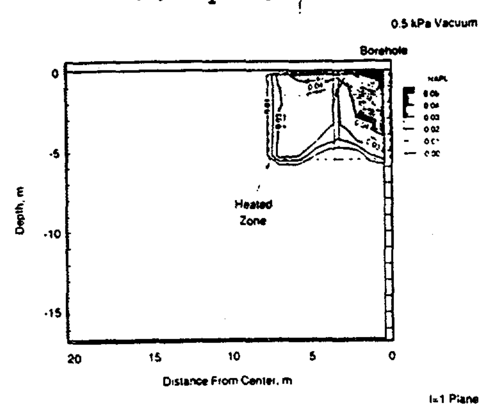
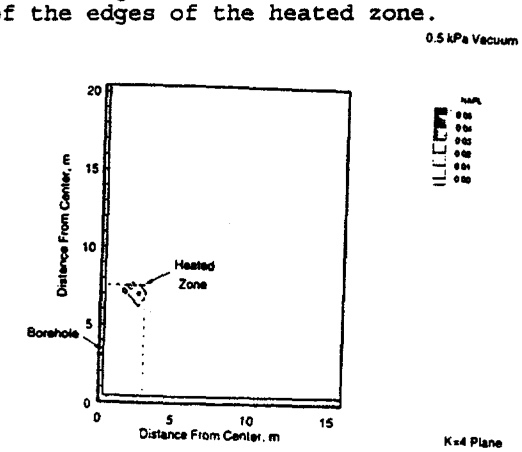


(b) Side View

Fig 7 NAPL Contours at 8 Days



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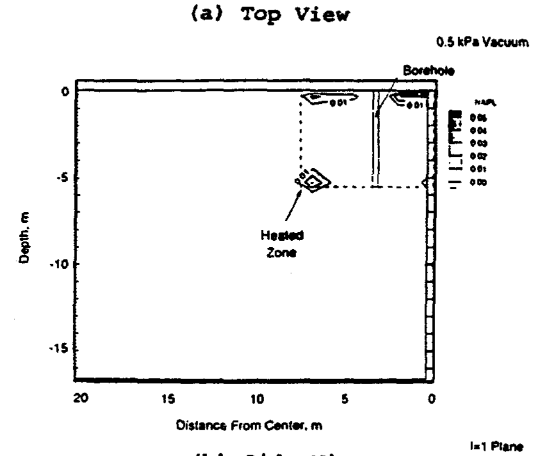


(b) Side View

Fig 8 NAPL Contours at 11.6 Days

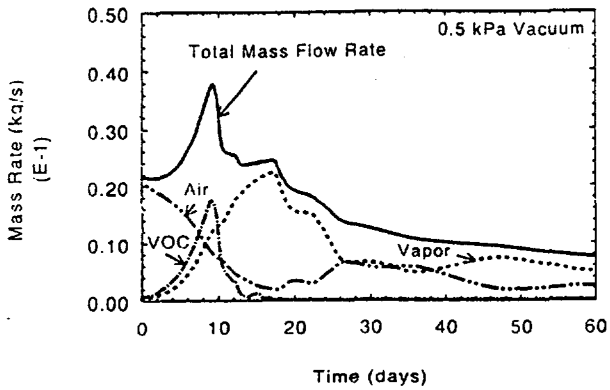
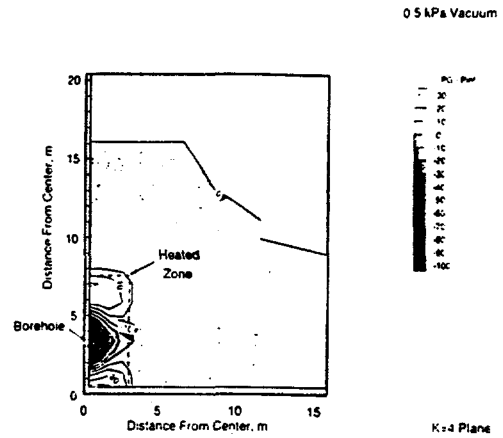


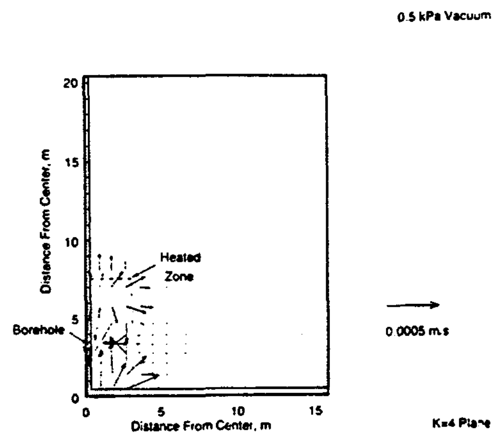
Fig 9 Mass Flow Rates Into the Borehole

Figure 9 shows the various mass flow rates into the borehole. The total mass flow rate into the borehole increases in the early stages of heating due to the evaporation of the NAPL (VOC) component in the heated soil. For much of the simulation, the mass fraction is predominantly vapor. The vapor flow rate into the borehole peaks at a value of about 0.022 kg/s, or about 1/2 of the maximum vapor generation rate given earlier; this value is significantly lower than the 0.032 kg/s rate for 2.5 kPa borehole vacuum. However, the air flow rate into the borehole is dramatically reduced from the 2.5 kPa case, from a peak of 0.094 kg/s to a peak of 0.02 kg/s for 0.5 kPa. The vapor mass fraction into the borehole peaks at about 92% at 15 days, indicating little air flow through the heated zone. For the 0.5 kPa case, the borehole vacuum is not sufficient to capture all the vapor generated, and some vapor flows into the unheated zone where it condenses. Some VOCs also flow along with the water vapor, condensing in the unheated soil. Obviously, a practical warning occurs when the vapor mass flow rate dominates the total mass flow rate into the borehole, indicating insufficient air flow and possible contaminant migration into the unheated soil.

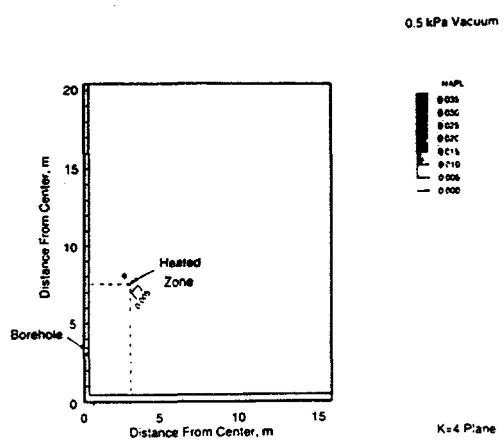
Figure 10 shows details of the NAPL migration into the unheated soil; the results are given for 15 days, which is the maximum rate of NAPL inflow into the unheated zone. Figure 10a shows the pressure difference compared to the far-field value; dark areas indicate gas pressures less than the far-field, while light areas indicate higher gas pressures. At the top of the heated zone, the gas pressure is significantly higher than the far-field value. Figure 10b shows the resulting gas velocity vectors indicating significant gas flow from the heated zone into the unheated soil. As shown in Figure 10c, this region corresponds to NAPL migration into the unheated soil, representing a loss of containment of the NAPL within the heated zone.



(a) Pressure Differential Contours



(b) Gas Velocity Vectors



(c) NAPL Contours

Fig 10 NAPL Migration Details at 15 Days

SUMMARY AND CONCLUSIONS

Detailed simulations have been performed for the soil-heated vapor extraction based on the TEVES Project using the TOUGH2 code considering air, water, and a single-component NAPL. A critical parameter varied in the simulations is the borehole vacuum which directly affects air flow through the system and indirectly influences soil temperatures and water and NAPL fluid masses. Contaminant migration from the heated zone into the unheated soil can occur if the borehole vacuum, or borehole flow rate, is not sufficient. Under these conditions, evaporation of liquids (water and NAPL) due to the heating can cause flow from the heated zone into the unheated soil. Insufficient air sweep may be indicated by a vapor dominated mass flow rate into the borehole, at least for the present configuration. Sufficient air flow through the heated zone must be provided to contain the contaminants within the heated zone.

The above analyses are greatly simplified since they assume homogeneous soil properties and a single-component NAPL. Further investigation into heterogeneity effects including layering and the influence of multicomponent NAPLs on contaminant migration should be performed. In this case, gas diffusion processes may dominate transport as discussed by Ho and Udell [11].

ACKNOWLEDGMENT

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