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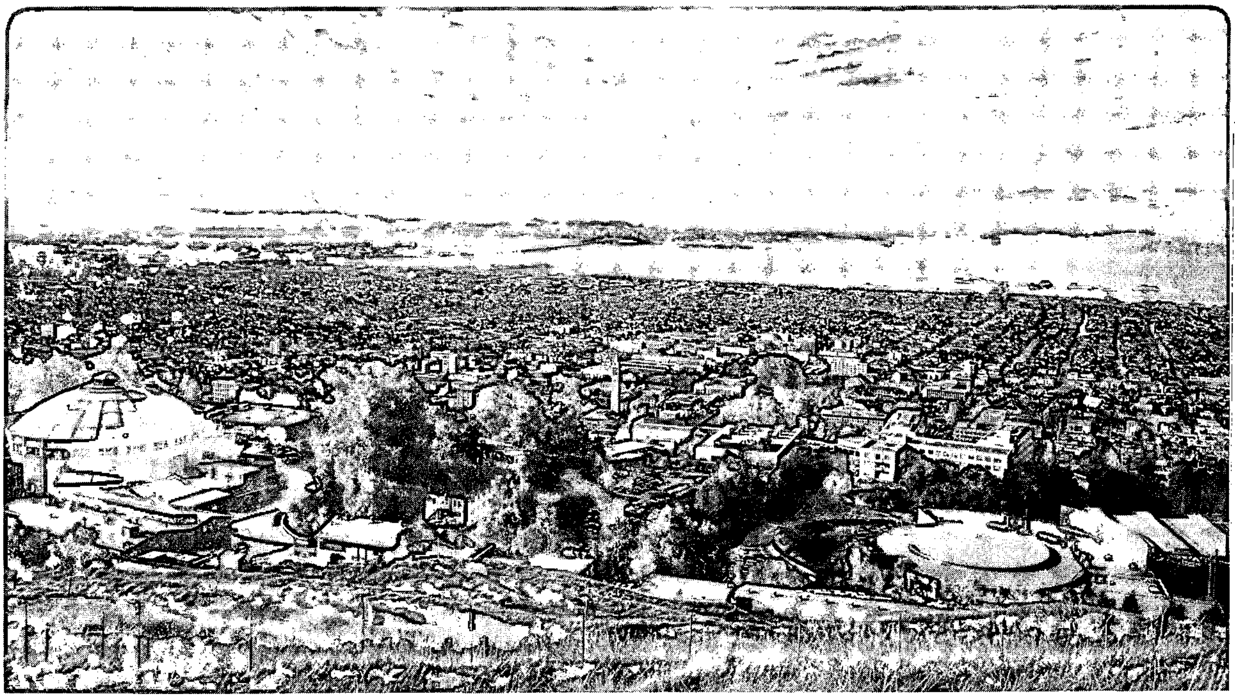

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Preliminary Studies of Thermally Enhanced Soil Vapor Extraction

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1 Introduction

In recent years, actual and potential contamination of air, soil and groundwater by organic compounds has become a field of increasing environmental interest in Germany. The main concern is the huge number of abandoned landfill sites, where organic liquids often infiltrate the unsaturated zone. Since non-aqueous phase liquids (NAPLs) - for example mineral oil or chlorinated hydrocarbons - are rather immobile if the NAPL-content of the soil is less than 10 %, contaminant spills with NAPL remain long term contaminant sources. They dissolve in groundwater and evaporate into the soil gas, and will be transported by diffusion into the atmosphere. For remediation the traditional "pump and treat" methods are inefficient because NAPL solubility in groundwater is small and because sorption and vaporization of the contaminant can be rate-limited processes.

With the aim of developing remediation technologies, the experimental VEGAS research facility for subsurface remediation [1] was built at the Institute of Hydraulic Engineering at the University of Stuttgart/Germany. The objective of VEGAS is to test and optimize existing techniques and to develop new approaches for in-situ remediation of contaminated aquifers and soils. VEGAS focusses on methods for determining the mobility of contaminants in the subsurface and for improving the assessment of contaminated sites. Furthermore, methods for determining the overall mass and distribution of contaminants in the subsurface, and techniques for identifying physical and chemical subsurface properties are to be developed and improved as well. This includes further development of finite element techniques for simulating 3-phase fluid and heat flow [2].

2 Aim

One of the ongoing studies in VEGAS is called "thermally enhanced soil vapor extraction" and concerns soil venting, which is an established technology for the remediation of organic contaminants in the vadose zone. Concurrent injection of heat may improve the effectiveness of soil venting by enhancing some physical processes, e.g. increasing NAPL vapor pressure and decreasing capillary forces. The aim of the present study is to develop a better understanding of the physical processes in existing thermally enhanced methods. Numerical modeling is used to explore effects of steam and hot air injection into homogeneous and heterogeneous soils. Subsequently it is planned to conduct laboratory experiments to investigate the remediation of contaminated soils on different scales. A bench scale experiment (Height=74cm, Length=135cm, Width=10cm) will lead through two-dimensional prestudies to a three-dimensional technical-scale experiment in the VEGAS-container (Height=450cm, Length=590cm, Width=600cm). Numerical models are used to provide a quantitative description of the relevant processes and mechanisms, and to aid in the design and analysis of the experiments.

For a better design of the experiments, numerical modeling was chosen as a tool to predict steam and hot air flow patterns for different injection scenarios. For this purpose the Integral-Finite-Difference simulator TOUGH2/T2VOC [3], [4], [5] was applied at Lawrence Berkeley Laboratory to various flow scenarios. TOUGH2/T2VOC is a version of the general-purpose multiphase fluid and heat flow simulator TOUGH2 that was specifically designed for 3-component, 3-phase flows of water, air and NAPL. A detailed discussion of physical processes modeled and mathematical and numerical methods used is given in the indicated references. The results of exploratory calculations are presented in this report.

3 Setup of the numerical examples

The flow system modeled is a two-dimensional rectangular container, placed vertically, which has three inlet and three outlet openings for the injection and withdrawal of fluids. The system was assumed 74 cm in height, 135 cm long, 10 cm thick, and the discretization is shown in Fig. 1. The figure shows lines connecting nodal points. Each of the six openings involves two adjacent nodes marked by arrows. No-flow boundary conditions are applied everywhere, except at the inlet and outlet ports. The investigations considered a homogeneous sand with and without a finer, less permeable sand lens, together with injection of steam only and steam with dry air with different spatial arrangements.

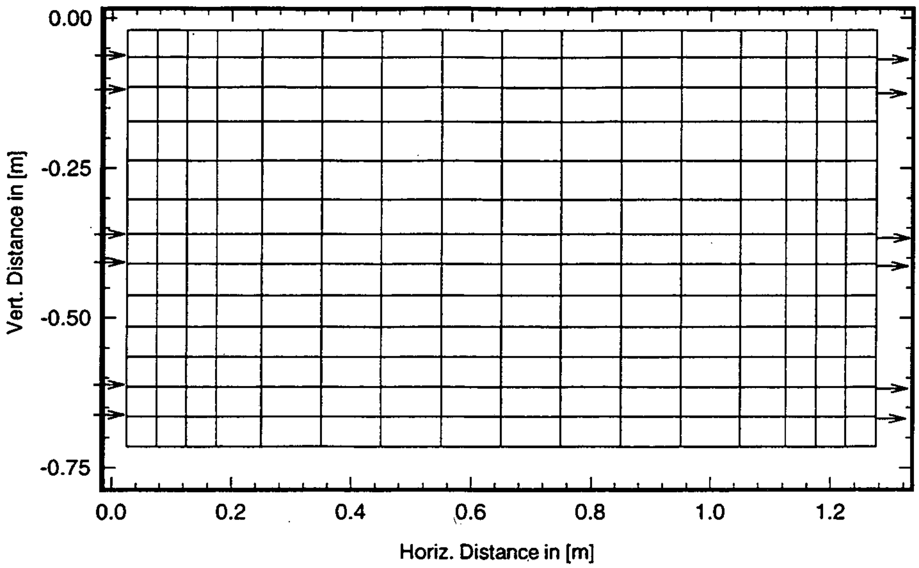


Figure 1: Discretization of container

The temperature of the injected fluids was always 100 ° C. As initial condition the sand was always at residual water saturation of $S_{wi} = 0.2$, whereas in the sand lens $S_{wi} = 0.3$. Initial gas pressure was 101330 Pa and was maintained constant at the outlet ports. Initial temperature was at $T = 10\,^{\circ}C$. Table 1 shows the different scenarios. The first three scenarios use homogeneous sand with an isotropic permeability of $5 \cdot 10^{-10} m^2$ while in the fourth scenario a rectangular fine sand lens with a 50 times lower permeability was included. The

Table 1: description of different scenarios

Scenario	homogeneous (h) / inhomogeneous (i)	permeability $[m^2]$		injection rate $[g/s]$	
		sand 1	sand 2	steam	dry air
1	h	$5 \cdot 10^{-10}$	-	$6.0^{(a)}$	-
2	h	$5 \cdot 10^{-10}$	-	$6.0^{(a)}$	$3.0^{(a)}$
3	h	$5 \cdot 10^{-10}$	-	2.0	1.0
4	i	$5 \cdot 10^{-10}$	$1 \cdot 10^{-11}$	$6.0^{(a)}$	$3.0^{(a)}$
sand grain parameters (constant for all scenarios): density : $2243 \left[\frac{kg}{m^3}\right]$ specific heat : $900 \left[\frac{J}{kg\,^{\circ}C}\right]$ thermal conductivity (dry/saturated): $1.0/2.5 \left[\frac{W}{m\,^{\circ}C}\right]$					

(a): total rate was equally partitioned among the three inlet ports porosity was kept constant at 0.3 in all runs. Figure 2 shows the van Genuchten capillary pressure – saturation relationships used in the simulations. The parameters are: $n = 1.8416$ and $\alpha = 0.001614$ for the coarse sand and $\alpha = 0.0002283$ for the fine sand. In Fig. 3 the relative permeability–saturation relationships for the wetting and non-wetting phase are shown. For the liquid phase a van Genuchten function was chosen whereas for the gas phase a Corey relationship seemed to be more realistic.

In scenario 1 steam was injected at a rate of $2g/s$ in each of the three inlet ports, while in the other scenarios steam ($2g/s$) and dry air ($1g/s$) were co-injected. In scenario 3 the fluids were injected in the lowest inlet port only.

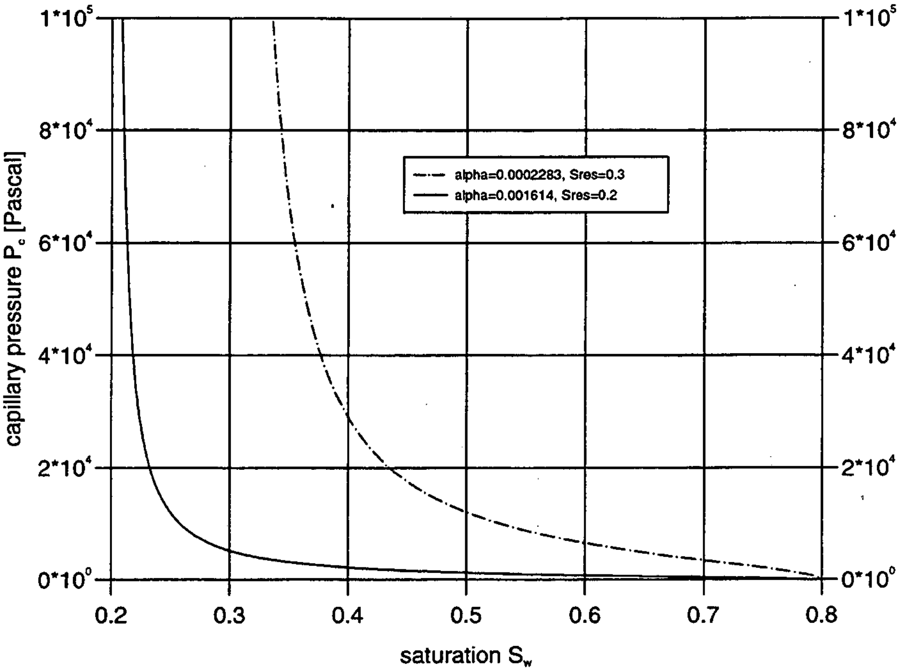


Figure 2: Capillary pressure–saturation relationship

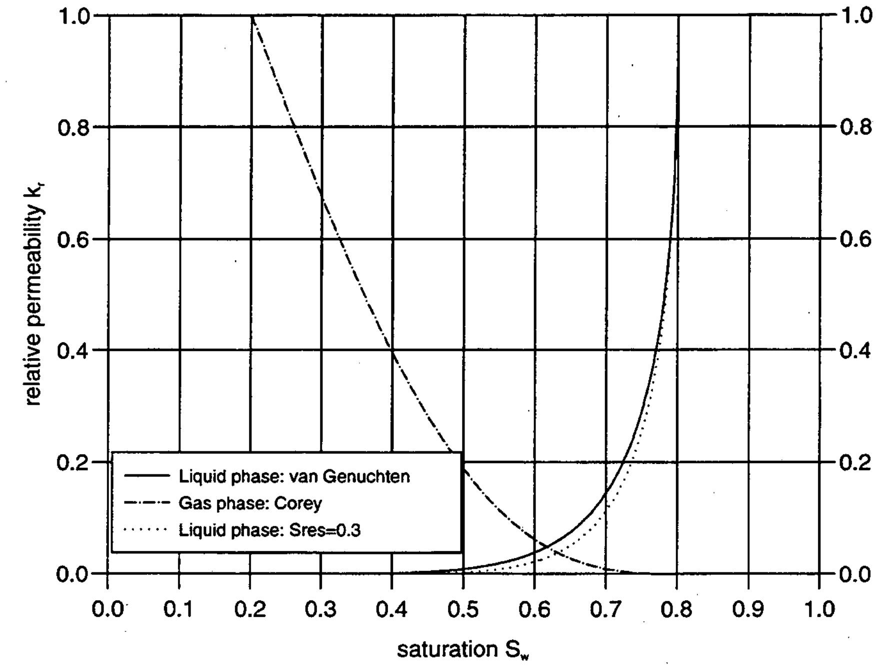


Figure 3: Relative permeability–saturation relationship

4 Discussion of the model results

4.1 Scenario 1

In the first scenario the system under investigation was a homogeneous sand, and steam at T = 100 ° C was injected in all three inlet ports. One purpose was to determine how strong the influence of gravity would be, and whether an almost vertical condensation front would be generated. The results show that at an injection rate of 6 g/s the condensation front moves rather slowly (see Fig. 4), so that condensed hot water can flow downward under gravity and accumulate at the bottom, where after 328 seconds a small region with 100 % liquid saturation has already formed. The condensate is sucked laterally by capillary force into residually saturated regions, causing a rise in temperature there (see Fig. 5). Thus, the system shows a strongly two-dimensional flow behaviour. To diminish generation of condensate and to try and achieve a more vertical displacement front, dry air was co-injected with vapor in all of the following scenarios.

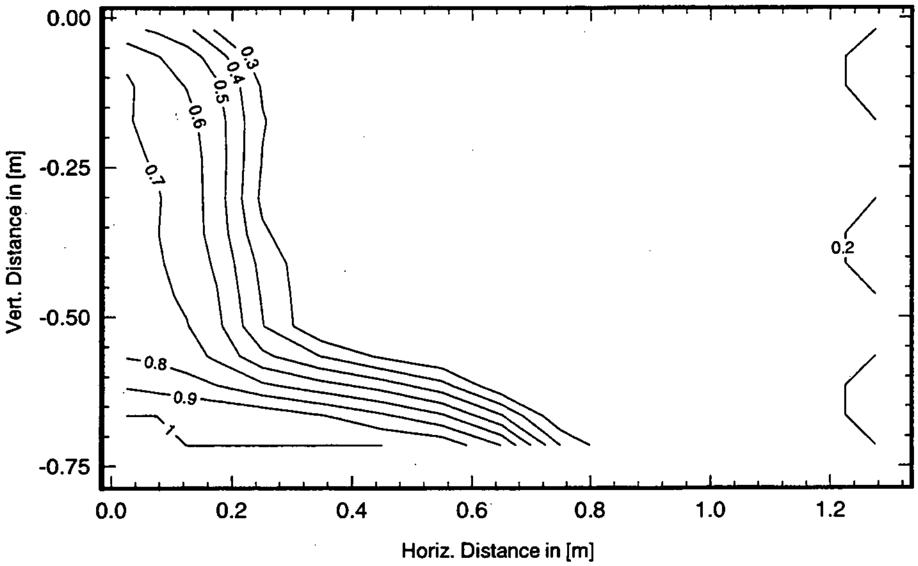


Figure 4: Scenario 1: liquid saturation after 328 sec.

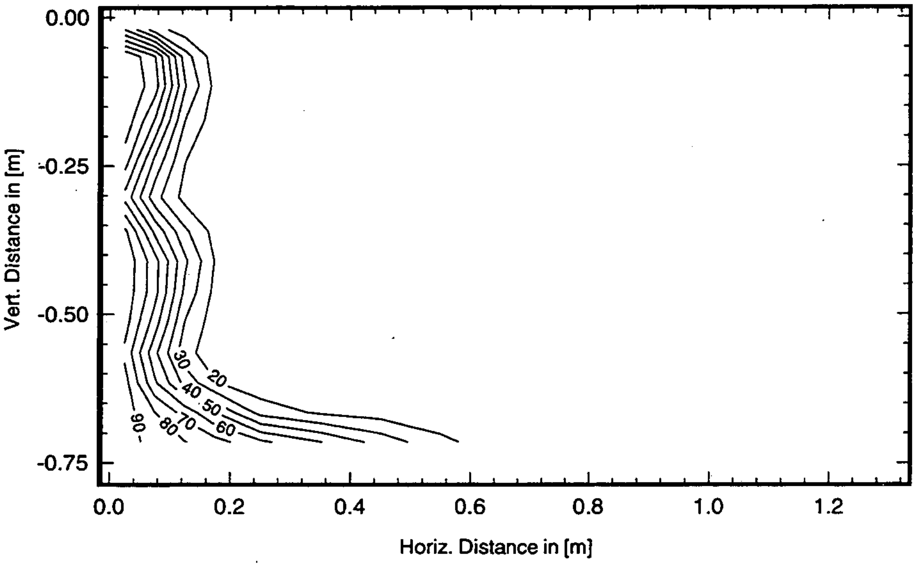


Figure 5: Scenario 1: temperature after 328 sec.

4.2 Scenario 2

In this scenario the same parameters were used as in scenario 1 except that dry air was injected at a rate of 3 g/s additionally to the steam (rate: 6 g/s), equally partitioned among the three inlet ports. The results after 270 seconds show a much faster movement of the saturation and temperature fronts (compare Figs. 6 and 7 with Figs. 4 and 5). This arises because 50 % more mass than in scenario 1 was injected, and because the introduction of dry air effectively suppresses steam condensation. Also, the temperature and saturation fronts are almost vertical in shape now. Behind the condensation front, some condensed water driven by gravity accumulates, as can be seen by looking at the shape of the left 0.4 and the 0.45 liquid saturation isolines. Between 0.2*m* and 0.7*m* downstream from the left boundary, a large region with more than 40 % liquid saturation has formed. The main reason for this is that the gas phase consists of more dry air now and is capable of taking up more vapor than in scenario 1. Fig. 8 shows that the pattern of air mass fraction in the gas phase is strongly correlated with the temperature distribution. The influence of the gas phase pressure is small.

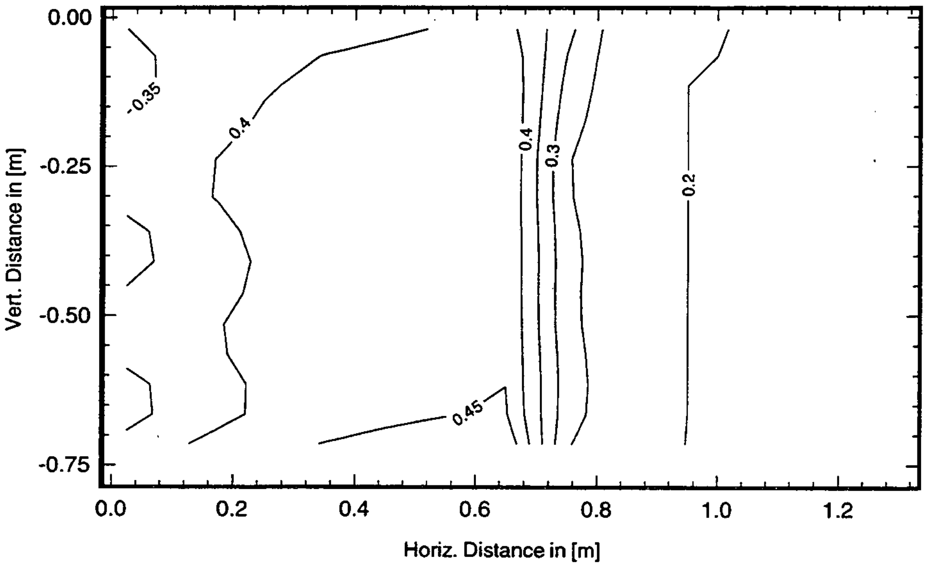


Figure 6: Scenario 2: liquid saturation after 270 sec.

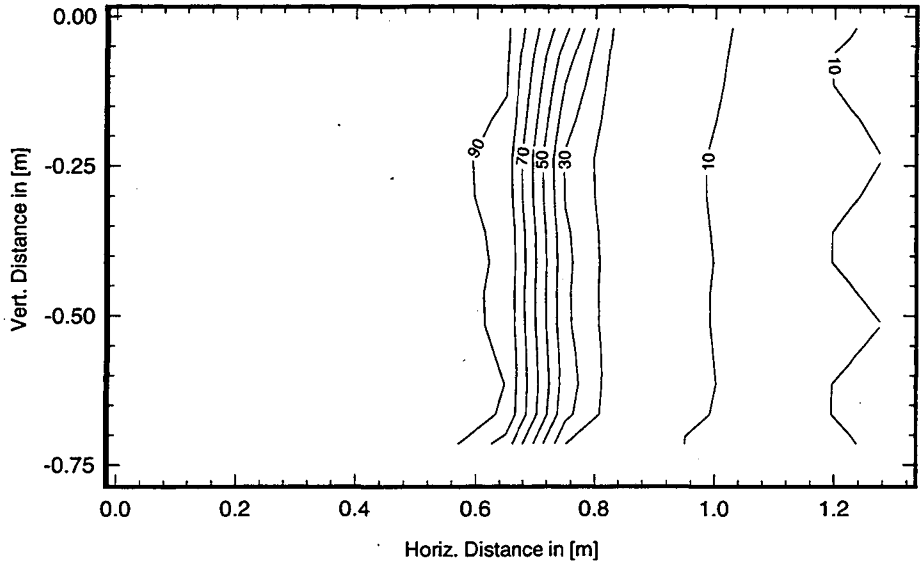


Figure 7: Scenario 2: temperature after 270 sec.

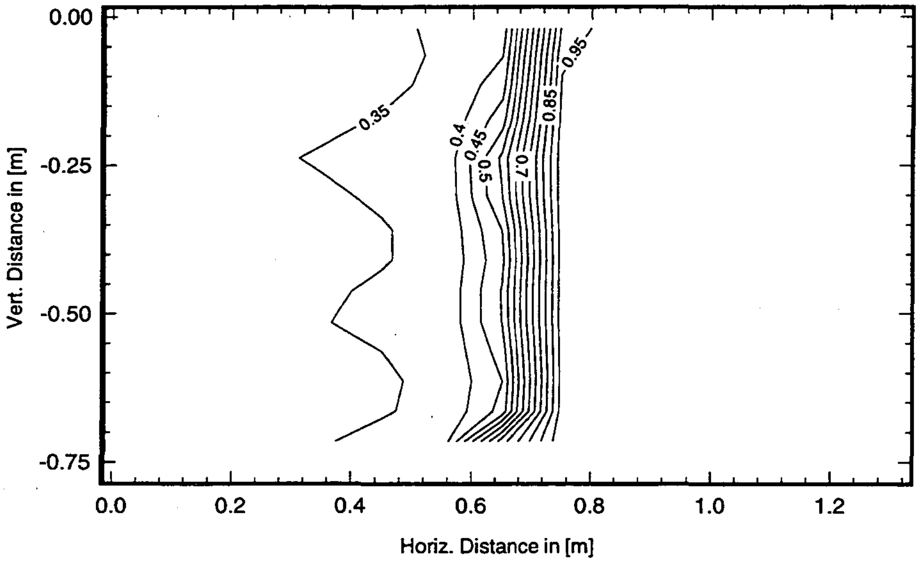


Figure 8: Scenario 2: air mass fraction in the gas phase after 270 sec.

4.3 Scenario 3

For remediation operations in the vadose zone it is generally desirable to avoid any downward movement of contaminants. The second scenario avoided the strong downflow of water seen in scenario 1. Here we attempt to achieve a generally upward displacement, by injecting only in the lowest inlet port. The results show a radial condensation front, but water still tends to flow downward in most of the swept region (see Figs. 9 and 10). A more effective approach may be to inject the hot air at a lower elevation than the steam. This will be tried in future studies. The temperature field (Fig. 11) would tend to drive volatile contaminants upward.

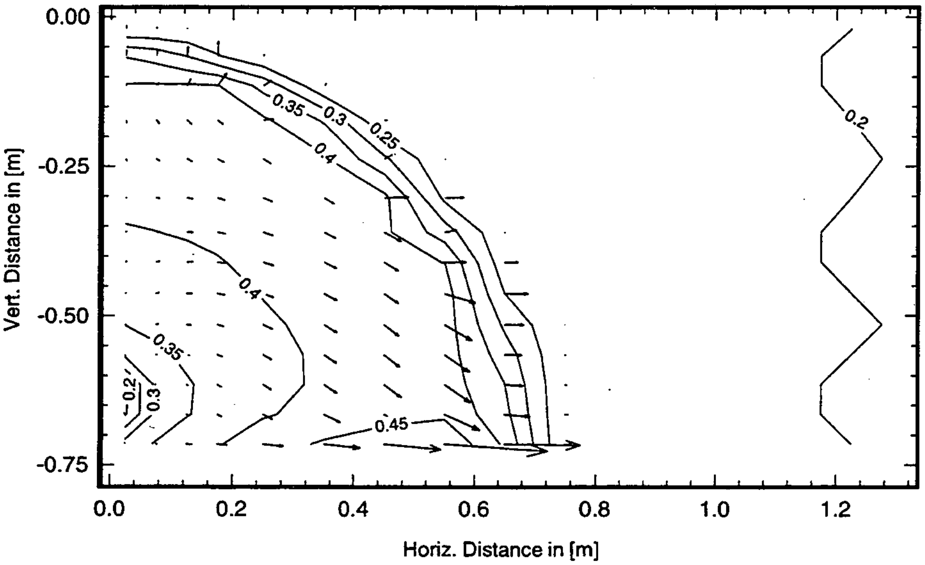


Figure 9: Scenario 3: liquid saturation and liquid flux after 500 sec.

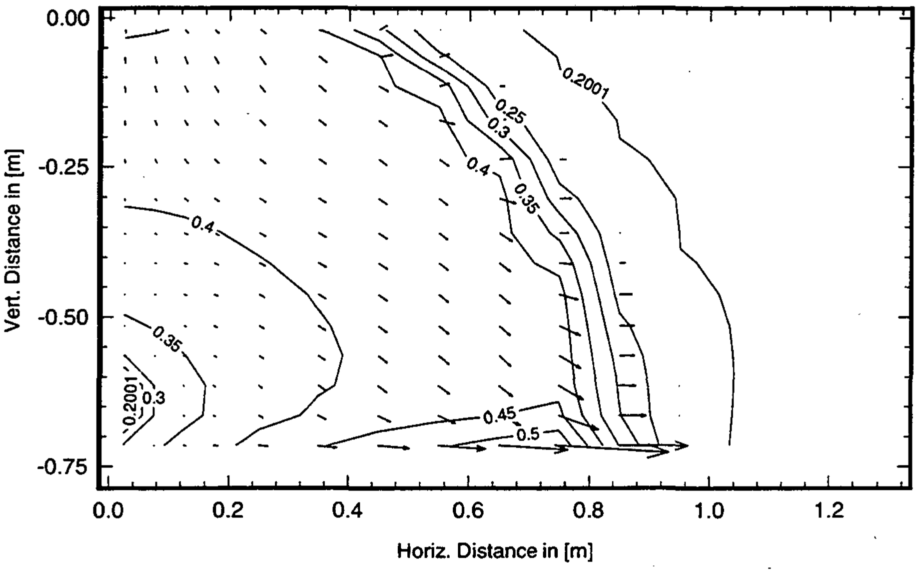


Figure 10: Scenario 3: liquid saturation and liquid flux after 756 sec.

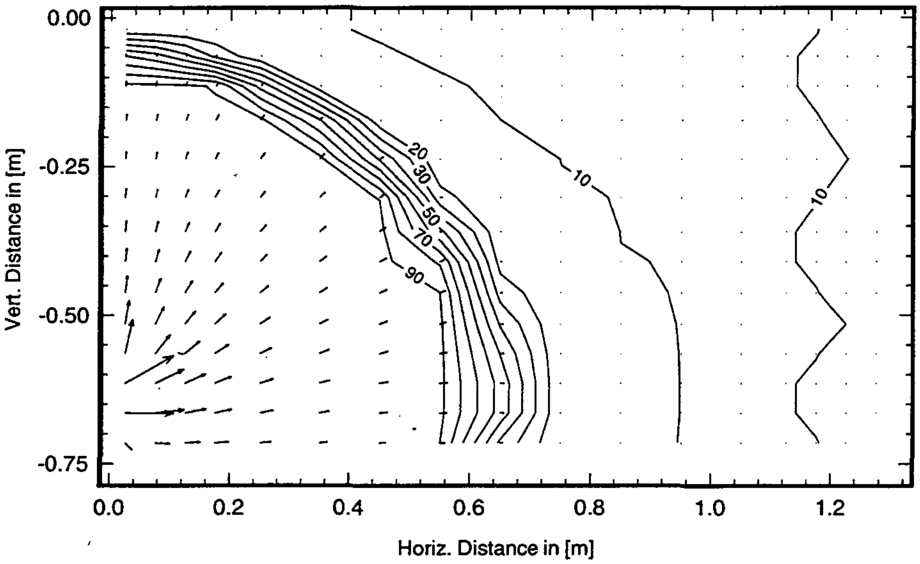
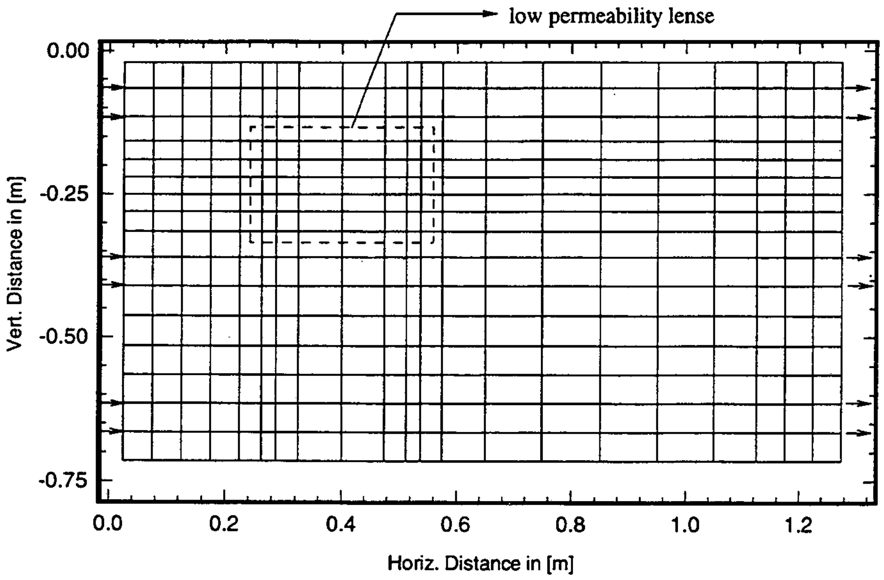


Figure 11: Scenario 3: temperature and heat flux after 500 sec.

4.4 Scenario 4

Finally the influence of a fine sand lens, rectangular in shape with 50 times lower permeability, was investigated. The modified discretization takes into account a finer resolution around the lens for a better representation of steeper gradients and is shown in Fig. 12. The results after 190 seconds show much of the gas phase flow bypassing the region of lower permeability (Fig. 13). Liquid saturation rises from initial 30 % up to 60 % in the left part of the lens and up to 45 % at the right end (see Fig. 14). This is because higher capillary pressure in the lens sucks in the condensing hot water at the arrival of the condensation front. This process of entering of condensed water into the lens continues as the front passes by the upper and lower bounds of the lens. The temperature and heat flux distribution (see Fig. 15) show that there is a very small heat flux in the lens which leads to a temperature of only 20 degree Celsius in the center, whereas at the outer bounds the temperature has reached approximately 90 degrees. The otherwise nearly vertical lines of equal temperature and liquid saturation are affected by a retardation effect caused by the lens. Behind the right-hand side of the lens the upper and lower streamtubes passing by the upper and lower edges of the lens approach each other while carrying hot fluid (see Figs. 13 - 15). There is almost no downstream flux out of the lens so the fluid of the just-mentioned streamtubes has to heat up the region behind the lens. Those streamtubes become larger in cross-sectional area behind the lens, leading to a reduced fluid velocity and the retardation effect seen in Figs. 13 - 15.

Figure 12: Discretization of the system with finer resolution around the fine sand lens



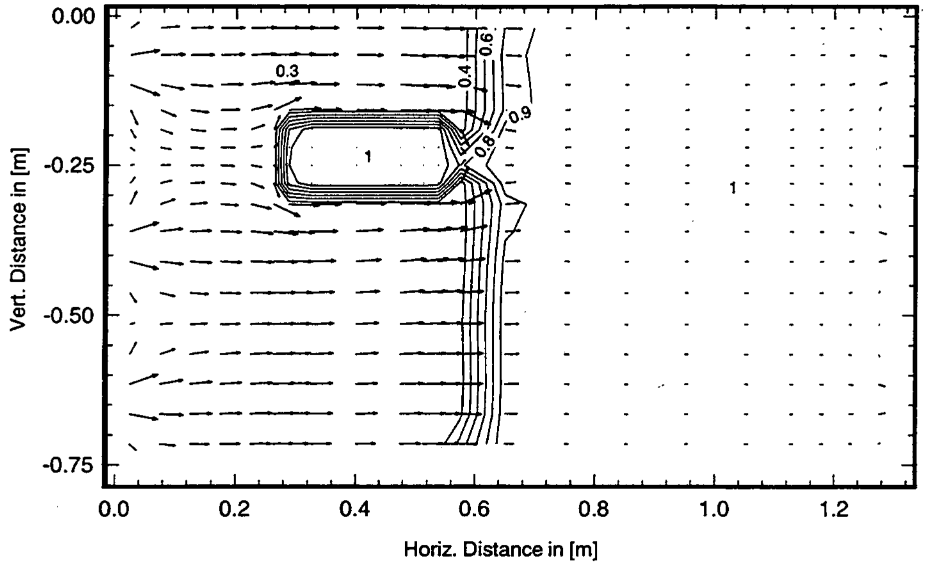


Figure 13: Scenario 4: air mass fraction in the gas phase and gas mass flux after 190 sec.

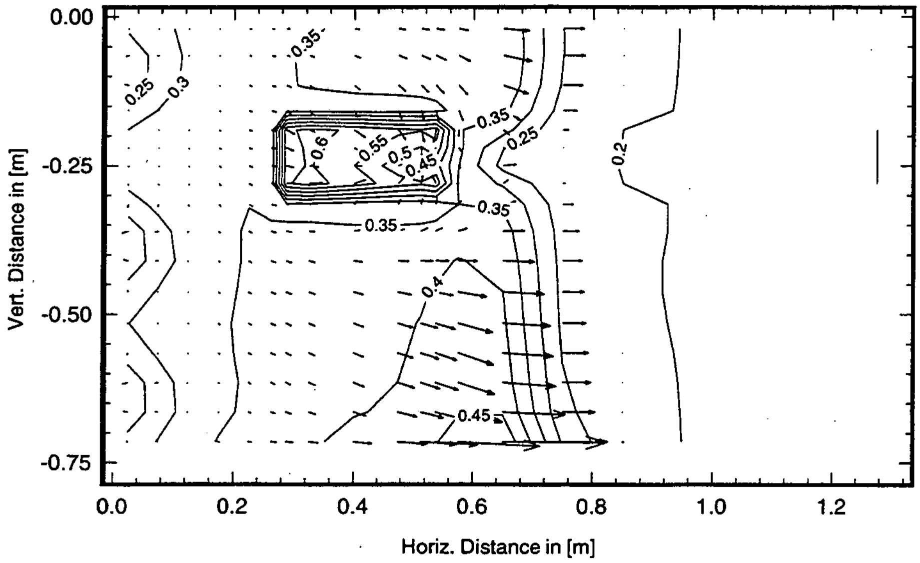


Figure 14: Scenario 4: liquid saturation and liquid mass flux after 190 sec.

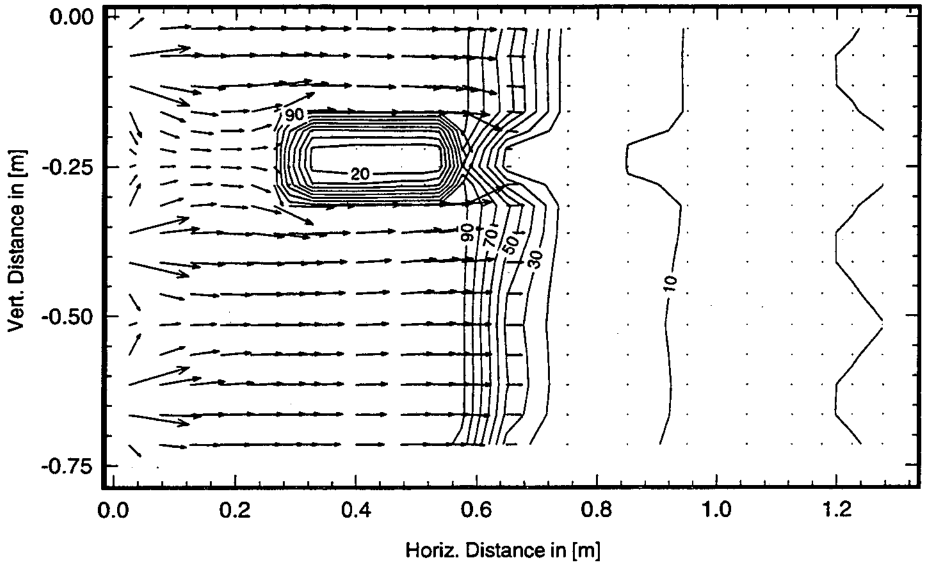


Figure 15: Scenario 4: temperature and heat flux after 190 sec.

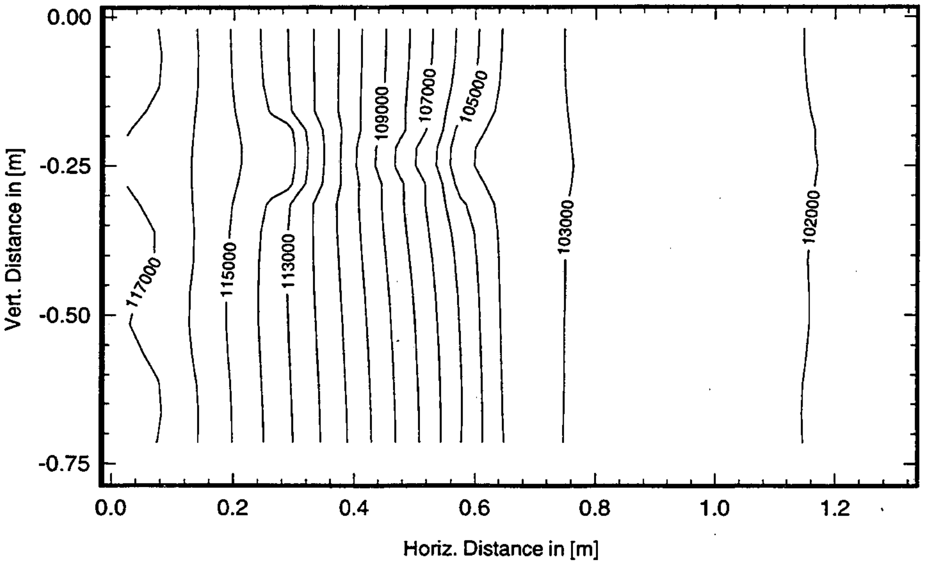


Figure 16: Scenario 4: gas pressure after 190 sec.

These results lead to the following considerations. If a contaminant would be at irreducible saturation in the low-permeability lens and a remediation process using steam and/or hot air injection is planned, it could be useful to continue with injection until the temperature everywhere in the lens is high enough to evaporate the contaminant into the gas phase. To avoid condensation of the contaminant vapor in cooler regions, additional soil vapor extraction would help to accelerate the remediation by inducing a gas pressure gradient.

5 Conclusions

Results of exploratory numerical simulation studies using TOUGH2/T2VOC were presented for steam and hot air injection. In four different scenarios, the influence of injection of steam only and steam together with air, the influence of injection at various locations, and the influence of a low-permeability lens were investigated. The results furthered the understanding of the governing processes and their interaction under different conditions.

The configurations used here were limited to purely two-dimensional flow fields. The implied assumption that there is no energy exchange across the vertical boundaries of the system may be difficult to realize in experimental practice. Heater tapes may be applied to achieve a simultaneous heating of the container walls with the moving condensation front in space and time, and prevent the flow field from becoming three-dimensional.

6 Acknowledgement

This work was part of the project "numerical modelling of nonisothermal multiphase processes" which is supported by PWAB of the state Baden-Württemberg, Germany. The project is also part of the main research topic "NAPLs in the vadose zone" of VEGAS. It aims at numerical modeling of nonisothermal multiphase processes in porous and heterogeneous media. Based on an existing Finite Element model [2] for isothermal multiphase flow problems, the mathematical-numerical formulation has to be further developed with particular respect to phase change effects caused by heat transfer mechanisms and the transport of components. The program system must be capable of modeling the governing processes of thermally enhanced soil vapor extraction. Therefore VEGAS includes intensive collaboration on the above mentioned project "thermally enhanced soil vapor extraction". The first author appreciates the hospitality of Lawrence Berkeley Laboratory, where the numerical simulations were carried out. Thanks are due to Curt Oldenburg and April James for a review of the manuscript, and the suggestion of improvements. This work was performed under U.S. Department of Energy Contract No. DE-AC-03-76SF00098.

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