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### Authors

Falta, R W

Pruess, K

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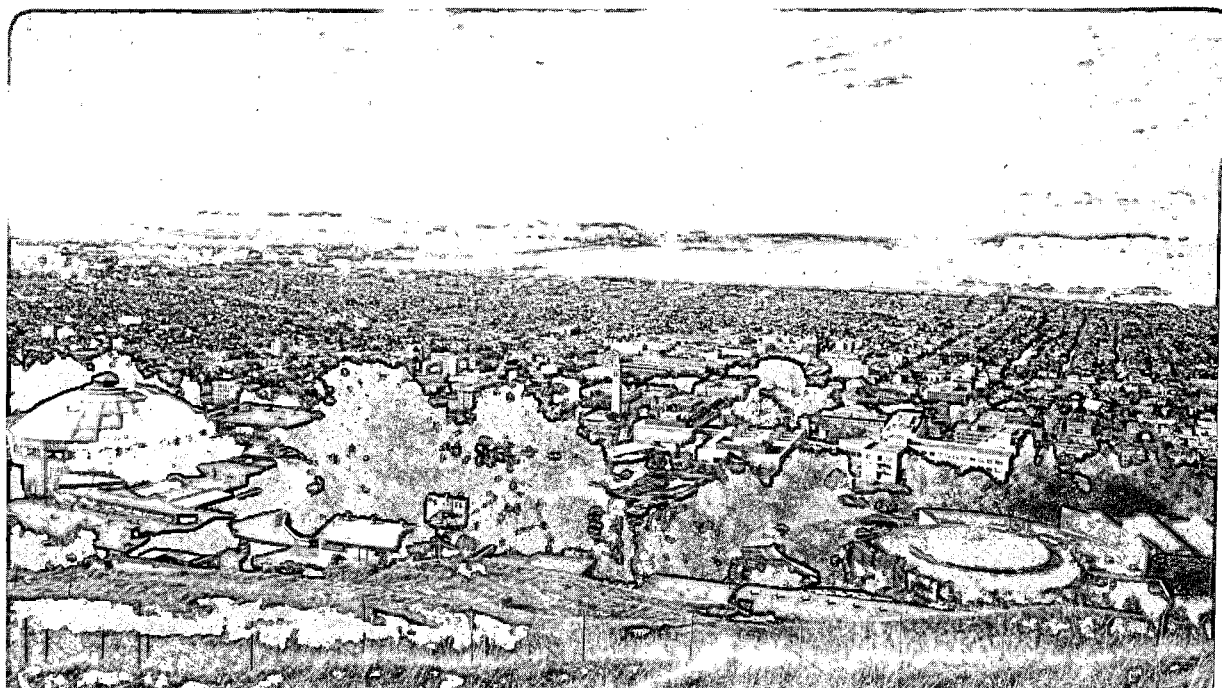
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## EARTH SCIENCES DIVISION

### STMVOC User's Guide

R.W. Falta and K. Pruess

June 1991



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## STMVOC User's Guide

*Ronald W. Falta and Karsten Pruess*

Earth Sciences Division  
Lawrence Berkeley Laboratory  
University of California  
Berkeley, California 94720

June 1991

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**ABSTRACT**

This report contains instructions for using the STMVOC numerical simulator. This code, which was developed at Lawrence Berkeley Laboratory, is an extension of the TOUGH geothermal code for use in problems involving subsurface contamination by nonaqueous phase liquids (NAPLs). The code is used for modeling the nonisothermal transport of air, water, and an organic chemical in three fluid phases. A discussion of the physical processes included in the simulator is given along with a brief outline of the mathematical formulation. A detailed guide to preparing the STMVOC input file with several illustrative examples is provided.

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## INTRODUCTION

The STMVOC code is a three dimensional numerical simulator developed for modeling the transport of organic chemical contaminants in nonisothermal multiphase systems. In particular, the code was designed to simulate steam injection for the removal of hazardous nonaqueous phase liquids (NAPLs) from contaminated soils and aquifers. Although it is expected that this will be the primary area of application of the code, the STMVOC simulator may be used to simulate many other multiphase contaminant transport problems such as NAPL migration in variably saturated media, forced vacuum extraction of organic chemical vapors from the unsaturated zone, and evaporation and diffusion of chemical vapors in the unsaturated zone.

STMVOC uses a general integral finite difference method formulation known as MULKOM [Pruess, 1983; 1988]. Several versions of MULKOM have been developed for solving different multiphase flow problems. The features and capabilities of these different versions have been summarized by Pruess [1988]. The most well known and widely used version of MULKOM is the TOUGH simulator [Pruess, 1987]. TOUGH (Transport of Unsaturated Groundwater and Heat) is a three dimensional code for simulating the coupled transport of water, water vapor, air, and heat in porous and fractured porous media. The STMVOC simulator has been developed directly from TOUGH, and for the purpose of this report, it is assumed that the reader is familiar with the TOUGH code. It is intended that this report be used in conjunction with the original TOUGH user's guide [Pruess, 1987] rather than as a "stand alone" user's guide.

This report contains a description of the physical processes included in the STMVOC simulator, and a limited discussion of the mathematical formulation. Instructions for generating the input file are given along with four illustrative sample problems. For more complete details concerning the STMVOC formulation, the reader is referred to Falta [1990] or Falta et al. [1990a]. Several problems other than those described in this report have been modeled using STMVOC, and these are discussed in Falta [1990] and Falta et al. [1990b].

The original STMVOC code development was carried out on a Cray XMP supercomputer. However, a double precision version of the code has been generated for use on 32-bit workstations, and the results of simulations performed on these machines have been quite satisfactory. For purposes of comparison, using the Cray XMP cpu time as a baseline, a given problem will run about 2-3 times slower on an IBM Series 6000 Model 320 workstation, about 5-6 times slower on a Solbourne Series 5 Model 502 workstation, and about 12-14 times slower on a Sun Sparcstation workstation.

## PHYSICAL PROCESSES AND ASSUMPTIONS

In the STMVOC formulation, the multiphase system is assumed to be composed of three mass components: air (or some other noncondensable gas), water, and a volatile, slightly water-soluble organic chemical. Although air consists of several components (nitrogen, oxygen, etc.), here it is treated as a single "pseudo" component with averaged properties. These three components may be present in different proportions in any of the three phases, gas, aqueous, and NAPL. The components and phases considered by the STMVOC simulator are listed in Table 1. Each phase flows in response to pressure and gravitational forces according to the multiphase extension of Darcy's law, including the effects of relative permeability and capillary pressure between the phases.

Transport of the three mass components occurs by advection in all three phases, and by multicomponent diffusion in the gas phase. At the present time, no allowance is made for molecular diffusion in the aqueous and NAPL phases, or for hydrodynamic dispersion. It is assumed that the three phases are in local chemical and thermal equilibrium, and that there are no chemical reactions taking place other than interphase mass transfer and adsorption of the chemical component to the solid phase. Mechanisms of interphase mass transfer for the organic chemical component include evaporation and boiling of the NAPL, dissolution of the NAPL into the aqueous phase, condensation of the organic chemical from the gas phase into the NAPL, and equilibrium phase partitioning of the organic chemical between the gas, aqueous, and solid phases. Interphase mass transfer of the water component includes the effects of evaporation and boiling of the aqueous phase, dissolution of water in the NAPL (not usually important), and condensation of water vapor from the gas phase. The interphase mass transfer of the air component consists of equilibrium phase partitioning of the air between the gas, aqueous, and NAPL phases.

Heat transfer occurs due to conduction, multiphase convection, and gaseous diffusion. The heat transfer effects of phase transitions between the NAPL, aqueous and gas phases are fully accounted for by considering the transport of both latent and sensible heat. The overall

**Table 1. Components and Phases**

Components	Phases
air water organic chemical heat	gas aqueous NAPL

porous media thermal conductivity is calculated as a function of water and NAPL saturation, and depends on the chemical characteristics of the NAPL.

Thermophysical properties of the aqueous and NAPL phases such as saturated vapor pressure and viscosity are calculated as functions of temperature, while specific enthalpy and density are computed as functions of both temperature and pressure. Vapor pressure lowering effects due to capillary forces are not presently included in the simulator. Gas phase thermophysical properties such as specific enthalpy, viscosity, density, and component molecular diffusivities are considered to be functions of temperature, pressure, and gas phase composition. The solubility of the organic chemical in water may be specified as a function of temperature, and the gas-aqueous Henry's constant for the organic chemical is calculated as a function of temperature. The gas-aqueous and gas-NAPL Henry's constants for air are assumed to be constant, as is the water solubility in the NAPL phase.

The necessary NAPL/organic chemical thermophysical and transport properties are computed by means of a very general equation of state. This equation of state is largely based on semi-empirical corresponding states methods in which chemical parameters are calculated as functions of the critical properties of the chemical such as the critical temperature and pressure. Because these data are available for hundreds of organic compounds, the NAPL/organic chemical equation of state is quite flexible in its application.

By virtue of the fact that the integral finite difference method [Narasimhan and Witherspoon, 1976] is used for spatial discretization, the present formulation makes no reference to a global coordinate system other than the direction of the gravitational acceleration vector, and no particular dimensionality is required. The STMVOC simulator may therefore be used for one, two, or three-dimensional anisotropic, heterogeneous porous or fractured systems having complex geometries. The porous medium porosity may be specified to be a function of pore pressure and temperature, but no stress calculations are made.

## GOVERNING EQUATIONS

In a nonisothermal system containing three mass components, three mass balance equations and an energy balance equation are needed to fully describe the system. The following summary of the governing transport equations follows Pruess [1987; 1988] with extensions to account for a NAPL phase and a chemical component. The balance equations are written in integral form for some flow region,  $V_l$ , having a surface area  $\Gamma_l$ , as follows

$$\frac{d}{dt} \int_{V_l} M^K dV_l = \int_{\Gamma_l} \mathbf{F}^K \cdot \mathbf{n} d\Gamma_l + \int_{V_l} q^K dV_l \quad (1)$$

$$K = a: \text{air}; K = w: \text{water}; K = c: \text{chemical}; K = h: \text{heat}$$

where  $M^K$  is the amount of component  $K$  per unit porous medium volume,  $\mathbf{F}^K$  is the total flux of component  $K$  into  $V_l$ ,  $\mathbf{n}$  is the outward unit normal vector, and  $q^K$  is the rate of generation of component  $K$  per unit volume. For  $K=a,w,c$ ,  $M^K$  is the mass of component  $K$  per unit porous medium volume,  $\mathbf{F}^K$  is the mass flux of component  $K$ , and  $q^K$  is the rate of mass generation of component  $K$  per unit volume. For  $K=h$ ,  $M^K$  is the amount of energy (heat) per unit porous medium volume,  $\mathbf{F}^K$  is the heat flux, and  $q^K$  is the rate of heat generation per unit volume.

### Accumulation Terms

The mass accumulation terms for air and water ( $K=a,w$ ) contain a sum over the gas, aqueous, and NAPL phases

$$M^K = \phi \sum_{\beta} S_{\beta} \rho_{\beta} \omega_{\beta}^K \quad (2)$$

$$\beta = g: \text{gas}; \beta = w: \text{aqueous}; \beta = n: \text{NAPL}$$

where  $\phi$  is the porosity,  $S_{\beta}$  is the  $\beta$  phase saturation,  $\rho_{\beta}$  is the  $\beta$  phase density, and  $\omega_{\beta}^K$  is the mass fraction of component  $K$  in phase  $\beta$ . The organic chemical accumulation term ( $K=c$ ) includes the effect of linear equilibrium adsorption onto the solid phase.



$$M^c = \rho_b \rho_w \omega_w^c K_D + \phi \sum_{\beta} S_{\beta} \rho_{\beta} \omega_{\beta}^c \quad (3)$$

where  $\rho_b$  is the dry bulk density of the soil,  $\omega_w^c$  is the mass fraction of the chemical in the aqueous phase, and  $K_D$  is the solid-aqueous distribution coefficient for the organic chemical [Freeze and Cherry, 1979]. The first term in (3) may be written as

$$C_s^c = \rho_b K_D C_w^c \quad (4)$$

where  $C_s^c$  is the adsorbed mass of chemical per unit volume of soil, and  $C_w^c$  is the chemical mass concentration in the aqueous phase. The use of (4) assumes that some liquid water is present in the system, and that the soil is preferentially wetted by the aqueous phase. In very dry systems, the use of (4) to describe vapor adsorption may lead to some error. Because it has been found that the degree of adsorption of organic chemicals depends largely on the amount of organic carbon present in the soil,  $K_D$  is often written as

$$K_D = K_{oc} f_{oc} \quad (5)$$

where  $K_{oc}$  is the organic carbon partition coefficient, and  $f_{oc}$  is the organic carbon fraction in the soil [Karickhoff et al., 1979; Schwarzenbach and Westall, 1981].

The heat accumulation term ( $K=h$ ) includes contributions from both the solid and the fluid phases

$$M^h = (1 - \phi) \rho_R C_R T + \phi \sum_{\beta} S_{\beta} \rho_{\beta} \mu_{\beta} \quad (6)$$

where  $\rho_R$  is the soil grain density,  $C_R$  is the heat capacity of the soil grains,  $T$  is the temperature, and  $\mu_{\beta}$  is the specific internal energy of phase  $\beta$ . Because the mass fractions of air and organic chemical in the aqueous phase are small, the specific internal energy of the aqueous phase is assumed to be independent of composition. Likewise, because the mass fractions of air and water in the NAPL phase are small, the specific internal energy of the NAPL phase is also assumed to be independent of composition. The gas phase internal energy is a very strong function of composition, and is calculated by

$$u_g = \sum_{K=a,w,c} \omega_g^K u_g^K \quad (7)$$

where  $u_g^K$  is the specific internal energy of component  $K$  in the gas phase.

### Flux Terms

The three mass flux terms (air, water, chemical) sum over the three phases (gas, aqueous, NAPL)

$$F^K = \sum_{\beta} F_{\beta}^K \quad (8)$$

The mass flux of each component in the gas phase includes both advection and diffusion

$$F_g^K = \frac{-kk_{r_g} \rho_g}{\mu_g} \omega_g^K (\nabla P_g - \rho_g \mathbf{g}) + \mathbf{J}_g^K \quad (9)$$

where  $k$  is the absolute permeability,  $k_{r_g}$  is the gas phase relative permeability,  $\mu_g$  is the gas phase dynamic viscosity,  $P_g$  is the gas phase pressure,  $\mathbf{g}$  is the gravitational acceleration vector, and  $\mathbf{J}_g^K$  is the diffusive mass flux of component  $K$  in the gas phase. In (9), Knudsen effects are neglected. The diffusive mass fluxes of water vapor and organic chemical vapor,  $\mathbf{J}_g^w$ , and  $\mathbf{J}_g^c$  are calculated by

$$\mathbf{J}_g^K = -\phi S_g \tau_g D_g^K \rho_g \nabla \omega_g^K \quad (10)$$

where  $D_g^K$  is the multicomponent molecular diffusion coefficient of component  $K$  in the gas phase, and  $\tau_g$  is the gas phase tortuosity computed from the Millington and Quirk [1961] model

$$\tau_g = \phi^{1/3} S_g^{7/3} \quad (11)$$

The use of (11) to predict the gas phase tortuosity does not account for possible enhancements to the diffusive flow of condensable vapors which may occur when the liquid condensate is also present [Walker et al., 1981]. With the water and chemical diffusive mass fluxes given by (10), the air diffusive mass flux,  $\mathbf{J}_g^a$  is determined from the requirement that

$$\mathbf{J}_g^a + \mathbf{J}_g^w + \mathbf{J}_g^c = 0 \quad (12)$$

The use of (12) ensures that the total gas phase diffusive mass flux summed over the three components is zero with respect to the mass average velocity [Bird et al., 1960]. Then, the total gas phase mass flux is the product of the gas phase Darcy velocity and the gas phase density.

The component mass fluxes in the aqueous and NAPL phases are calculated by considering only advection,

$$\mathbf{F}_w^K = \frac{-kk_{rw}\rho_w}{\mu_w} \omega_w^K (\nabla P_w - \rho_w \mathbf{g}) \quad (13)$$

$$\mathbf{F}_n^K = \frac{-kk_{rn}\rho_n}{\mu_n} \omega_n^K (\nabla P_n - \rho_n \mathbf{g}) \quad (14)$$

The aqueous phase pressure in (13) is related to the gas phase pressure in (9) by

$$P_w = P_g + P_{cgw} \quad (15)$$

where  $P_{cgw}$  is the gas-water capillary pressure. The NAPL phase pressure in (14) is related to the gas phase pressure by

$$P_n = P_g + P_{cgn} \quad (16)$$

where  $P_{cgn}$  is the gas-NAPL capillary pressure. It follows that the NAPL-water capillary pressure,  $P_{cnw}$ , is

$$P_{cnw} = P_{cgw} - P_{cgn} = P_w - P_n \quad (17)$$

The heat flux includes both conduction and convection

$$\mathbf{F}^h = -\lambda \nabla T + \sum_{\beta} h_{\beta} \mathbf{F}_{\beta} \quad (18)$$

where  $\lambda$  is the overall porous medium thermal conductivity,  $h_{\beta}$  is the  $\beta$  phase specific enthalpy, and  $\mathbf{F}_{\beta}$  is the total  $\beta$  phase mass flux (not to be confused with the component mass flux). As in the case of the aqueous and NAPL phase internal energies, the aqueous and

NAPL phase specific enthalpies are assumed to be independent of composition. The gas phase specific enthalpy is calculated as

$$h_g = \sum_{K=a,w,c} \omega_g^K h_g^K \quad (19)$$

and is a very strong function of composition. From thermodynamics, the relationship between the enthalpy and the internal energy of a fluid is  $h = u + P/\rho$  [Sonntag and van Wylen, 1982].

The nonlinear coupled balance equations given by (1) are linearized using an iterative Newton-Raphson technique, and the linearized equations are solved directly. Complete details of the numerical solution method used in STMVOC are given in Falta [1990] and Falta et al. [1990a].

## PRIMARY VARIABLES AND VARIABLE SUBSTITUTION

In order to describe the thermodynamic state of a four-component (three mass components and heat) system in which local thermal and chemical phase equilibrium is assumed, it is necessary to choose four primary variables. In addition to the four primary variables, a complete set of "secondary variables" is needed for the solution of the four coupled balance equations. These secondary variables include thermodynamic and transport properties such as enthalpies, densities, relative permeabilities, viscosities, and mass fractions. The four primary variables must be chosen so that the entire set of secondary variables may be calculated as functions of the primary variables, and so that all of the primary variables are independent.

In multiphase flow problems involving phase transitions (ie. appearance or disappearance of a phase), the number of possible phase combinations may become large. In a system in which a maximum of three fluid phases may be present, there are seven possible phase combinations. These combinations include three single phase systems (eg. gas, aqueous, NAPL), three two-phase systems (eg. gas-aqueous, gas-NAPL, aqueous-NAPL), and one three-phase system (eg. gas-aqueous-NAPL).

Ideally, a different set of primary variables should be used for each different phase combination. With this technique, during each phase transition (in each element) the primary variables are switched so that the system is always fully defined thermodynamically by the primary variables.

While the technique of variable substitution during phase transitions is quite attractive, implementing this procedure for a three-phase system with seven possible phase combinations would require seven sets of primary variables and would be cumbersome to code. An alternative method is to prohibit complete phase transitions; that is, each phase must be present to some degree in each element. The phases are prevented from completely disappearing by artificially reducing rates of interphase mass transfer from a phase when its

saturation becomes small. In practical terms, the minimum saturation of each phase using this method may be very small, on the order of  $10^{-3}$  or  $10^{-4}$ , and numerical results using this method are usually satisfactory.

A drawback of this method is that it is not possible to rigorously simulate the complete removal of a phase (for example, a NAPL) from the porous medium. Although the minimum phase saturation may be as small as  $10^{-4}$ , in some problems this may be a significant amount of the phase. Consider a system with a porosity of 0.4. A NAPL saturation of  $10^{-4}$  corresponds to 40 ml of NAPL per  $m^3$  of porous medium. For toxic organic chemicals, this is a substantial level of contamination.

In the STMVOC simulator, a compromise is made between the robustness and elegance of the variable substitution method, and the simplicity of the minimum saturation method. To reduce the number of phase combinations to two, it is assumed that the gas and aqueous phases never totally disappear, although the phase saturations may be quite small ( $\approx 10^{-4}$ ). In regions where the NAPL phase is present, the system is considered to be under three-phase conditions (gas-aqueous-NAPL), and the primary variables are gas phase pressure  $P_g$ , gas phase saturation  $S_g$ , aqueous phase saturation  $S_w$ , and temperature  $T$ . The disappearance of the NAPL phase is recognized when  $S_g + S_w \geq 1$ . In this case, the system is in two-phase conditions (gas-aqueous), and the variables are switched to  $P_g$ ,  $\chi_g^c$ ,  $S_w$ ,  $T$  where  $\chi_g^c$  is the mole fraction of the organic chemical in the gas phase. If at any point the partial pressure of the chemical ( $\chi_g^c P_g$ ) becomes greater than the saturated vapor pressure of the chemical ( $P_{sat}^c$ ), the NAPL phase evolves and the variables are switched to the three-phase set of variables. In either case, the minimum saturation method is used for the gas and aqueous phases in order to prevent complete disappearance of these phases. Because these phases must always be present to some degree, the initial conditions for STMVOC simulations must always include at least a small amount of the gas and aqueous phases ( $S_g$  and  $S_w > 10^{-4}$ ). The different primary variables used under two-phase and three-phase conditions are summarized in Table 2.

Table 2. Primary Variables.

Fluid Mixture	Variables
two-phase (no NAPL)	$P_g, T, \chi_g^c, S_w^\dagger$
three-phase (w/NAPL)	$P_g, S_g^\dagger, T, S_w^\dagger$

$^\dagger$  must be specified  $> 10^{-4}$

## SECONDARY VARIABLES

In nonisothermal multiphase flow simulations, major nonlinearities in the governing equations occur due to large variations of secondary thermodynamic and transport parameters that arise from changes in the values of the primary variables. For this reason, the accurate calculation of secondary variables from the primary variables is of considerable importance. In the formulation of STMVOC an effort has been made to include all of the secondary variables which significantly contribute to the nonlinearity of the problem. A complete list of all of the variable secondary parameters along with their dependence on the primary variables is given in Table 3. The dependence of the secondary variables on specific primary variables may change under different phase conditions due to the primary variable switching. In Table 3, it is assumed that the pressure used as a primary variable is the gas phase pressure. For this reason, it is not necessary to compute a gas phase capillary pressure. A detailed discussion of how all of the secondary variables used in STMVOC are computed may be found in Falta [1990] and Falta et al. [1990a].



Table 3. Secondary Variables and Functional Dependence

Parameter	Phase		
	gas	aqueous	NAPL
Saturation	$S_g(S_w)$	-	$S_n(S_g, S_w)$
Relative Permeability	$k_{rg}(S_g, S_w)$	$k_{rw}(S_w)$	$k_{rn}(S_g, S_w)$
Viscosity	$\mu_g(P, \chi_g^c, T)$	$\mu_w(P, T)$	$\mu_n(T)$
Density	$\rho_g(P, \chi_g^c, T)$	$\rho_w(P, T)$	$\rho_n(P, T)$
Specific Enthalpy	$h_g(P, \chi_g^c, T)$	$h_w(P, T)$	$h_n(P, T)$
Capillary Pressure	-	$P_{cgw}(S_g, S_w)$	$P_{cgn}(S_g, S_w)$
Air Mass Fraction	$\omega_g^a(P, \chi_g^c, T)$	$\omega_w^a(P, \chi_g^c, T)$	$\omega_n^a(P, \chi_g^c, T)$
Water Mass Fraction	$\omega_g^w(P, \chi_g^c, T)$	$\omega_w^w(P, \chi_g^c, T)$	$\omega_n^w(P, \chi_g^c, T)$
Chemical Mass Fraction	$\omega_g^c(P, \chi_g^c, T)$	$\omega_w^c(P, \chi_g^c, T)$	$\omega_n^c(P, \chi_g^c, T)$
Water Molecular Diffusivity	$D_g^w(P, \chi_g^c, T)$	-	-
Chemical Molecular Diffusivity	$D_g^c(P, \chi_g^c, T)$	-	-
Tortuosity	$\tau_g(S_g, S_w)$	-	-
Chemical Henry's Constant	$H_{gw}^c(T)$		
Thermal Conductivity	$\lambda(S_g, S_w, T)$		

## INCORPORATION OF SOURCE TERMS AND INITIAL AND BOUNDARY CONDITIONS

Several options are available in the STMVOC simulator for specifying the injection or production of fluids and heat. For the injection of fluids, any of the three mass components (air, water, chemical) may be injected in an element at a constant or time-dependent rate. Alternately, a total gas or aqueous phase mass injection rate may be specified in which the injected phase composition (water and air components only) is given by the user. The specific enthalpy of the injected fluid is input by the user as either a constant or time-dependent value. Heat sources/sinks (with no mass injection) may be either constant or time-dependent.

Fluid production from an element is handled using one of two options. With the first option, the total mass rate of production is given as a constant or time-dependent value. In this case, the phase composition of the produced fluids may be determined by the relative phase mobilities in the source element. Alternately, the produced phase composition may be specified to be the same as the phase composition in the producing element. In either case, the mass fraction of each component in each of the produced phases is determined by the component mass fractions in each phase in the producing element.

The second production option is a well deliverability model in which production occurs against a prescribed flowing wellbore pressure,  $P_{wb}$ , with a productivity index  $PI$  [Coats, 1977]. With this option, the mass production rate of phase  $\beta$  is

$$q_{\beta} = \frac{k_{r\beta}}{\mu_{\beta}} \rho_{\beta} \cdot PI \cdot (P_{\beta} - P_{wb}) \quad (20)$$

and the rate at which each mass component ( $K \neq h$ ) is removed is

$$\hat{q}^K = \sum_{\beta} \omega_{\beta}^K q_{\beta} \quad (21)$$

For wells which are screened in more than one layer (element), the flowing wellbore pressure is approximately corrected for gravity effects according to the depth-dependent flowing

density in the wellbore. Further details of this method are given by Pruess [1987].

During fluid production or injection, the rate of heat removal or injection is determined by

$$\hat{q}^h = \sum_{\beta} q_{\beta} h_{\beta} \quad (22)$$

where  $h_{\beta}$  is the specific enthalpy of phase  $\beta$ .

The initial conditions for a simulation are introduced by specifying the values of the four primary variables in all volume elements. As discussed earlier, the choice of these primary variables depends on the phase conditions in a given element. In many instances, it is convenient to use the results of an earlier simulation as the initial conditions for a later simulation. This feature is particularly useful for simulations in which the initial conditions consist of a steady-state flow field, or static equilibrium.

Boundary conditions are normally applied through the use of appropriately chosen volume elements, nodal point to interface distances, and source/sink terms. Boundary conditions of the "no flow" type are applied by simply not including any elements beyond the "no flow" boundary. Specified flux boundary conditions (Neumann) are maintained by means of source/sink terms in elements adjacent to the boundary on the outside of the flow region. Boundary conditions in which the primary variables are constant (Dirichlet) are specified by introducing boundary elements having a very large volume ( $\approx 10^{20} m^3$ ). In this case, the distance from the nodal point of the boundary element to the boundary is given a very small value. Specifying a very large volume for the boundary element ensures that the primary variables at the boundary will not change during the course of the simulation. Several other types of boundary conditions are made possible by assigning special values of certain parameters such as capillary pressures, relative permeabilities, thermal conductivity, or heat capacity to the boundary elements. In the assembly and solution of the linear equations, boundary elements are not distinguished from other elements, and no special numerical treatment is required.

## STMVOC INPUT FORMATS

The input data used by STMVOC is read in a format which is nearly identical to that used by the TOUGH simulator. The primary difference in the two input files is the addition of a data block called CHEMP after the ROCKS data block. CHEMP contains all of the information about a given chemical needed to compute the various thermophysical properties of the NAPL/chemical.

This section, which is intended to be used as an addendum to the original TOUGH User's Guide [Pruess, 1987], gives the specific changes needed for the STMVOC input file with respect to the TOUGH input file. Unless otherwise stated, all formats and variables in the STMVOC input file are identical to those in the TOUGH input file.

TITLE                    unchanged from TOUGH.

### ROCKS

Record ROCKS.1        unchanged from TOUGH.

Record ROCKS.1.1    unchanged from TOUGH except that if TORTX = 0, the gas phase tortuosity will be calculated using the Millington and Quirk [1961] model as  $\tau_g = \phi^{1/3} S_g^{7/3}$ .

Record ROCKS.1.2    unchanged from TOUGH except that three additional three phase relative permeability relationships are available (see Appendix 1). If one of the TOUGH two phase relative permeability functions is chosen, the NAPL relative permeability will be set to zero.

Record ROCKS.1.3    unchanged from TOUGH except that a three phase capillary pressure relationship is available (see Appendix 2). If one of the TOUGH two phase capillary pressure functions is chosen, the gas-NAPL capillary pressure will be set to zero.

Record ROCKS.2 a blank record closes the ROCKS data block.

CHEMP This data block provides the constants for a given organic chemical that are used to calculate the thermophysical properties of the NAPL/chemical. The units of many of these constants are not standard metric units, and care must be taken to ensure that the appropriate units are used. Most of the data used in this block is from Appendix A of Reid et al. [1987], where it appears in the same units used here. Details of the methods used to compute the properties of the NAPL/chemical may be found in Falta [1990] or Falta et al. [1990a].

Record CHEMP.1

Format (5E12.5)

TCRIT, PCRIT, ZCRIT, OMEGA, DIPOLM

TCRIT chemical critical temperature, K.

PCRIT chemical critical pressure, bar (1 bar =  $10^5$  Pa).

ZCRIT chemical critical compressibility.

OMEGA Pitzer's acentric factor for the chemical.

DIPOLM chemical dipole moment, debyes.

Record CHEMP.2

Format (5E12.5)

TBOIL, VPA, VPB, VPC, VPD

TBOIL chemical normal boiling point, K.

VPA chemical vapor pressure constant from Reid et al. [1987].

VPB chemical vapor pressure constant from Reid et al. [1987].

VPC chemical vapor pressure constant from Reid et al. [1987].

VPD chemical vapor pressure constant from Reid et al. [1987].

## Record CHEMP.3

Format (5E12.5)

AMO, CPA, CPB, CPC, CPD

AMO chemical molecular weight, g/mole.

CPA chemical ideal gas heat capacity constant from Reid et al. [1987].

CPB chemical ideal gas heat capacity constant from Reid et al. [1987].

CPC chemical ideal gas heat capacity constant from Reid et al. [1987].

CPD chemical ideal gas heat capacity constant from Reid et al. [1987].

## Record CHEMP.4

Format (5E12.5)

RHOREF, TDENRF, DIFV0, TDIFRF, TEXPO

RHOREF reference NAPL (liquid) density,  $\text{kg}/\text{m}^3$ .

TDENRF reference temperature for NAPL density, K.

DIFV0 reference chemical gas diffusivity,  $m^2/s$ .  
 TDIFRF reference temperature for gas diffusivity, K.  
 TEXPO exponent for calculation of chemical diffusivity.

Record CHEMP.5 two options are available for calculating the NAPL liquid viscosity. If the liquid viscosity constants VLOA - VL0D for the desired NAPL are found in Table 9-8 of Reid et al. [1987], then the viscosity is calculated using a polynomial fit to actual viscosity data. Otherwise, VLOA and VLOB should be set equal to 0, and VLOC becomes a reference liquid viscosity with VL0D equal to the reference temperature. In this case, the viscosity is calculated from a more general (and less accurate) empirical relationship.

Format (5E12.5)

VLOA, VLOB, VLOC, VL0D, VOLCRT

VLOA liquid NAPL viscosity constant from Reid et al. [1987].  
 VLOB liquid NAPL viscosity constant from Reid et al. [1987].  
 VLOC liquid NAPL viscosity constant from Reid et al. [1987], or, if VLOA and VLOB = 0, reference NAPL viscosity, cP.  
 VL0D liquid NAPL viscosity constant from Reid et al. [1987], or, if VLOA and VLOB = 0, reference temperature for NAPL viscosity, K.  
 VOLCRT chemical critical volume,  $cm^3/mole$ .

Record CHEMP.6 the chemical solubility is calculated from the polynomial SOLUBILITY = SOLA + SOLB\*T + SOLC\*T\*\*2 + SOLD\*T\*\*3. If data for the solubility as a function of temperature are available, then SOLA,

SOLB, SOLC, and SOLD are calculated from a polynomial fit of the data. If these data are not available (the usual case), the solubility will be assumed to be constant, and SOLA should be set equal to the known solubility with SOLB, SOLC, and SOLD set equal to 0.

Format (4E12.5)

SOLA, SOLB, SOLC, SOLD

SOLA constant for chemical solubility in water, *mole fraction*.

SOLB constant for chemical solubility in water, *mole fraction /K*.

SOLC constant for chemical solubility in water, *mole fraction /K<sup>2</sup>*.

SOLD constant for chemical solubility in water, *mole fraction /K<sup>3</sup>*.

Record CHEMP.7

Format (2E12.5)

OCC, FOC

OCC chemical organic carbon partition coefficient, *m<sup>3</sup>/kg*.

FOC fraction of organic carbon in soil.

START unchanged from TOUGH.

PARAM

Record PARAM.1 unchanged from TOUGH except that if DIFFO=0, there will be no gas phase diffusion of chemical vapor.



## Record PARAM.2

Format (4E10.4,I5,5X,3E10.4)

TSTART, TIMAX, DELTEN, DELTMX, NELST, GF, REDLT,

SCALE

TSTART unchanged from TOUGH.

TIMAX unchanged from TOUGH.

DELTEN unchanged from TOUGH.

DELTMX unchanged from TOUGH.

NELST the number of elements (up to 20) for which a short printout after every timestep will be provided.

GF unchanged from TOUGH.

REDLT unchanged from TOUGH.

SCALE unchanged from TOUGH.

Record PARAM.2.1 optional for NELST greater than 0.

Format (20A5)

ELST(K), K=1,NELST

ELST(K) name of each element for which a short printout at every timestep is desired.

Record PARAM.2.2, 2.3, etc

Format (8E10.4)

DLT(I), I=1,100

DLT(I) unchanged from TOUGH.

Record PARAM.3

## Format (7E10.4)

RE1, RE2, U, WUP, WNR, DFAC, RERMAX

RE1 unchanged from TOUGH.

RE2 unchanged from TOUGH.

U unchanged from TOUGH.

WUP unchanged from TOUGH.

WNR unchanged from TOUGH.

DFAC unchanged from TOUGH.

RERMAX maximum relative residual. If the maximum relative residual exceeds RERMAX at any iteration, the timestep will be reduced (default= $\infty$ ).

Record PARAM.4 this record contains the default initial values of the four primary variables for all elements not specified in block INCON if option START is used. Note that  $S_g$  and  $S_w$  must be at least  $10^{-4}$ .

## Format (4E20.14)

DEP(I), I = 1,4

DEP(1) pressure, Pa.

DEP(2)  $\geq 1.5$ : temperature,  $^{\circ}C$ ; two phase gas/aqueous points.

$< 1.5$ : gas saturation; three phase gas/aqueous/NAPL points.

DEP(3)  $\geq 1.5$ : temperature,  $^{\circ}C$ ; three phase gas/aqueous/NAPL points.

$< 1.5$ : chemical vapor mole fraction in the gas phase; two phase gas/aqueous points.

DEP(4) aqueous phase saturation.

RPCAP

Record RPCAP.1 unchanged from TOUGH except that three additional three phase relative permeability relationships are available (see Appendix 1). If one of the TOUGH two phase relative permeability functions is chosen, the NAPL relative permeability will be set to zero.

Record RPCAP.2 unchanged from TOUGH except that a three phase capillary pressure relationship is available (see Appendix 2). If one of the TOUGH two phase capillary pressure functions is chosen, the gas-NAPL capillary pressure will be set to zero.

TIMES unchanged from TOUGH.

ELEME unchanged from TOUGH.

CONNE unchanged from TOUGH.

GENER

Record GENER.1

Format (A3,I2,A3,I2,4I5,A4,A1,4E11.4)

EL, NE, SL, NS, NSEQ, NADD, NADS, LTAB, TYPE, ITAB, GX,  
EX, HG, XMAW,

EL, NE unchanged from TOUGH.

SL, NS unchanged from TOUGH.

NSEQ unchanged from TOUGH.

NADD unchanged from TOUGH.

NADS unchanged from TOUGH.

LTAB unchanged from TOUGH.

TYPE HEAT - heat sink/source.

COM1 - water injection.

WATE - water injection.

COM2 - air injection.

AIR - air injection.

OIL - chemical injection.

MASS - mass production rate specified (extended to three phase flow).

DELV - well on deliverability, extended to three phase flow. See TOUGH user's guide for details of use.

ITAB unchanged from TOUGH.

GX unchanged from TOUGH except that OIL is an additional generation type.

EX unchanged from TOUGH.

HG unchanged from TOUGH.

XMAW for WATE or COM1, XMAW is the mass fraction of air in the injected water. For AIR or COM2, XMAW is the mass fraction of water in the injected air.

Record GENER.1.1 unchanged from TOUGH.  
 Record GENER.1.2 unchanged from TOUGH.  
 Record GENER.1.3 unchanged from TOUGH.  
 Record GENER.2 a blank record closes the GENER data block.

## INCON

Record INCON.1 unchanged from TOUGH.  
 Record INCON.2 Note that  $S_g$  and  $S_w$  must be at least  $10^{-4}$ .  
 Format (4E20,4)  
 X1, X2, X3, X4  
 X1 pressure, Pa.  
 X2  $\geq 1.5$ : temperature,  $^{\circ}C$ ; two phase gas/aqueous points.  
 $< 1.5$ : gas saturation; three phase gas/aqueous/NAPL points.  
 X3  $\geq 1.5$ : temperature,  $^{\circ}C$ ; three phase gas/aqueous/NAPL points.  
 $< 1.5$ : chemical vapor mole fraction in the gas phase; two phase gas/aqueous points.  
 X4 aqueous phase saturation.

ENDCY closes the STMVOC data file.

## STMVOC OUTPUT

The output produced by STMVOC is similar to that produced by TOUGH, and consists mainly of two types of output. The first type of output is printed at every time step for elements specified in record PARAM.2.1. For each of these elements, the following quantities are printed:

P	gas phase pressure, Pa.
T	temperature, °C.
SO	NAPL phase saturation.
SG	gas phase saturation.
PCW	gas-water capillary pressure, Pa.
PCO	gas-NAPL capillary pressure, Pa.
CG	chemical concentration in the gas phase, $kg/m^3$ .
CW	chemical concentration in the aqueous phase, $kg/m^3$ .

The second type of output occurs at times specified by the user (as in TOUGH), and includes a listing of the conditions in all elements at that time. The STMVOC output lists each element twice in order to give a more complete description of the conditions present. The first time the elements are listed, the following quantities are tabulated:

P	gas phase pressure, Pa.
T	temperature, °C.
SO	NAPL phase saturation.
SW	aqueous phase saturation.
SG	gas phase saturation.
PVOC	chemical vapor partial pressure, Pa.

PAIR	air partial pressure, Pa.
PSATO	chemical saturated vapor pressure, Pa.
PSATW	water saturated vapor pressure, Pa.
PCO	gas-NAPL capillary pressure, Pa.
PCW	gas-water capillary pressure, Pa.

The second time the elements are listed, the following quantities are tabulated:

CVOCG	chemical concentration in the gas phase, $kg/m^3$ .
CVOCW	chemical concentration in the aqueous phase, $kg/m^3$ .
DGAS	gas phase density, $kg/m^3$ .
DOIL	NAPL density, $kg/m^3$ .
VISGAS	gas phase viscosity, kg/m s.
VISOIL	NAPL viscosity, kg/m s.
DIFFO	multicomponent chemical vapor diffusivity, $m^2/s$ .
DIFFW	multicomponent water vapor diffusivity, $m^2/s$ .
KRGAS	gas phase relative permeability.
KRWAT	aqueous phase relative permeability.
KROIL	NAPL relative permeability.

The remaining output options are similar to those produced by TOUGH with appropriate modifications for three phases and three mass components.

**SAMPLE PROBLEMS**

The following problems were run on a Solbourne Series 5 Model 502 workstation using a double precision version of STMVOC. The execution times listed for these problems pertain only to this machine. For the purpose of comparison, simulations performed on a Cray XMP would run about 5-6 times faster, simulations performed on an IBM Series 6000 Model 320 would run about 2-3 times faster, and simulations performed on a Sun Sparcstation would run about 2-3 times slower.



### Problem No. 1 - One Dimensional Gas Diffusion of an Organic Chemical With Phase Partitioning

In this problem, chlorobenzene vapor diffuses through an initially clean one dimensional column. Phase partitioning of the vapor into an immobile aqueous phase and the solid phase (adsorption) is included. Initially, the column does not contain any chlorobenzene, and the aqueous phase saturation is 0.25. The initial temperature and pressure are 10 °C and 101325 Pa, respectively. A listing of the input file used for this problem is provided in Figure 1. The mesh consists of 100 interior elements with two boundary elements. For the first 5 m, the mesh spacing is 0.1 m. After 5 m, the mesh spacing is increased to 0.2 m to a total length of 15 m. The constants needed to calculate the properties of chlorobenzene are included in the data block CHEMP. Adsorption to the solid phase is included by specifying the fraction of organic carbon in the soil to be 0.005. Due to the relatively high aqueous solubility and organic carbon partition coefficient of chlorobenzene, the chlorobenzene vapor is strongly retarded. Calculating the gas phase retardation coefficient from [Falta et al., 1989]

$$R_g = \frac{S_w}{HS_g} + \frac{\rho_b K_{oc} f_{oc}}{H \phi S_g} + 1 \quad (23)$$

gives a value of 67.8 indicating that the vapor is very strongly retarded in this problem.

For this problem, the source of chlorobenzene is provided by giving the inner boundary element a NAPL saturation of 0.05. The initial time step size is set equal to 1 second, and is allowed to grow to a maximum value of 5 days. After one year, the simulation is terminated. A printout of the STMVOC simulation results after one year is given in Figure 2.

These results are compared with an analytical solution for transient gas diffusion with phase partitioning [Baehr, 1987] in Figure 3. The numerical solution calculated using STMVOC is in excellent agreement with the analytical solution. It should be mentioned here that this example has been specifically designed so that there will be no deviation from

```

cccc***** 1d gas diffusion of chlorobenzene with phase partitioning *****
rocks-----1-----2-----3-----4-----5-----6-----7-----8
dirt1          2650.0      .400 1.0000e-141.0000e-141.0000e-14      3.1      1000.0

champ-----1-----2-----3-----4-----5-----6-----7-----8
632.4          45.2        0.265      0.249      1.6
404.9          -7.58700     2.26551    -4.09418    0.17038
112.559        -3.3890e+01    5.631e-01  -4.522e-04  1.426e-07
1106.0         293.00         8.000e-06  283.15     1.00
              -4.573      1.196e+3    1.37e-3    -1.378e-6    308.0
              7.996e-5  0.          0.          0.
0.15          0.005
start
param-----1-----2-----3-----4-----5-----6-----7-----8
  1 350        3501000000000100010410000000  2.13e-5
              3.1558e+7      1.0  4.32e+5      1      9.8060
aa  1
    1.e-5      1.e00
101325.00      10.00      0.0      1.e-8  0.00
rpcap-----1-----2-----3-----4-----5-----6-----7-----8
  6          0.4        0.1        0.001      1.
  9
elem-----1-----2-----3-----4-----5-----6-----7-----8
aa  1  49      1dirt1      0.100
bb  1  49      1dirt1      0.200
bn  1  1      1dirt1      1.e+20

conne-----1-----2-----3-----4-----5-----6-----7-----8
bn  1aa  1          1          1          .0001      .0500      1.00      0.0
aa  1aa  2  48      1          1          .0500      .0500      1.00      0.0
aa  50bb 1          1          1          .0500      .1000      1.00      0.0
bb  1bb  2  48      1          1          .1000      .1000      1.00      0.0
bb  50bn 2          1          .1000      .0001      1.00      0.0

incon-----1-----2-----3-----4-----5-----6-----7-----8
bn  1          .4
101325.00      0.750      10.0      0.200

gener-----1-----2-----3-----4-----5-----6-----7-----8
endcy

```

Figure 1. STMVOC input file for problem 1.









\*\*\*\*\* volume- and mass-balances \*\*\*\*\*

\*\*\*\*\* [kyc,iter] = [ 91, 2] \*\*\*\*\* the time is 0.31558E+08 seconds, or 0.36525E+03 days

phase volumes in place  
gas 0.60000E+20 m\*\*3; water 0.18000E+20 m\*\*3; hydrocarbon 0.20000E+19 m\*\*3

phase mass in place  
gas 0.75165E+20 kg aqueous 0.17996E+23 kg liquid hydrocarbon 0.22321E+22 kg

air/water component mass in place  
air 0.73924E+20 kg water vapor 0.56291E+18 kg liquid water 0.17992E+23 kg

hydrocarbon component mass in place  
voc vapor 0.96667E+18 kg dissolved voc 0.39976E+19 kg liquid voc 0.22321E+22 kg total voc 0.22370E+22 kg

\*\*\*\*\*

write file \*save\* after 91 time steps --- the time is 0.31558E+08 seconds

end of tough simulation job --- elapsed time = 481.7710 sec  
-- calculation time = 481.3100 sec-- data input time = 0.4610 sec

Figure 2. Printed output for problem 1 (continued).

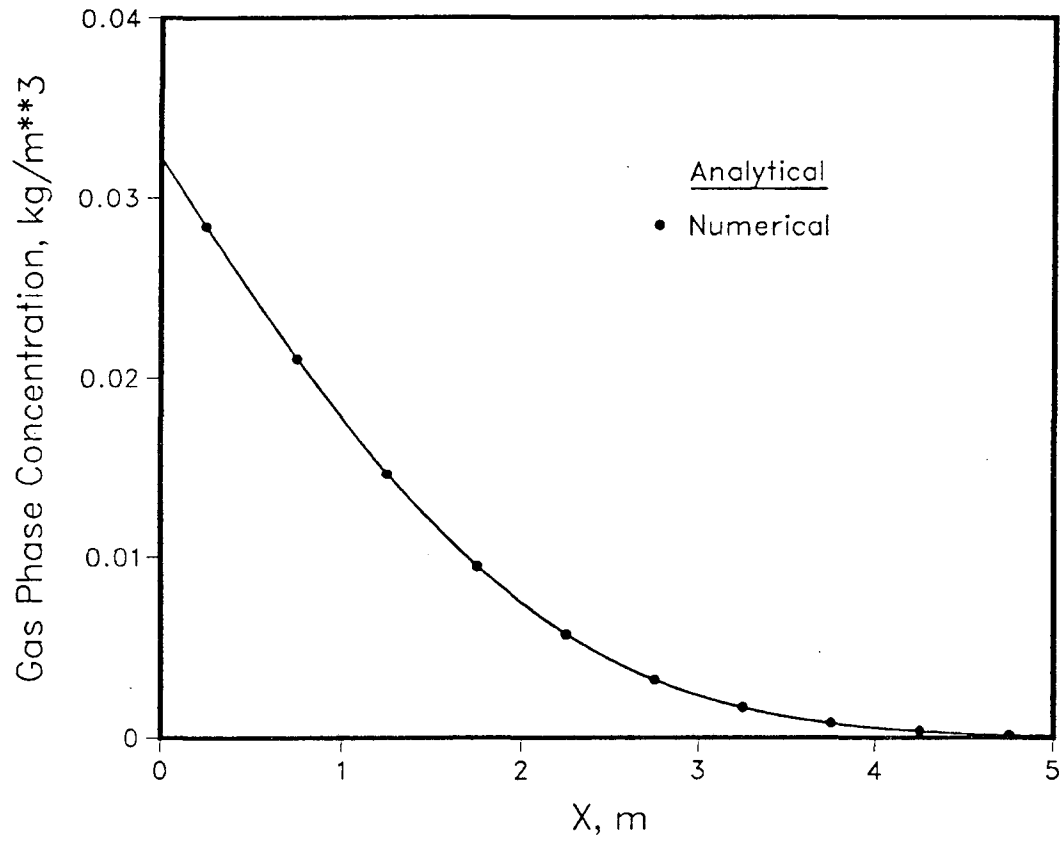


Figure 3. Comparison of STMVOC results with analytical solution of Baehr [1987] for transient diffusion with phase partitioning.



Fick's law during evaporation of the NAPL, and so that there will be no density driven flow of the chlorobenzene vapor. Under certain conditions, these phenomena (which are not accounted for in the analytical solution) are very important and these transport mechanisms are included in the STMVOC simulator. For a discussion of the effects of evaporation on deviations from Fick's second law of diffusion, the reader is referred to Falta [1990]. A study of the effects of density driven gas flow on gas phase chemical transport may be found in Falta et al. [1989]. It should also be mentioned that for problems in which the expected contaminant concentrations are very small, say less than about  $1 \mu\text{g}/\text{l}$ , the value of RE1 in record PARAM.3 should be reduced from the default value of  $1 \times 10^{-5}$  to a value of  $1 \times 10^{-7}$  or less. The value of DFAC in this record should also be reduced from the default value. Reducing RE1 will result in an increased number of iterations for a given problem, but will increase the accuracy of the simulation for very low concentrations.

**Problem No. 2 - Buckley-Leverett One Dimensional Two Phase Flow Problem**

This problem consists of water injection into a porous medium filled with NAPL and water. The initial water saturation in the matrix is 0.159, and at this saturation, the water is immobile. As water is injected, NAPL is displaced, and a shock front develops at the leading edge of the invading water. In this isothermal problem, capillary pressure effects are neglected, and the NAPL does not undergo interphase mass transfer with the aqueous phase. Details of the problem specification are given by Faust [1985], and may be read off the input file for the STMVOC simulation which is given in Figure 4. The two phase relative permeability curves used for this problem (IRP = 11 in record RPCAP.1) are described in Appendix 1. By setting ICP in record RPCAP.2 equal to 9, capillary pressure effects are neglected.

Because the NAPL is not chemically active ("black oil"), the data in block CHEMP must be appropriately modified. For this problem, the chemical constants for chlorobenzene used in the previous problem are used (rather arbitrarily). However, for this problem, the NAPL density is  $998.3 \text{ kg/m}^3$ , the viscosity is 1.00 cP, and the NAPL is not soluble. These properties are specified by changing RHOREF in record CHEMP.4 to 998.3 with TDENRF equal to 292.15, by making VLOA and VLOB in record CHEMP.5 equal to 0, by making VLOC in record CHEMP.5 equal to 1.0 with VLOD equal to 292.15, and by setting SOLA in record CHEMP.6 equal to a very small number. Because adsorption of the chemical to the solid matrix is not included in this problem, OCK and FOC in record CHEMP.7 are set equal to 0. In record ROCKS.1, DROCK is given a very large number to ensure that isothermal conditions prevail.

Initially, a small gas saturation (0.001) is specified for every element. This is necessary because the STMVOC simulator assumes that at least a small amount of both gas and water are present in every element. The small initial gas saturation used in this problem does not significantly affect the results. The temperature of  $19 \text{ }^\circ\text{C}$  used here is chosen so that the water viscosity will be equal to 1.0 cP (with a density of  $998.3 \text{ kg/m}^3$ ).

```

cccc*****1d Buckley-Leverett problem for two phase flow*****
rocks---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
dirt1      1.e+20      .200 2.9600e-132.9600e-132.9600e-13      3.1      1000.0

chemp---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
632.4      45.2      0.265      0.249      1.6
404.9      -7.58700      2.26551      -4.09418      0.17038
112.559     -3.3890e+01      5.631e-01      -4.522e-04      1.426e-07
998.3      292.15      8.000e-06 273.15      1.00
      1.000e-7 0.      0.      1.00      292.15      308.
0.00      0.000
start
param---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
1 150      150100000000100010100000000 0.00e-5
      1.296e+8 8.64e+5 8.64e+5 1 9.8060
aa 10
      1.e-5      1.e00      1.e-8 0.00
689500.00      0.001      19.0      .1590
rpcap---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
11
9
elem---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
aa 1 39 1dirt1 7078.980
bn 1 1 1dirt1 7078.980

conne---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
bn 1aa 1      1      .0010 3.810 929.00 0.0
aa 40bn 2      1      3.810 .0010 929.00 0.0
aa 1aa 2 38 1 1 1 3.810 3.810 929.00 0.0

gener---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
bn 1inj 1      wate 0.1399 8.4960e+4
bn 2pro 1      mass -0.1399

incon---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
bn 1      .2
689500.00      0.001      19.0      0.799

endcy

```

Figure 4. STMVOC input file for problem 2.

The time step size for this problem is constant at 10 days, and the simulation is stopped after 1500 days. A printout from the STMVOC simulation for the first few time steps, and for the results after 1500 days is given in Figure 5. These results are compared with the Buckley-Leverett analytical solution [Buckley and Leverett , 1942] in Figure 6. The numerical results match the analytical solution well although some smearing of the sharp front is evident.

1

```

00000 00 0 0 000 0 0      000 0 0 0 0 0 0      00 00000 0 00 0 0      0 00 000
0 0 0 0 0 0 0 0      0 0 00 00 0 0 0      0 0 0 0 0 0 0      0 0 0 0 0 0
0 0 0 0 0 0 00 0000      00 0 0 0 0 0 0      0000 0 0 0 0 0 0      0 0 0 000
0 0 0 0 0 0 0 0      0 0 0 0 0 0 0      0 0 0 0 0 0 00      0 0 0 0 0 0
0 00 00 000 0 0      000 0 0 0 00 0000 0 0 0 0 00 0 0      000 00 000

```

tough is a program for two-phase two-component flow of water and air, including heat flow.  
it was developed by k. pruess at lawrence berkeley laboratory.

\*\*\*\*\*  
\*\*\*\*\*

summary of optional files

file \*mesh\* exists --- open as an old file  
file \*incon\* exists --- open as an old file  
file \*gener\* exists --- open as an old file  
file \*save\* exists --- open as an old file  
file \*lineq\* exists --- open as an old file

\*\*\*\*\*  
\*\*\*\*\*

problem title: cccc\*\*\*\*\*1d Buckley-Leverett problem for two phase flow\*\*\*\*\*

domain no. 1 material name -- dirt1  
0.63240E+03 0.45200E+02 0.26500E+00 0.24900E+00 0.16000E+01  
0.40490E+03-0.75870E+01 0.22655E+01-0.40942E+01 0.17038E+00  
0.11256E+03-0.33890E+02 0.56310E+00-0.45220E-03 0.14260E-06  
0.99830E+03 0.29215E+03 0.80000E-05 0.27315E+03 0.10000E+01  
0.00000E+00 0.00000E+00 0.10000E+01 0.29215E+03 0.30800E+03  
0.10000E-06 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00  
0.00000E+00 0.00000E+00  
write file \*mesh\* from input data  
write file \*gener\* from input data  
write file \*incon\* from input data

\*mesh\* has 42 elements and 41 connections (interfaces) between them  
\*gener\* has 2 sinks/sources

end of tough input job --- elapsed time = 0.2100 seconds

===== equation of state for water/air mixtures =====

table of primary variables, in dependence upon composition and phases present

```

*****
components + water      air      water and air
*****
phases  gas      * p,t,x      p,t,x      p,t,x
        liquid * p,t,x      ./      p,t,x
        two-phase * p,s,t      ./      p,s,t
*****

```

the primary variables are

43

Figure 5. Printed output for problem 2.

```

p - pressure (pa)      t - temperature (deg-c)      x - air mass fraction      s - gas phase saturation
1***** volume- and mass-balances *****
***** [kycy,iter] = [ 0, 0] *****           the time is 0.00000E+00 seconds, or 0.00000E+00 days

phase volumes in place
gas 0.59472E+02 m**3;  water 0.10362E+05 m**3;  hydrocarbon 0.49050E+05 m**3

phase mass in place
gas 0.49069E+03 kg  aqueous 0.10350E+08 kg  liquid hydrocarbon 0.48967E+08 kg

air/water component mass in place
air 0.48769E+03 kg  water vapor 0.96771E+00 kg  liquid water 0.10350E+08 kg

hydrocarbon component mass in place
voc vapor 0.31833E+01 kg  dissolved voc 0.64720E+01 kg  liquid voc 0.48967E+08 kg  total voc 0.48967E+08 kg

*****

no convergence at [ 1, 1] --- deltex = 0.86400E+06  max. res. = 0.10697E+00  at element *bn 1* equation 1
no convergence at [ 1, 2] --- deltex = 0.86400E+06  max. res. = 0.25148E-01  at element *aa 2* equation 3
no convergence at [ 1, 3] --- deltex = 0.86400E+06  max. res. = 0.14859E-03  at element *aa 2* equation 3
***** kycy = 1 iter = 4 st = 0.86400E+06 dt = 0.86400E+06 *****
aa 10 p = 757372. t = 19.00 so = 0.8401E+00 sg = 0.9099E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 2, 1] --- deltex = 0.86400E+06  max. res. = 0.34429E+00  at element *aa 1* equation 1
no convergence at [ 2, 2] --- deltex = 0.86400E+06  max. res. = 0.18049E-01  at element *aa 2* equation 1
no convergence at [ 2, 3] --- deltex = 0.86400E+06  max. res. = 0.10906E-04  at element *aa 2* equation 3
***** kycy = 2 iter = 4 st = 0.17200E+07 dt = 0.86400E+06 *****
aa 10 p = 758167. t = 19.00 so = 0.8401E+00 sg = 0.9089E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 3, 1] --- deltex = 0.86400E+06  max. res. = 0.24139E+00  at element *aa 1* equation 1
no convergence at [ 3, 2] --- deltex = 0.86400E+06  max. res. = 0.17613E-01  at element *aa 2* equation 1
no convergence at [ 3, 3] --- deltex = 0.86400E+06  max. res. = 0.42741E-04  at element *aa 2* equation 1
***** kycy = 3 iter = 4 st = 0.25920E+07 dt = 0.86400E+06 *****
aa 10 p = 757389. t = 19.00 so = 0.8401E+00 sg = 0.9098E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 4, 1] --- deltex = 0.86400E+06  max. res. = 0.17170E+00  at element *aa 1* equation 1
no convergence at [ 4, 2] --- deltex = 0.86400E+06  max. res. = 0.10121E-01  at element *aa 2* equation 1
no convergence at [ 4, 3] --- deltex = 0.86400E+06  max. res. = 0.31939E-04  at element *aa 2* equation 1
***** kycy = 4 iter = 4 st = 0.34560E+07 dt = 0.86400E+06 *****
aa 10 p = 756593. t = 19.00 so = 0.8401E+00 sg = 0.9108E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 5, 1] --- deltex = 0.86400E+06  max. res. = 0.14061E+00  at element *aa 2* equation 1
no convergence at [ 5, 2] --- deltex = 0.86400E+06  max. res. = 0.36886E-02  at element *aa 3* equation 1
***** kycy = 5 iter = 3 st = 0.43200E+07 dt = 0.86400E+06 *****
aa 10 p = 755804. t = 19.00 so = 0.8401E+00 sg = 0.9118E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 6, 1] --- deltex = 0.86400E+06  max. res. = 0.15489E+00  at element *aa 2* equation 1
no convergence at [ 6, 2] --- deltex = 0.86400E+06  max. res. = 0.61707E-02  at element *aa 3* equation 1
***** kycy = 6 iter = 3 st = 0.51840E+07 dt = 0.86400E+06 *****
aa 10 p = 755015. t = 19.00 so = 0.8401E+00 sg = 0.9127E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 7, 1] --- deltex = 0.86400E+06  max. res. = 0.14866E+00  at element *aa 2* equation 1
no convergence at [ 7, 2] --- deltex = 0.86400E+06  max. res. = 0.75920E-02  at element *aa 3* equation 1
***** kycy = 7 iter = 3 st = 0.60480E+07 dt = 0.86400E+06 *****
aa 10 p = 754226. t = 19.00 so = 0.8401E+00 sg = 0.9137E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 8, 1] --- deltex = 0.86400E+06  max. res. = 0.13093E+00  at element *aa 2* equation 1
no convergence at [ 8, 2] --- deltex = 0.86400E+06  max. res. = 0.67031E-02  at element *aa 3* equation 1
no convergence at [ 8, 3] --- deltex = 0.86400E+06  max. res. = 0.11876E-04  at element *aa 3* equation 1
***** kycy = 8 iter = 4 st = 0.69120E+07 dt = 0.86400E+06 *****
aa 10 p = 753439. t = 19.00 so = 0.8401E+00 sg = 0.9146E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 9, 1] --- deltex = 0.86400E+06  max. res. = 0.10911E+00  at element *aa 2* equation 1

```

Figure 5. Printed output for problem 2 (continued).

```

no convergence at [ 9, 2] --- deltex = 0.86400E+06 max. res. = 0.39603E-02 at element aa 3* equation 1
***** kcyc = 9 iter = 3 st = 0.77760E+07 dt = 0.86400E+06 *****
aa 10 p = 752656. t = 19.00 so = 0.8401E+00 sg = 0.9156E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 10, 1] --- deltex = 0.86400E+06 max. res. = 0.12230E+00 at element aa 3* equation 1
no convergence at [ 10, 2] --- deltex = 0.86400E+06 max. res. = 0.29234E-02 at element aa 4* equation 1
***** kcyc = 10 iter = 3 st = 0.86400E+07 dt = 0.86400E+06 *****
aa 10 p = 751875. t = 19.00 so = 0.8401E+00 sg = 0.9166E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 11, 1] --- deltex = 0.86400E+06 max. res. = 0.13087E+00 at element aa 3* equation 1
no convergence at [ 11, 2] --- deltex = 0.86400E+06 max. res. = 0.45080E-02 at element aa 4* equation 1
***** kcyc = 11 iter = 3 st = 0.95040E+07 dt = 0.86400E+06 *****
aa 10 p = 751093. t = 19.00 so = 0.8401E+00 sg = 0.9175E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 12, 1] --- deltex = 0.86400E+06 max. res. = 0.12727E+00 at element aa 3* equation 1
no convergence at [ 12, 2] --- deltex = 0.86400E+06 max. res. = 0.54786E-02 at element aa 4* equation 1
***** kcyc = 12 iter = 3 st = 0.10368E+08 dt = 0.86400E+06 *****
aa 10 p = 750309. t = 19.00 so = 0.8401E+00 sg = 0.9185E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 13, 1] --- deltex = 0.86400E+06 max. res. = 0.11542E+00 at element aa 3* equation 1
no convergence at [ 13, 2] --- deltex = 0.86400E+06 max. res. = 0.50874E-02 at element aa 4* equation 1
***** kcyc = 13 iter = 3 st = 0.11232E+08 dt = 0.86400E+06 *****
aa 10 p = 749527. t = 19.00 so = 0.8401E+00 sg = 0.9195E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 14, 1] --- deltex = 0.86400E+06 max. res. = 0.99513E-01 at element aa 3* equation 1
no convergence at [ 14, 2] --- deltex = 0.86400E+06 max. res. = 0.34053E-02 at element aa 4* equation 1
***** kcyc = 14 iter = 3 st = 0.12096E+08 dt = 0.86400E+06 *****
aa 10 p = 748748. t = 19.00 so = 0.8401E+00 sg = 0.9204E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 15, 1] --- deltex = 0.86400E+06 max. res. = 0.10997E+00 at element aa 4* equation 1
no convergence at [ 15, 2] --- deltex = 0.86400E+06 max. res. = 0.21674E-02 at element aa 5* equation 1
***** kcyc = 15 iter = 3 st = 0.12960E+08 dt = 0.86400E+06 *****
aa 10 p = 747972. t = 19.00 so = 0.8401E+00 sg = 0.9214E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 16, 1] --- deltex = 0.86400E+06 max. res. = 0.12038E+00 at element aa 4* equation 1
no convergence at [ 16, 2] --- deltex = 0.86400E+06 max. res. = 0.34486E-02 at element aa 5* equation 1
***** kcyc = 16 iter = 3 st = 0.13824E+08 dt = 0.86400E+06 *****
aa 10 p = 747194. t = 19.00 so = 0.8401E+00 sg = 0.9223E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 17, 1] --- deltex = 0.86400E+06 max. res. = 0.12047E+00 at element aa 4* equation 1
no convergence at [ 17, 2] --- deltex = 0.86400E+06 max. res. = 0.44772E-02 at element aa 5* equation 1
***** kcyc = 17 iter = 3 st = 0.14688E+08 dt = 0.86400E+06 *****
aa 10 p = 746414. t = 19.00 so = 0.8401E+00 sg = 0.9233E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 18, 1] --- deltex = 0.86400E+06 max. res. = 0.11254E+00 at element aa 4* equation 1
no convergence at [ 18, 2] --- deltex = 0.86400E+06 max. res. = 0.46182E-02 at element aa 5* equation 1
***** kcyc = 18 iter = 3 st = 0.15552E+08 dt = 0.86400E+06 *****
aa 10 p = 745634. t = 19.00 so = 0.8401E+00 sg = 0.9243E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 19, 1] --- deltex = 0.86400E+06 max. res. = 0.99764E-01 at element aa 4* equation 1
no convergence at [ 19, 2] --- deltex = 0.86400E+06 max. res. = 0.36355E-02 at element aa 5* equation 1
***** kcyc = 19 iter = 3 st = 0.16416E+08 dt = 0.86400E+06 *****
aa 10 p = 744858. t = 19.00 so = 0.8401E+00 sg = 0.9253E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 20, 1] --- deltex = 0.86400E+06 max. res. = 0.97725E-01 at element aa 5* equation 1
no convergence at [ 20, 2] --- deltex = 0.86400E+06 max. res. = 0.19418E-02 at element aa 5* equation 1
***** kcyc = 20 iter = 3 st = 0.17280E+08 dt = 0.86400E+06 *****
aa 10 p = 744085. t = 19.00 so = 0.8401E+00 sg = 0.9262E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 21, 1] --- deltex = 0.86400E+06 max. res. = 0.11188E+00 at element aa 5* equation 1
no convergence at [ 21, 2] --- deltex = 0.86400E+06 max. res. = 0.25488E-02 at element aa 6* equation 1
***** kcyc = 21 iter = 3 st = 0.18144E+08 dt = 0.86400E+06 *****
aa 10 p = 743311. t = 19.00 so = 0.8401E+00 sg = 0.9272E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 22, 1] --- deltex = 0.86400E+06 max. res. = 0.11666E+00 at element aa 5* equation 1
no convergence at [ 22, 2] --- deltex = 0.86400E+06 max. res. = 0.36379E-02 at element aa 6* equation 1
***** kcyc = 22 iter = 3 st = 0.19008E+08 dt = 0.86400E+06 *****
aa 10 p = 742538. t = 19.00 so = 0.8401E+00 sg = 0.9282E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 23, 1] --- deltex = 0.86400E+06 max. res. = 0.11305E+00 at element aa 5* equation 1
no convergence at [ 23, 2] --- deltex = 0.86400E+06 max. res. = 0.42498E-02 at element aa 6* equation 1
***** kcyc = 23 iter = 3 st = 0.19872E+08 dt = 0.86400E+06 *****
aa 10 p = 741759. t = 19.00 so = 0.8401E+00 sg = 0.9291E-03 pcw = 0. pco = 0. cg = 0.5353E-01 cw = 0.6246E-03
no convergence at [ 24, 1] --- deltex = 0.86400E+06 max. res. = 0.10344E+00 at element aa 5* equation 1

```

Figure 5. Printed output for problem 2 (continued).









```

***** volume- and mass-balances *****
***** [kcyc,iter] = [ 150,  3] *****           the time is  0.12960E+09 seconds, or  0.15000E+04 days

phase volumes in place
gas  0.68176E+02 m**3;  water  0.28515E+05 m**3;  hydrocarbon  0.30888E+05 m**3

phase mass in place
gas  0.48942E+03 kg   aqueous  0.28481E+08 kg   liquid hydrocarbon  0.30836E+08 kg

air/water component mass in place
air  0.48776E+03 kg   water vapor  0.11093E+01 kg   liquid water  0.28481E+08 kg

hydrocarbon component mass in place
voc vapor  0.36492E+01 kg   dissolved voc  0.17810E+02 kg   liquid voc  0.30836E+08 kg   total voc  0.30836E+08 kg
*****

write file *save* after 150 time steps --- the time is  0.12960E+09 seconds

end of tough simulation job --- elapsed time =    274.8300 sec
-- calculation time =    274.5800 sec-- data input time =    0.2500 sec

```

Figure 5. Printed output for problem 2 (continued).

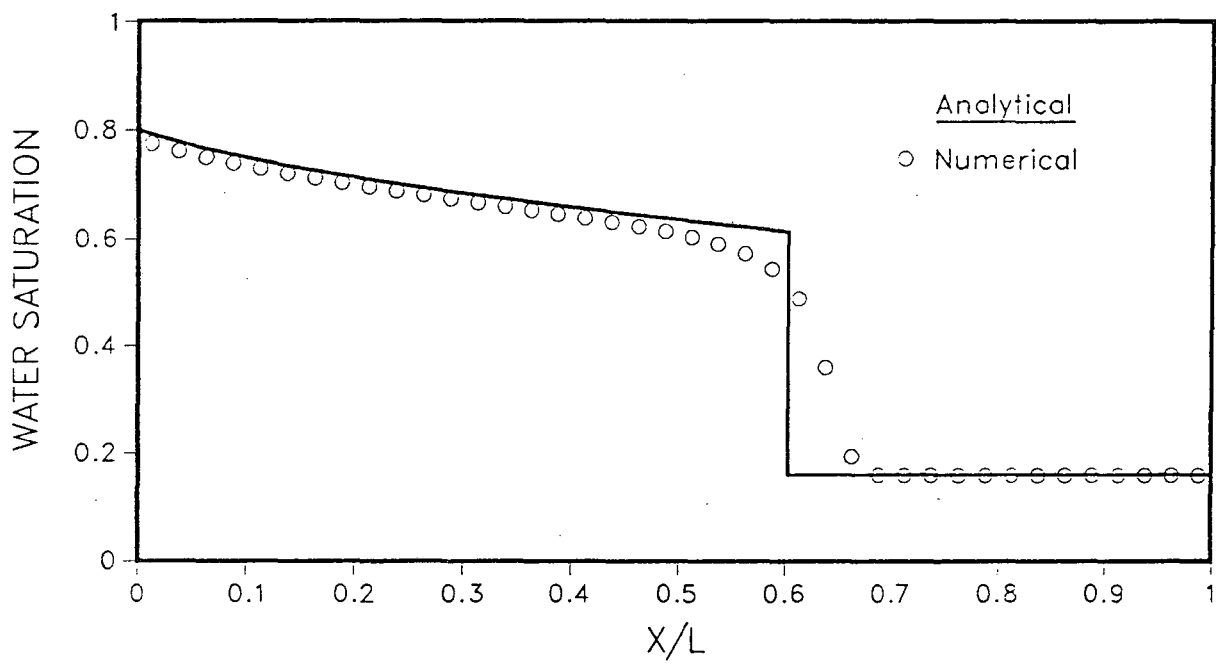


Figure 6. Comparison of STMVOC results with analytical solution for two phase flow.

### Problem No. 3 - Steam Displacement of a NAPL in a Laboratory Column

This simulation, which consists of three parts, is patterned after a simulation in which the STMVOC simulator was validated with experimental data. A discussion of the STMVOC validation with experimental data may be found in Falta [1990] and in Falta et al., [1990b]. The present problem has been simplified somewhat, but captures the essential features of the original validation simulation for steam displacement of trichloroethylene from a laboratory column.

The first part of the simulation involves the injection of liquid trichloroethylene into a horizontal water filled column. The column is 91 cm long with a cross sectional area of  $20.428 \text{ cm}^2$ . The mesh used for this simulation consists of 50 evenly spaced elements with a mesh spacing of 1.82 cm. Initially, the column is water saturated except for a small amount of gas (a gas saturation of 0.005). As in the previous example, it is necessary to include a small gas saturation for numerical reasons. The initial temperature in the column is  $22^\circ \text{C}$ , and deliverability boundary conditions are used at each end of the column. The deliverability boundary condition is specified by setting TYPE in record GENER.1 equal to DELV and by specifying a productivity index (GX in record GENER.1) and a wellbore pressure (EX in record GENER.1). Trichloroethylene is injected at a constant rate into the 15 th element by choosing the OIL option for TYPE in record GENER.1. The specific enthalpy of the injected trichloroethylene (EX in record GENER.1) corresponds to liquid trichloroethylene at a temperature of about  $22^\circ \text{C}$ . The various constants used to compute the thermophysical properties of trichloroethylene are contained in data block CHEMP. Additional problem parameters for this part of the simulation may be read from the input file which is shown in Figure 7. Details of the three phase relative permeability functions (IRP = 6 in record RPCAP.1) and the three phase capillary pressure functions (ICP = 8 in record RPCAP.2) may be found in Appendices 1 and 2, respectively.

Trichloroethylene is injected into the column for a period of 120 s, with an initial time step size of 2 seconds. A printout of the STMVOC simulation results at this time is given in

```

cccc--injection of trichloroethylene into a column ccccccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1 1 2650. .385 1.6000e-111.6000e-11 3.1 1000.0
0. 0. 2.85 0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
572.0 50.5 0.265 0.213 0.9
360.4 -7.38190 1.94817 -3.03294 -5.34536
131.389 3.0170e+01 2.287e-01 -2.229e-04 8.244e-08
1462. 293.0 8.000e-06273.0 1.60
1.50954e-40. 0. 0.
0. 0.
start
param---1-----2-----3-----4-----5-----6-----7-----8
1 20 20100000000100010410000000 0.00e-5
120.00 2. 120.000 2 9.8060
aa 1aa 15
1.e-5 1.e00 1.e-8 500.
101330.00 22.0 0.00 .9950
rpcap---1-----2-----3-----4-----5-----6-----7-----8
6 .150 .05 .001 3.
8 0.000 1.84 10. 11.
eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 49 1dirt1 3.7179e-5
conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 48 1 1 1 .0091 .0091 2.0428e-3 0.0
incon---1-----2-----3-----4-----5-----6-----7-----8
gener---1-----2-----3-----4-----5-----6-----7-----8
aa 1inj 1 delv 3.5917e-12 1.0140e+5
aa 50pro 1 delv 3.5917e-12 1.0140e+5
aa 15ino 1 oil 2.1900e-04 2.2100e+4
endcy

```

Figure 7. STMVOC input file for part 1 of problem 3.

Figure 8, and the liquid trichloroethylene (NAPL) phase saturation profile is shown graphically in Figure 9.

The second part of this simulation consists of injecting cold water ( $22\text{ }^{\circ}\text{C}$ ) into one end of the column and allowing fluids to drain from the other end of the column according to a deliverability boundary condition (TYPE = DELV in record GENER.1, etc.). The initial conditions for this part of the simulation are the conditions at the end of the first part of the simulation. To start the second part of the simulation, the SAVE file generated by the first part of the simulation must be renamed INCON, and the INCON section of the input file must be removed. The input file used for the waterflood part of the simulation is shown in Figure 10. This file is similar to the previous input file (Figure 7), except that data block GENER has been changed. These changes consist of removing the NAPL injection, and changing the inlet condition at the first element to cold water injection. Water with a specific enthalpy of  $9.2332 \times 10^4\text{ J/kg}$  is injected at a rate of  $3.5395 \times 10^{-4}\text{ kg/s}$  (a Darcy velocity of 15 m/day) for a period of 17880 s with an initial time step size of 2 s. A printout of the simulation results after a total time of 18000 s (120 s + 17880 s) is given in Figure 11, and the NAPL saturation profile in the column at this time is shown graphically in Figure 9.

The final part of the simulation consists of steam injection into the column. Again, the initial conditions for this part of the problem are the conditions at the end of the previous part of the problem, and the file SAVE generated during the waterflood part of the simulation must be renamed INCON. During this final part of the simulation, steam with an enthalpy of  $1.562 \times 10^6\text{ J/kg}$  is injected at a rate of  $3.5341 \times 10^{-5}\text{ kg/s}$  for a period of 9000 s. A printout is specified after 5000 s of steam injection (a total time of 23000 s) using data block TIMES. The input file used for the steam injection part of the simulation is shown in Figure 12, and is similar to the input file used in the previous part of the simulation (Figure 10), except that the inlet condition for the first element specified in data block GENER has been changed to represent steam injection.











```

***** volume- and mass-balances *****
***** [kcy,iter] = [ 10, 4] ***** the time is 0.12000E+03 seconds, or 0.13889E-02 days

phase volumes in place
gas 0.35967E-05 m**3; water 0.69455E-03 m**3; hydrocarbon 0.17951E-04 m**3

phase mass in place
gas 0.44829E-05 kg aqueous 0.69309E+00 kg liquid hydrocarbon 0.26181E-01 kg

air/water component mass in place
air 0.42712E-05 kg water vapor 0.69725E-07 kg liquid water 0.69299E+00 kg

hydrocarbon component mass in place
voc vapor 0.24544E-06 kg dissolved voc 0.98889E-04 kg liquid voc 0.26181E-01 kg total voc 0.26280E-01 kg
*****

write file *save* after 10 time steps --- the time is 0.12000E+03 seconds

end of tough simulation job --- elapsed time = 36.0000 sec
-- calculation time = 35.7700 sec-- data input time = 0.2300 sec

```

Figure 8. Printed output for part 1 of problem 3 (continued).

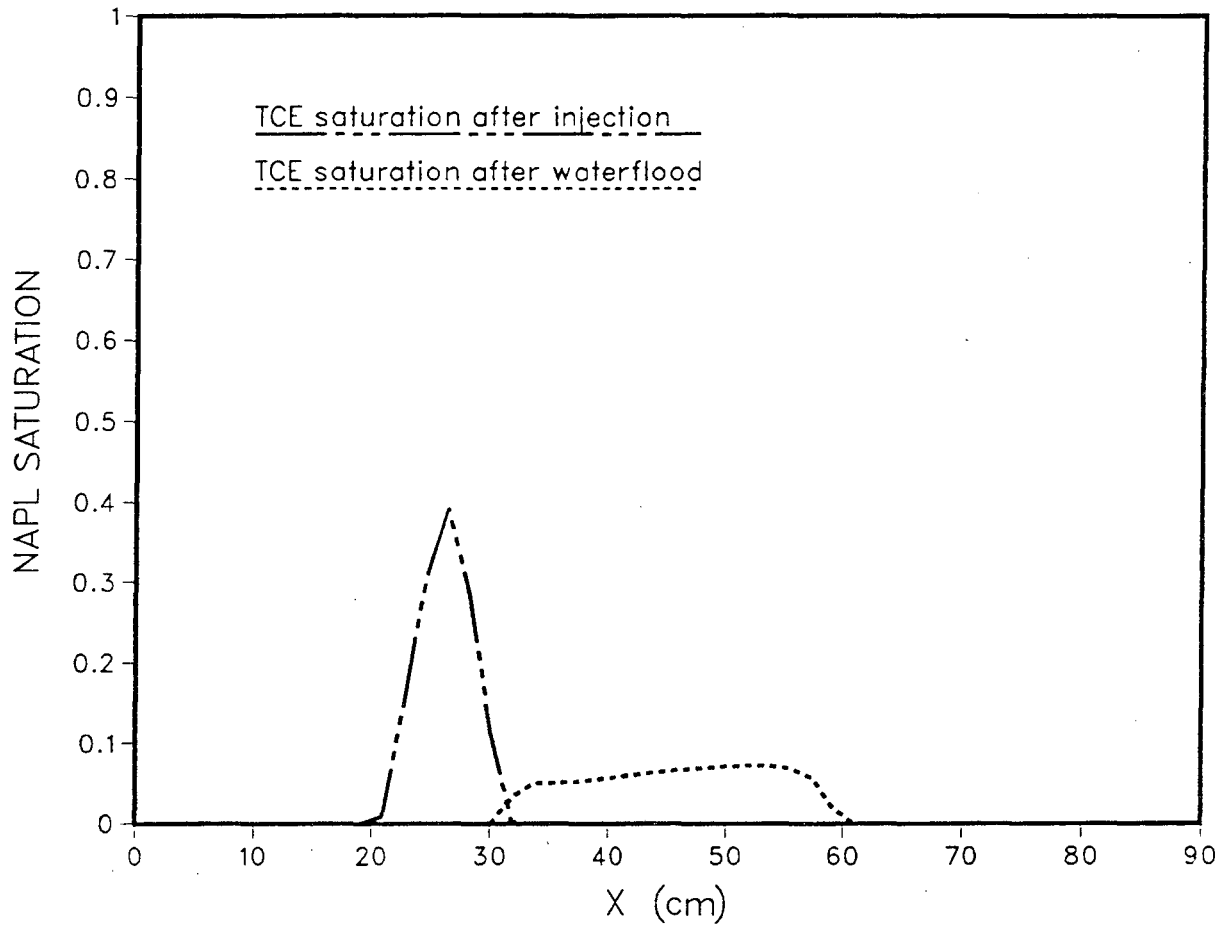


Figure 9. NAPL phase saturation distribution after trichloroethylene injection, and after waterflood.

```

cccc--cold waterflood at a rate of 15 m/day ----cccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1  1      2650.      .385 1.6000e-11 1.6000e-11 1.6000e-11      3.1      1000.0
      0.      0.      2.85      0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
572.0      50.5      0.265      0.213      0.9
360.4      -7.38190      1.94817      -3.03294      -5.34536
131.389      3.0170e+01      2.287e-01      -2.229e-04      8.244e-08
1462.      293.0      8.000e-06 273.0      1.60
      0.59      293.15256.0
1.50954e-40.      0.      0.
0.      0.
start
param---1-----2-----3-----4-----5-----6-----7-----8
1 80      80100000000100010410000000 0.00e-5
      18000.      2.0      8000.      1      9.8060
aa 15
      1.e-5      1.e00      22.0      0.00      1.e-8 0.00
101330.00      0.00      .9950
rpcap---1-----2-----3-----4-----5-----6-----7-----8
6      .150      .05      .005      3.
8      0.000      1.84      10.      11.
eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 49      1dirt1 3.7179e-5

conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 48 1 1 1 .0091 .0091 2.0428e-3 0.0

gener---1-----2-----3-----4-----5-----6-----7-----8
aa 1inj 1      wate 3.5395e-04 9.2332e+4
aa 50pro 1      delv 3.5917e-12 1.0140e+5

endcy

```

Figure 10. STMVOC input file for part 2 of problem 3.











```

***** volume- and mass-balances *****
***** [kcyc,iter] = [ 40, 4] ***** the time is 0.18000E+05 seconds, or 0.20833E+00 days

phase volumes in place
gas 0.27994E-05 m**3; water 0.70007E-03 m**3; hydrocarbon 0.13228E-04 m**3

phase mass in place
gas 0.41916E-05 kg aqueous 0.69860E+00 kg liquid hydrocarbon 0.19294E-01 kg

air/water component mass in place
air 0.32705E-05 kg water vapor 0.54216E-07 kg liquid water 0.69810E+00 kg

hydrocarbon component mass in place
voc vapor 0.92738E-06 kg dissolved voc 0.50299E-03 kg liquid voc 0.19294E-01 kg total voc 0.19798E-01 kg
*****

write file *save* after 40 time steps --- the time is 0.18000E+05 seconds

end of tough simulation job --- elapsed time = 135.0300 sec
-- calculation time = 134.7200 sec-- data input time = 0.3100 sec

```

Figure 11. Printed output for part 2 of problem 3 (continued).

```

cccccc-----inject steam at 105c with quality of .5 ----ccc
rocks-----1-----2-----3-----4-----5-----6-----7-----8
dirt1 1 2650. .385 1.6000e-11 1.6000e-11 1.6000e-11 3.1 1000.0
0. 0. 2.85 0.0

chemp-----1-----2-----3-----4-----5-----6-----7-----8
572.0 50.5 0.265 0.213 0.9
360.4 -7.38190 1.94817 -3.03294 -5.34536
131.389 3.0170e+01 2.287e-01 -2.229e-04 8.244e-08
1462. 293.0 8.000e-08 273.0 1.60
1.50954e-40. 0. 0.
0. 0.
start
param-----1-----2-----3-----4-----5-----6-----7-----8
1 400 100100000000100010410000000 0.00e-5
27000. 20.0 2000. 2 9.8060
aa laa 50
1.e-5 1.e00 1.e-8 500.
101330.00 22.0 0.00 .9950
rpcap-----1-----2-----3-----4-----5-----6-----7-----8
8 .150 .05 .005 3.
8 0.000 1.84 10.0 11.0
times-----1-----2-----3-----4-----5-----6-----7-----8
1
23000.0
eleme-----1-----2-----3-----4-----5-----6-----7-----8
aa 1 49 1dirt1 3.7179e-5

conne-----1-----2-----3-----4-----5-----6-----7-----8
aa laa 2 48 1 1 1 .0091 .0091 2.0428e-3 0.0

gener-----1-----2-----3-----4-----5-----6-----7-----8
aa linj 1 wate 3.5341e-05 1.5620e+6
aa 50pro 1 delv 3.5917e-12 1.0140e+5

endcy

```

Figure 12. STMVOC input file for part 3 of problem 3.

The output after 5000 s of steam injection is shown in Figure 13. These results are shown graphically in Figure 14 in which it is apparent that the steam is effectively displacing the trichloroethylene. By the end of the simulation, after 9000 s of steam injection, the entire column is at the steam temperature, and the trichloroethylene has been completely removed. A printout of the STMVOC output at this time is given in Figure 15.











```

***** volume- and mass-balances *****
***** [kcyc,iter] = [ 301, 4] ***** the time is 0.23000E+05 seconds, or 0.26620E+00 days

phase volumes in place
gas 0.35702E-03 m**3; water 0.34567E-03 m**3; hydrocarbon 0.13414E-04 m**3

phase mass in place
gas 0.24320E-03 kg aqueous 0.33660E+00 kg liquid hydrocarbon 0.19024E-01 kg

air/water component mass in place
air 0.31702E-05 kg water vapor 0.23042E-03 kg liquid water 0.33643E+00 kg

hydrocarbon component mass in place
voc vapor 0.10166E-04 kg dissolved voc 0.17099E-03 kg liquid voc 0.19024E-01 kg total voc 0.19205E-01 kg

*****

**** max res. = 0.18189E+04 at elem aa 38 equation 1 is greater than rermx 0.50000E+03
***** kcyc = 302 iter = 4 st = 0.23006E+05 dt = 0.56348E+01 *****
aa 50 p = 101580. t = 22.04 so = 0.7072E-07 sg = 0.5025E-02 pcw = -160. pco = -84. cg = 0.4270E+00 cw = 0.1098E+01
***** kcyc = 303 iter = 5 st = 0.23017E+05 dt = 0.11270E+02 *****
aa 50 p = 101588. t = 22.04 so = 0.7066E-07 sg = 0.5024E-02 pcw = -160. pco = -84. cg = 0.4271E+00 cw = 0.1098E+01
***** kcyc = 304 iter = 4 st = 0.23020E+05 dt = 0.28174E+01 *****
aa 50 p = 101597. t = 22.04 so = 0.7073E-07 sg = 0.5024E-02 pcw = -160. pco = -84. cg = 0.4271E+00 cw = 0.1098E+01
***** kcyc = 305 iter = 8 st = 0.23025E+05 dt = 0.56348E+01 *****
aa 50 p = 101625. t = 22.04 so = 0.7098E-07 sg = 0.5022E-02 pcw = -160. pco = -84. cg = 0.4271E+00 cw = 0.1098E+01
***** kcyc = 306 iter = 6 st = 0.23031E+05 dt = 0.56348E+01 *****
aa 50 p = 101641. t = 22.04 so = 0.7101E-07 sg = 0.5022E-02 pcw = -160. pco = -84. cg = 0.4272E+00 cw = 0.1098E+01
***** kcyc = 307 iter = 4 st = 0.23037E+05 dt = 0.56348E+01 *****
aa 50 p = 101625. t = 22.05 so = 0.7056E-07 sg = 0.5022E-02 pcw = -160. pco = -84. cg = 0.4272E+00 cw = 0.1098E+01
***** kcyc = 308 iter = 7 st = 0.23048E+05 dt = 0.11270E+02 *****
aa 50 p = 101607. t = 22.05 so = 0.6993E-07 sg = 0.5023E-02 pcw = -160. pco = -84. cg = 0.4273E+00 cw = 0.1098E+01
***** kcyc = 309 iter = 5 st = 0.23059E+05 dt = 0.11270E+02 *****
aa 50 p = 101610. t = 22.06 so = 0.6958E-07 sg = 0.5023E-02 pcw = -160. pco = -84. cg = 0.4274E+00 cw = 0.1098E+01
***** kcyc = 310 iter = 5 st = 0.23070E+05 dt = 0.11270E+02 *****
aa 50 p = 101590. t = 22.06 so = 0.6895E-07 sg = 0.5025E-02 pcw = -160. pco = -84. cg = 0.4275E+00 cw = 0.1098E+01
***** kcyc = 311 iter = 5 st = 0.23082E+05 dt = 0.11270E+02 *****
aa 50 p = 101566. t = 22.06 so = 0.6840E-07 sg = 0.5026E-02 pcw = -160. pco = -84. cg = 0.4276E+00 cw = 0.1098E+01
***** kcyc = 312 iter = 4 st = 0.23093E+05 dt = 0.11270E+02 *****
aa 50 p = 101571. t = 22.07 so = 0.6826E-07 sg = 0.5026E-02 pcw = -160. pco = -84. cg = 0.4276E+00 cw = 0.1098E+01
***** kcyc = 313 iter = 4 st = 0.23116E+05 dt = 0.22539E+02 *****
aa 50 p = 101575. t = 22.07 so = 0.6782E-07 sg = 0.5026E-02 pcw = -160. pco = -84. cg = 0.4278E+00 cw = 0.1098E+01
***** kcyc = 314 iter = 9 st = 0.23161E+05 dt = 0.45078E+02 *****
aa 50 p = 101601. t = 22.10 so = 0.3874E-07 sg = 0.5025E-02 pcw = -160. pco = -84. cg = 0.4284E+00 cw = 0.1098E+01
***** kcyc = 315 iter = 9 st = 0.23206E+05 dt = 0.45078E+02 *****
aa 50 p = 101598. t = 22.14 so = 0.0000E+00 sg = 0.5027E-02 pcw = -160. pco = -84. cg = 0.4291E+00 cw = 0.1098E+01
***** kcyc = 316 iter = 8 st = 0.23251E+05 dt = 0.45078E+02 *****
aa 50 p = 101573. t = 22.16 so = 0.0000E+00 sg = 0.5029E-02 pcw = -160. pco = -84. cg = 0.4295E+00 cw = 0.1098E+01
***** kcyc = 317 iter = 5 st = 0.23262E+05 dt = 0.11270E+02 *****
aa 50 p = 101581. t = 22.17 so = 0.0000E+00 sg = 0.5029E-02 pcw = -160. pco = -84. cg = 0.4297E+00 cw = 0.1098E+01
***** kcyc = 318 iter = 4 st = 0.23265E+05 dt = 0.28174E+01 *****
aa 50 p = 101586. t = 22.17 so = 0.0000E+00 sg = 0.5029E-02 pcw = -160. pco = -84. cg = 0.4297E+00 cw = 0.1098E+01
***** kcyc = 319 iter = 5 st = 0.23270E+05 dt = 0.56348E+01 *****
aa 50 p = 101601. t = 22.18 so = 0.0000E+00 sg = 0.5028E-02 pcw = -160. pco = -84. cg = 0.4298E+00 cw = 0.1098E+01
***** kcyc = 320 iter = 8 st = 0.23276E+05 dt = 0.56348E+01 *****
aa 50 p = 101635. t = 22.19 so = 0.0000E+00 sg = 0.5027E-02 pcw = -160. pco = -84. cg = 0.4300E+00 cw = 0.1098E+01
***** kcyc = 321 iter = 8 st = 0.23282E+05 dt = 0.56348E+01 *****

```

Figure 13. Printed output for part 3 of problem 3 after 5000 s of steam injection (continued).

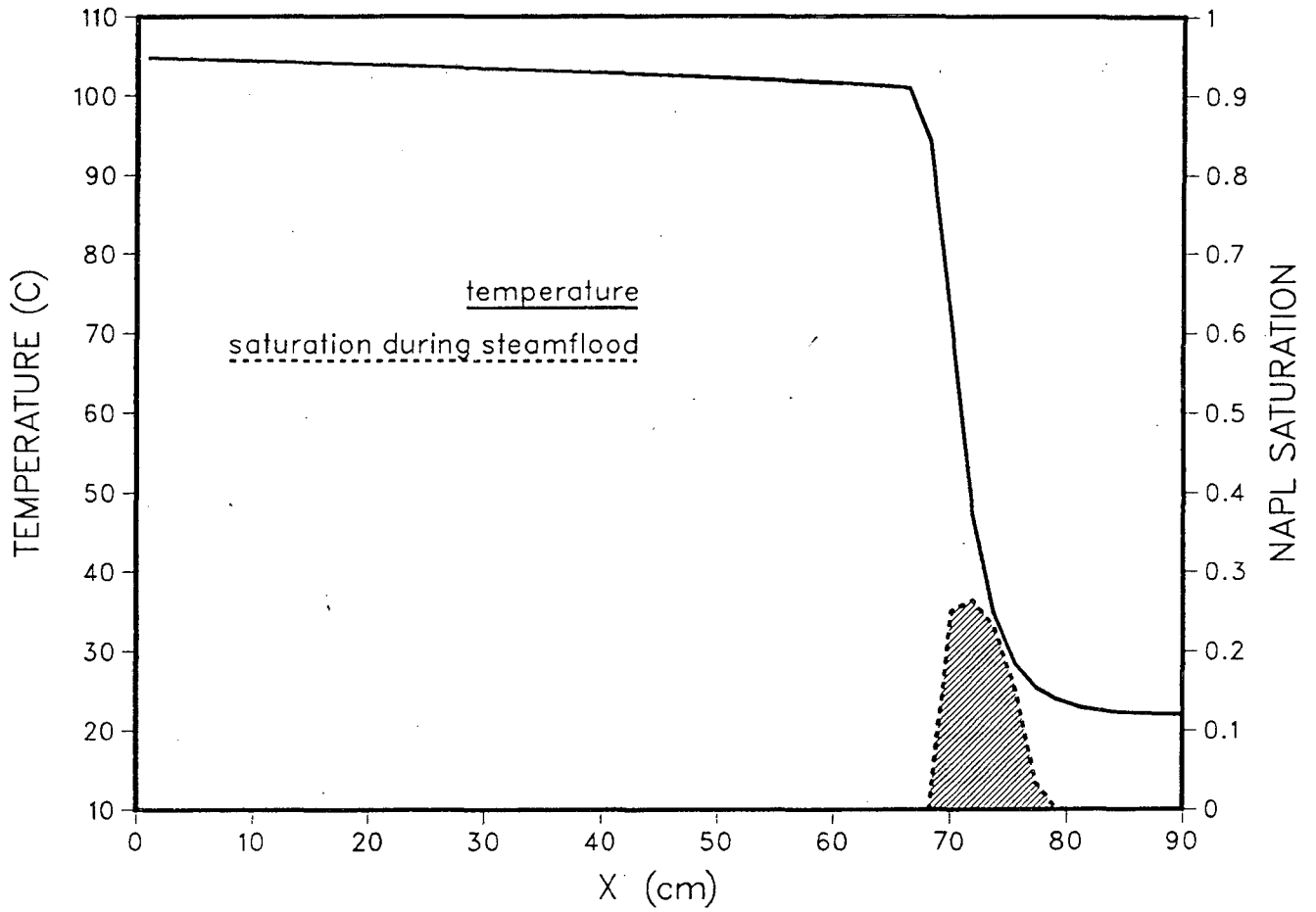


Figure 14. Calculated separate phase trichloroethylene distribution and temperature profile after 5000 s of steam injection.









```

***** volume- and mass-balances *****
***** [kyc,iter] = [ 399,  3] *****           the time is  0.27000E+05 seconds, or  0.31250E+00 days

phase volumes in place
gas  0.47186E-03 m**3;   water  0.24424E-03 m**3;   hydrocarbon  0.00000E+00 m**3

phase mass in place
gas  0.31139E-03 kg   aqueous  0.23343E+00 kg   liquid hydrocarbon  0.00000E+00 kg

air/water component mass in place
air  0.35495E-15 kg   water vapor  0.31139E-03 kg   liquid water  0.23343E+00 kg

hydrocarbon component mass in place
voc vapor  0.48329E-21 kg   dissolved voc  0.41341E-22 kg   liquid voc  0.00000E+00 kg   total voc  0.52463E-21 kg

*****

write file *save* after  399 time steps --- the time is  0.27000E+05 seconds

end of tough simulation job --- elapsed time =   1981.7100 sec
-- calculation time =   1981.3800 sec-- data input time =   0.3300 sec

```

Figure 15. Printed output at the end of part 3 of problem 3 (continued).

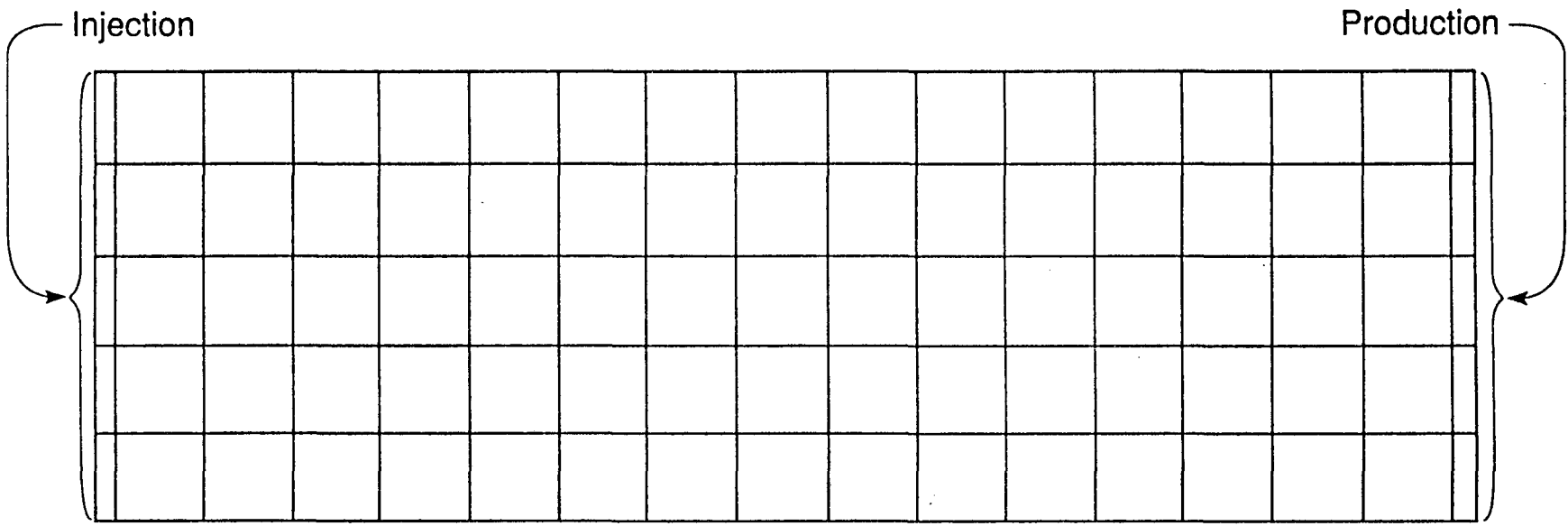


#### Problem No. 4 - Steam Displacement of a NAPL in a Two Dimensional Field Scale System

This example is nearly identical to a simulation discussed by Falta [1990] in which o-xylene is displaced by steam injection in a two dimensional field scale system. As in the previous example, this simulation consists of several parts due to changes in boundary conditions which occur over the course of the simulation.

For this problem, a rather coarse two dimensional (vertical cartesian) mesh is used with 75 interior elements, and 10 boundary elements. A scale diagram of the mesh is shown in Figure 16. The interior elements are 1.2 m by 1.2 m squares with a thickness of 1 m. These elements are named aa 1 through aa 75, with aa 1 through aa 15 corresponding to the top row, aa 16 through aa 30 corresponding to the second row, etc. The boundary elements are somewhat smaller, having dimensions of 0.3 m by 1.2 m. These elements are also given different material properties and are intended to approximately represent wells. The boundary elements are named bn 1 through bn 10, with bn 1 through bn 5 corresponding to injection elements (numbered from top to bottom), and bn 6 through bn 10 corresponding to the production elements (also numbered from top to bottom).

The first part of the simulation is the generation of an undisturbed water table with a static pressure distribution. The input file used for this part of the simulation is shown in Figure 17. This initial condition generation part of the simulation is run for a period of  $6.312 \times 10^8$  s (20 years), and the printed output from STMVOC at this time is shown in Figure 18. As in the earlier examples, for numerical reasons a small gas saturation must be present in all elements, including those which would normally be fully water saturated. The capillary pressure and relative permeability functions used throughout this simulation are similar to those used in the previous example, except that the capillary pressure between the gas phase and the NAPL is neglected. Even though no NAPL is present in the system during this first part of the simulation, data block CHEMP must be included for any STMVOC simulation. In the input file shown in Figure 17 (and in the other input files used for this



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lg/Mac

Figure 16. Scale diagram of the mesh used in problem 4.

```

cccc--- 2-d steamflood -- initial condition generation-----ccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1 1 2650. .400 2.5000e-132.5000e-132.5000e-13 3.1 1000.0
0. 0. 2.85 0.0
bndr1 1 1200. .400 2.5000e-132.5000e-132.5000e-13 3.1 600.0
0. 0. 2.85 0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
630.3 37.3 0.262 0.310 0.5
417.6 -7.53357 1.40968 -3.10985 -2.85992
106.168 -1.5850e+01 5.962e-01 -3.443e-04 7.528e-08
880.0 293.0 8.000e-06273.0 1.60
-3.332e+0 1.039e+3 -1.768e-3 1.076e-6 369.
2.97500e-50. 0. 0.
0. 0.

start
param---1-----2-----3-----4-----5-----6-----7-----8
1 30 3010000000010001041000000 0.00e-5
6.312e+8 1.6e+5 5.00e+8 1 9.8060

aa 37
1.e-5 1.e00 1.e-8 100.
112000.00 22.00 0.00 .9800

rpcap---1-----2-----3-----4-----5-----6-----7-----8
6 .100 .05 .01 3.
8 0.000 1.84 5.e+5 5.24

eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 74 1dirt1 1.4400e+0
bn 1 9 1bndr1 3.6000e-1

conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 16aa 17 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 31aa 32 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 46aa 47 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 61aa 62 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 1aa 16 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 16aa 31 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 31aa 46 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 46aa 61 14 1 1 1 .6000 .6000 1.2000e+0 1.0
bn 1aa 1 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 6aa 15 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 1bn 2 3 1 1 1 .6000 .6000 0.3000e+0 1.0
bn 6bn 7 3 1 1 1 .6000 .6000 0.3000e+0 1.0

incon---1-----2-----3-----4-----5-----6-----7-----8
bn 1 1 5 .40
101000.00 22.00 0.00 .1000
aa 1 29 1 .40
101000.00 22.00 0.00 .1000
bn 2 1 5 .40
101000.00 22.00 0.00 .1000
bn 3 1 5 .40
101000.00 22.00 0.00 .950
aa 31 14 1 .40
101000.00 22.00 0.00 .950

gener---1-----2-----3-----4-----5-----6-----7-----8
endcy

```

Figure 17. STMVOC input file for part 1 of problem 4.



elem	index	p (pa)	t (deg-c)	so	sw	sg	pvoc (pa)	pair (pa)	psato (pa)	psatw (pa)	pco (pa)	pcw (pa)	
aa	46	46	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	47	47	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	48	48	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	49	49	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	50	50	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	51	51	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	52	52	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	53	53	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	54	54	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	55	55	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	56	56	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	57	57	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	58	58	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	59	59	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	60	60	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
aa	61	61	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	62	62	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	63	63	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	64	64	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	65	65	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	66	66	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	67	67	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	68	68	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	69	69	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	70	70	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	71	71	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	72	72	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	73	73	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	74	74	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
aa	75	75	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
bn	1	76	102158.	22.000	0.0000E+00	0.1138E+00	0.8864E+00	0.	99514.	741.	2642.	0.	-24726.
bn	2	77	102170.	22.000	0.0000E+00	0.1931E+00	0.8069E+00	0.	99528.	741.	2642.	0.	-13020.
bn	3	78	102184.	22.000	0.0000E+00	0.8289E+00	0.1711E+00	0.	99542.	741.	2642.	0.	-1292.
bn	4	79	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
bn	5	80	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.
bn	6	81	102158.	22.000	0.0000E+00	0.1138E+00	0.8864E+00	0.	99514.	741.	2642.	0.	-24726.
bn	7	82	102170.	22.000	0.0000E+00	0.1931E+00	0.8069E+00	0.	99528.	741.	2642.	0.	-13020.
bn	8	83	102184.	22.000	0.0000E+00	0.8289E+00	0.1711E+00	0.	99542.	741.	2642.	0.	-1292.
bn	9	84	112911.	22.000	0.0000E+00	0.9866E+00	0.1337E-01	0.	110268.	741.	2642.	0.	-276.
bn	10	85	124641.	22.000	0.0000E+00	0.9876E+00	0.1236E-01	0.	121999.	741.	2642.	0.	-264.

Figure 18. Printed output for part 1 of problem 4 (continued).



		(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m*s)	(kg/m*s)	(m**2/s)	(m**2/s)				
aa 54	54	0.4357E-16	0.2379E-15	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 55	55	0.1176E-13	0.6422E-13	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 56	56	0.1314E-13	0.7174E-13	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 57	57	0.2175E-14	0.1188E-13	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 58	58	0.3202E-16	0.1749E-15	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 59	59	0.3847E-12	0.1991E-11	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 60	60	0.1686E-07	0.9208E-07	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
aa 61	61	0.1071E-13	0.5850E-13	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 62	62	0.3193E-12	0.1744E-11	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 63	63	0.1230E-14	0.6717E-14	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 64	64	0.3365E-12	0.1838E-11	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 65	65	0.1923E-17	0.1050E-16	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 66	66	0.0000E+00	0.0000E+00	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 67	67	0.5487E-14	0.2997E-13	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 68	68	0.5486E-12	0.2996E-11	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 69	69	0.2808E-18	0.1533E-17	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 70	70	0.9799E-15	0.5351E-14	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 71	71	0.2328E-13	0.1272E-12	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 72	72	0.1258E-15	0.6867E-15	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 73	73	0.1308E-18	0.7145E-18	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 74	74	0.7914E-16	0.4322E-14	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
aa 75	75	0.2298E-10	0.1255E-09	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
bn 1	76	0.1592E-15	0.8695E-15	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.9233E+00	0.3477E-05	0.0000E+00	0.0000E+00
bn 2	77	0.6011E-15	0.3283E-14	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.6941E+00	0.1108E-02	0.0000E+00	0.0000E+00
bn 3	78	0.0000E+00	0.0000E+00	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5733E-02	0.5313E+00	0.0000E+00	0.0000E+00
bn 4	79	0.4848E-10	0.2647E-09	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
bn 5	80	0.0000E+00	0.0000E+00	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00
bn 6	81	0.1749E-15	0.9554E-15	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.9233E+00	0.3477E-05	0.0000E+00	0.0000E+00
bn 7	82	0.8150E-15	0.4451E-14	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.6941E+00	0.1108E-02	0.0000E+00	0.0000E+00
bn 8	83	0.0000E+00	0.0000E+00	0.1194E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5733E-02	0.5313E+00	0.0000E+00	0.0000E+00
bn 9	84	0.0000E+00	0.0000E+00	0.1321E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.5247E-07	0.9561E+00	0.0000E+00	0.0000E+00
bn 10	85	0.0000E+00	0.0000E+00	0.1459E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.1806E-07	0.9594E+00	0.0000E+00	0.0000E+00

Figure 18. Printed output for part 1 of problem 4 (continued).

```

***** volume- and mass-balances *****
***** [kcyc,iter] = [ 13, 4] ***** the time is 0.63120E+09 seconds, or 0.73056E+04 days

phase volumes in place
gas 0.16874E+02 m**3; water 0.27766E+02 m**3; hydrocarbon 0.00000E+00 m**3

phase mass in place
gas 0.20191E+02 kg aqueous 0.27707E+05 kg liquid hydrocarbon 0.00000E+00 kg

air/water component mass in place
air 0.20103E+02 kg water vapor 0.32704E+00 kg liquid water 0.27707E+05 kg

hydrocarbon component mass in place
voc vapor 0.13377E-09 kg dissolved voc 0.53649E-07 kg liquid voc 0.00000E+00 kg total voc 0.53782E-07 kg

*****

write file *save* after 13 time steps --- the time is 0.63120E+09 seconds

end of tough simulation job --- elapsed time = 83.8900 sec
-- calculation time = 83.2910 sec-- data input time = 0.5990 sec

```

Figure 18. Printed output for part 1 of problem 4 (continued).



problem), the data in block CHEMP corresponds to o-xylene.

In the next part of the simulation, o-xylene is injected into the top center element (aa 8) at a rate of  $1.4667 \times 10^{-4} \text{ kg/s}$  for a period of  $4.8 \times 10^6 \text{ s}$  (55.6 days). This amounts to a total of 704 kg of o-xylene which is injected and allowed to drain down towards the water table. A deliverability boundary condition, which will be maintained for the remainder of the simulation, is used in the production elements. The input file used for this part of the problem is shown in Figure 19, and the STMVOC output after a total time of  $6.36 \times 10^8 \text{ s}$  is given in Figure 20. With respect to the earlier input file (Figure 17), several changes have been made to the input file used for this part of the problem (Figure 19). Data block INCON has been removed, and data block GENER has been changed to include the o-xylene injection in element aa 8, and the deliverability boundary condition in elements bn 6 through bn 10. In order to run this part of the problem, the SAVE file from the first part of the simulation must be renamed INCON.

In the next part of the simulation, the previously injected xylene is simply allowed to distribute itself over the water table. No additional fluids are injected or produced, except that the deliverability boundary condition is still maintained at the production end of the mesh. A listing of the input file is given in Figure 21, and this file is similar to the last input file (Figure 19) except that the o-xylene injection specified in block GENER has been removed. As before, in order to run this part of the simulation, the SAVE file from the previous part of the simulation must be renamed INCON. This part of the simulation is run for a period of  $3.156 \times 10^8 \text{ s}$  (10 years), and the STMVOC output at this time (a total time of  $9.516 \times 10^8 \text{ s}$ ) is shown in Figure 22. A contour plot of the separate phase xylene (NAPL) saturation distribution is shown in Figure 23.

In the final part of this simulation, steam with a specific enthalpy of  $2.676 \times 10^6 \text{ J/kg}$  (a quality of one) is injected in the injection boundary elements for a period of  $1.48 \times 10^7 \text{ s}$  (171.3 days). The total steam injection rate of  $7.4 \times 10^{-4} \text{ kg/s}$  is uniformly divided between the five injection elements. Again, at the production boundary, the deliverability boundary

```

cccc--- 2-d steamflood -- inject xylene -----ccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1 1 2650. .400 2.5000e-132.5000e-132.5000e-13 3.1 1000.0
0. 0. 2.85 0.0
bndr1 1 1200. .400 2.5000e-132.5000e-132.5000e-13 3.1 600.0
0. 0. 2.85 0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
630.3 37.3 0.282 0.310 0.5
417.6 -7.53357 1.40968 -3.10985 -2.85992
106.168 -1.5850e+01 5.962e-01 -3.443e-04 7.528e-08
880.0 293.0 8.000e-06273.0 1.60
-3.332e+0 1.039e+3 -1.768e-3 1.076e-6 369.
2.97500e-50. 0. 0.
0. 0.

start
param---1-----2-----3-----4-----5-----6-----7-----8
1 100 80100000000100010410000000 0.00e-5
8.360e+8 1.6e+5 8.0e+5 1 9.8060

aa 8
1.e-5 1.e00 1.e-8 100.
101000.00 22.00 0.00 .1000

rpcap---1-----2-----3-----4-----5-----6-----7-----8
8 .100 .05 .01 3.
8 0.000 1.84 5.e+04 5.240

eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 74 1dirt1 1.4400e+0
bn 1 9 1bndr1 3.6000e-1

conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 16aa 17 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 31aa 32 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 46aa 47 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 61aa 62 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 1aa 16 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 16aa 31 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 31aa 46 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 46aa 61 14 1 1 1 .6000 .6000 1.2000e+0 1.0
bn 1aa 1 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 6aa 15 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 1bn 2 3 1 1 1 .6000 .6000 0.3000e+0 1.0
bn 6bn 7 3 1 1 1 .6000 .6000 0.3000e+0 1.0

gener---1-----2-----3-----4-----5-----6-----7-----8
aa 8ino 1 oil 1.4667e-04 3.8000e+4
bn 10pro 5 5delv 2.0000e-12 1.0100e+5 1.2
bn 9pro 4 delv 2.0000e-12 1.0100e+5 1.2
bn 8pro 3 delv 2.0000e-12 1.0100e+5 1.2
bn 7pro 2 delv 2.0000e-12 1.0100e+5 1.2
bn 6pro 1 delv 2.0000e-12 1.0100e+5 1.2

endcy

```

Figure 19. STMVOC input file for part 2 of problem 4.











```

***** volume- and mass-balances *****
***** [kyc,iter] = [ 23, 3] ***** the time is 0.63600E+09 seconds, or 0.73611E+04 days

phase volumes in place
gas 0.16073E+02 m**3; water 0.27768E+02 m**3; hydrocarbon 0.80100E+00 m**3

phase mass in place
gas 0.19092E+02 kg aqueous 0.27708E+05 kg liquid hydrocarbon 0.70346E+03 kg

air/water component mass in place
air 0.18935E+02 kg water vapor 0.31141E+00 kg liquid water 0.27707E+05 kg

hydrocarbon component mass in place
voc vapor 0.84253E-01 kg dissolved voc 0.61699E+00 kg liquid voc 0.70346E+03 kg total voc 0.70416E+03 kg
*****

write file *save* after 23 time steps --- the time is 0.63600E+09 seconds

end of tough simulation job --- elapsed time = 82.1890 sec
-- calculation time = 81.5490 sec-- data input time = 0.6400 sec

```

Figure 20. Printed output for part 2 of problem 4 (continued).



```

cccc---2-d steamflood -- equilibration of xylene on water table -----ccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1  1      2650.      .400 2.5000e-132.5000e-132.5000e-13      3.1      1000.0
0.      0.      2.85      0.0
bndr1  1      1200.      .400 2.5000e-132.5000e-132.5000e-13      3.1      600.0
0.      0.      2.85      0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
630.3      37.3      0.262      0.310      0.5
417.6      -7.53357      1.40968      -3.10985      -2.65992
106.168      -1.5850e+01      5.962e-01      -3.443e-04      7.528e-08
880.0      293.0      8.000e-06273.0      1.60
-3.332e+0      1.039e+3      -1.768e-3      1.076e-6 369.
2.97500e-50.      0.      0.
0.      0.

start
param---1-----2-----3-----4-----5-----6-----7-----8
1 100      100100000000100010410000000 0.00e-5
9.516e+8      3.2e+6      1.6e+7      1      9.8060

aa 8
1.e-5      1.e00      1.e-8 100.
102200.00      22.00      0.00      .9700

rpcap---1-----2-----3-----4-----5-----6-----7-----8
6      .100      .05      .01      3.
8.      0.000      1.84      5.e+4      5.240

eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 74 1dirt1 1.4400e+0
bn 1 9 1bndr1 3.6000e-1

conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 16aa 17 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 31aa 32 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 46aa 47 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 61aa 62 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 1aa 16 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 16aa 31 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 31aa 46 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 46aa 61 14 1 1 1 .6000 .6000 1.2000e+0 1.0
bn 1aa 1 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 6aa 15 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 1bn 2 3 1 1 1 .6000 .6000 0.3000e+0 1.0
bn 6bn 7 3 1 1 1 .6000 .6000 0.3000e+0 1.0

gener---1-----2-----3-----4-----5-----6-----7-----8
bn 10pro 5 5delv 2.0000e-12 1.0100e+5 1.2
bn 9pro 4 delv 2.0000e-12 1.0100e+5 1.2
bn 8pro 3 delv 2.0000e-12 1.0100e+5 1.2
bn 7pro 2 delv 2.0000e-12 1.0100e+5 1.2
bn 6pro 1 delv 2.0000e-12 1.0100e+5 1.2

endcy

```

Figure 21. STMVOC input file for part 3 of problem 4.







		(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m*s)	(kg/m*s)	(m**2/s)	(m**2/s)			
aa 54	54	0.3206E-01	0.1751E+00	0.1336E+01	0.8782E+03	0.1792E-04	0.7868E-03	0.0000E+00	0.0000E+00	0.2385E-07	0.8285E+00	0.0000E+00
aa 55	55	0.1973E-02	0.1077E-01	0.1310E+01	0.0000E+00	0.1820E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2471E-07	0.9585E+00	0.0000E+00
aa 56	56	0.8474E-03	0.4628E-02	0.1309E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2403E-07	0.9586E+00	0.0000E+00
aa 57	57	0.5233E-03	0.2858E-02	0.1309E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2413E-07	0.9586E+00	0.0000E+00
aa 58	58	0.1284E-05	0.7015E-05	0.1308E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2421E-07	0.9586E+00	0.0000E+00
aa 59	59	0.1455E-08	0.7950E-08	0.1308E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2424E-07	0.9586E+00	0.0000E+00
aa 60	60	0.1565E-07	0.8548E-07	0.1308E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2425E-07	0.9586E+00	0.0000E+00
aa 61	61	0.4074E-12	0.2225E-11	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
aa 62	62	0.2762E-10	0.1508E-09	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
aa 63	63	0.5274E-08	0.2881E-07	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
aa 64	64	0.2006E-05	0.1096E-04	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8045E-08	0.9612E+00	0.0000E+00
aa 65	65	0.4176E-05	0.2281E-04	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8043E-08	0.9612E+00	0.0000E+00
aa 66	66	0.3310E-04	0.1808E-03	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8037E-08	0.9612E+00	0.0000E+00
aa 67	67	0.6700E-03	0.3660E-02	0.1447E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8045E-08	0.9612E+00	0.0000E+00
aa 68	68	0.2042E-02	0.1116E-01	0.1448E+01	0.0000E+00	0.1820E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8271E-08	0.9611E+00	0.0000E+00
aa 69	69	0.6915E-03	0.3777E-02	0.1447E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8479E-08	0.9611E+00	0.0000E+00
aa 70	70	0.3006E-04	0.1642E-03	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8271E-08	0.9611E+00	0.0000E+00
aa 71	71	0.4348E-05	0.2375E-04	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
aa 72	72	0.2006E-05	0.1096E-04	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8039E-08	0.9612E+00	0.0000E+00
aa 73	73	0.4747E-08	0.2593E-07	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8043E-08	0.9612E+00	0.0000E+00
aa 74	74	0.1830E-10	0.9993E-10	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
aa 75	75	0.2280E-09	0.1246E-08	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
bn 1	76	0.2026E-14	0.1107E-13	0.1180E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.9205E+00	0.4180E-05	0.0000E+00
bn 2	77	0.1696E-12	0.9264E-12	0.1180E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.6908E+00	0.1154E-02	0.0000E+00
bn 3	78	0.3176E-11	0.1735E-10	0.1181E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.4048E-02	0.5708E+00	0.0000E+00
bn 4	79	0.4569E-10	0.2496E-09	0.1308E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2424E-07	0.9586E+00	0.0000E+00
bn 5	80	0.5922E-12	0.3235E-11	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00
bn 6	81	0.6583E-06	0.3595E-05	0.1180E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.9205E+00	0.4205E-05	0.0000E+00
bn 7	82	0.3718E-08	0.2031E-07	0.1180E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.6908E+00	0.1154E-02	0.0000E+00
bn 8	83	0.4310E-10	0.2354E-09	0.1181E+01	0.0000E+00	0.1821E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.4047E-02	0.5708E+00	0.0000E+00
bn 9	84	0.3258E-09	0.1779E-08	0.1308E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.2426E-07	0.9586E+00	0.0000E+00
bn 10	85	0.4745E-11	0.2592E-10	0.1447E+01	0.0000E+00	0.1822E-04	0.1000E+01	0.0000E+00	0.0000E+00	0.8046E-08	0.9612E+00	0.0000E+00

Figure 22. Printed output for part 3 of problem 4 (continued).



\*\*\*\*\* volume- and mass-balances \*\*\*\*\*

\*\*\*\*\* [kyc,iter] = [ 47, 2] \*\*\*\*\*

the time is 0.95160E+09 seconds, or 0.11014E+05 days

phase volumes in place

gas 0.16073E+02 m\*\*3; water 0.27767E+02 m\*\*3; hydrocarbon 0.80037E+00 m\*\*3

phase mass in place

gas 0.19090E+02 kg aqueous 0.27708E+05 kg liquid hydrocarbon 0.70289E+03 kg

air/water component mass in place

air 0.18897E+02 kg water vapor 0.31145E+00 kg liquid water 0.27707E+05 kg

hydrocarbon component mass in place

voc vapor 0.10557E+00 kg dissolved voc 0.11654E+01 kg liquid voc 0.70289E+03 kg total voc 0.70416E+03 kg

\*\*\*\*\*

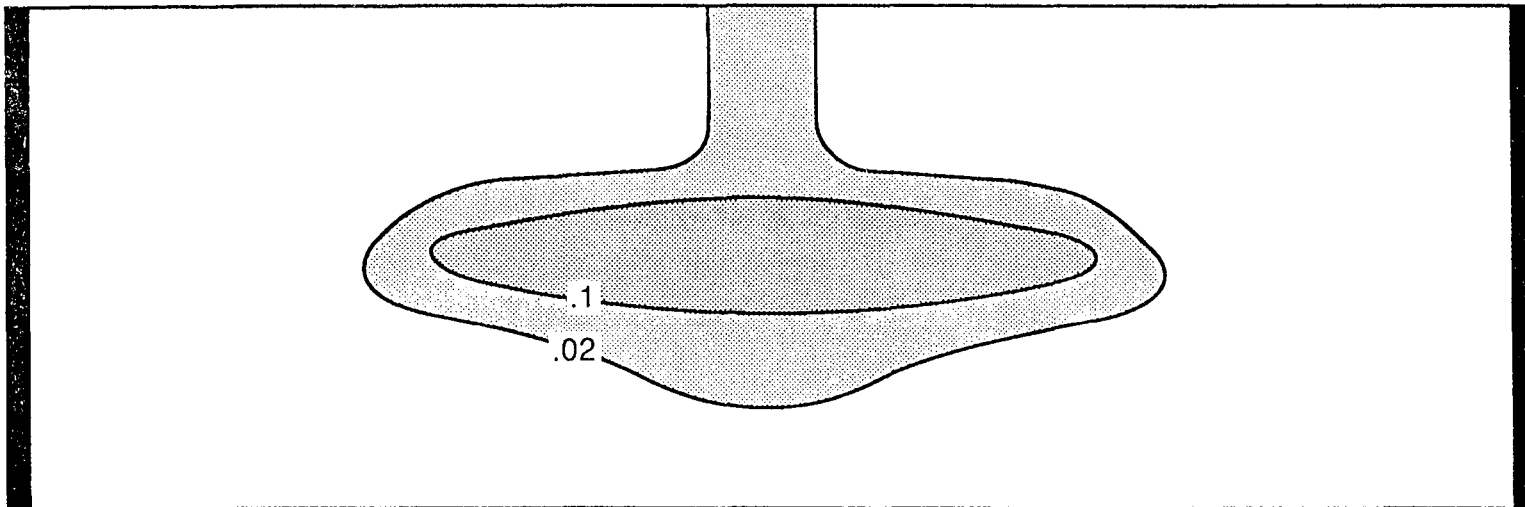
write file \*save\* after 47 time steps --- the time is 0.95160E+09 seconds

end of tough simulation job --- elapsed time = 157.8900 sec

-- calculation time = 157.2500 sec-- data input time = 0.6400 sec

Figure 22.

Printed output for part 3 of problem 4 (continued).



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lg/Mac

Figure 23. Separate phase xylene saturation distribution prior to steam injection.



condition is used. The input file for this part of the simulation is shown in Figure 24, and as before, the SAVE file from the previous part of the simulation must be renamed INCON. This input file is similar to the previous input file (Figure 21), except that data block GENER has been changed to include steam injection in the boundary elements bn 1 through bn 5. A printout after  $9.2 \times 10^6$  s (106.5 days) of steam injection is specified in data block TIMES (a total time of  $9.608 \times 10^8$  s), and this output is given in Figure 25. A contour plot of the xylene saturation distribution along with the steam front location at this time is shown in Figure 26. From this figure, it is evident that the steam is effectively sweeping the xylene from the system. By the end of the simulation, after  $1.48 \times 10^7$  s (171.3 days) of steam injection, all of the xylene has been removed, and the entire system is at the steam temperature. The STMVOC output at this time is given in Figure 27.

```

cccc--- 2-d steamflood -- steam injection-----ccc
rocks---1-----2-----3-----4-----5-----6-----7-----8
dirt1   1     2650.   .400 2.5000e-132.5000e-132.5000e-13   3.1   1000.0
0.      0.      2.85   0.0      0.0
bndr1   1     1200.   .400 2.5000e-132.5000e-132.5000e-13   3.1   600.0
0.      0.      2.85   0.0      0.0

chemp---1-----2-----3-----4-----5-----6-----7-----8
630.3   37.3      0.262   0.310   0.5
417.6   -7.53357  1.40968  -3.10985  -2.85992
106.168 -1.5850e+01  5.962e-01 -3.443e-04  7.528e-08
880.0   293.0      8.000e-06273.0   1.60
-3.332e+0  1.039e+3  -1.768e-3  1.076e-6 369.
2.97500e-50.      0.      0.
0.      0.

start
param---1-----2-----3-----4-----5-----6-----7-----8
1 300   4501000000000100010410000000 0.00e-5
9.664e+8 1.6e+5 1.6e+7 1 9.8060

aa 52
1.e-5 1.e00 .2 1.e-8 100.
102200.00 22.00 0.00 .9700

rpcap---1-----2-----3-----4-----5-----6-----7-----8
6      .100 .05 .01 3.
8      0.000 1.84 5.e+4 5.240

times---1-----2-----3-----4-----5-----6-----7-----8
1
9.608e+8

eleme---1-----2-----3-----4-----5-----6-----7-----8
aa 1 74 1dirt1 1.4400e+0
bn 1 9 1bndr1 3.6000e-1

conne---1-----2-----3-----4-----5-----6-----7-----8
aa 1aa 2 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 16aa 17 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 31aa 32 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 46aa 47 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 61aa 62 13 1 1 1 .6000 .6000 1.2000e+0 0.0
aa 1aa 16 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 16aa 31 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 31aa 46 14 1 1 1 .6000 .6000 1.2000e+0 1.0
aa 46aa 61 14 1 1 1 .6000 .6000 1.2000e+0 1.0
bn 1aa 1 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 6aa 15 4 1 15 1 .0200 .6000 1.2000e+0 0.0
bn 1bn 2 3 1 1 1 .6000 .6000 0.3000e+0 1.0
bn 6bn 7 3 1 1 1 .6000 .6000 0.3000e+0 1.0

gener---1-----2-----3-----4-----5-----6-----7-----8
bn 1inj 1 wate 1.480e-04 2.676e+06
bn 2inj 2 wate 1.480e-04 2.676e+06
bn 3inj 3 wate 1.480e-04 2.676e+06
bn 4inj 4 wate 1.480e-04 2.676e+06
bn 5inj 5 wate 1.480e-04 2.676e+06
bn 10pro 5 5delv 2.0000e-12 1.0100e+5 1.2
bn 9pro 4 delv 2.0000e-12 1.0100e+5 1.2
bn 8pro 3 delv 2.0000e-12 1.0100e+5 1.2
bn 7pro 2 delv 2.0000e-12 1.0100e+5 1.2
bn 6pro 1 delv 2.0000e-12 1.0100e+5 1.2

endcy

```

Figure 24.

STMVOC input file for part 4 of problem 4.



elem	index	p (pa)	t (deg-c)	so	sw	sg	pvoc (pa)	pair (pa)	psato (pa)	psatw (pa)	pco (pa)	pcw (pa)	
aa	46	48	243797.	126.605	0.0000E+00	0.1839E+00	0.8161E+00	0.	0.	61582.	243797.	-1.	-12982.
aa	47	47	235956.	125.536	0.0000E+00	0.1918E+00	0.8082E+00	0.	0.	59677.	235956.	-1.	-12349.
aa	48	48	227804.	124.394	0.0000E+00	0.1989E+00	0.8011E+00	0.	0.	57693.	227804.	-1.	-11820.
aa	49	49	219342.	123.173	0.0000E+00	0.2058E+00	0.7942E+00	0.	0.	55631.	219342.	-1.	-11350.
aa	50	50	210562.	121.865	0.0000E+00	0.2130E+00	0.7870E+00	0.	0.	53488.	210562.	-1.	-10891.
aa	51	51	201447.	120.459	0.0000E+00	0.2218E+00	0.7784E+00	0.	0.	51258.	201447.	-1.	-10387.
aa	52	52	191965.	118.940	0.0000E+00	0.2338E+00	0.7684E+00	0.	0.	48934.	191965.	-1.	-9740.
aa	53	53	182036.	117.282	0.0000E+00	0.2560E+00	0.7440E+00	0.	0.	46495.	182036.	-1.	-8702.
aa	54	54	171512.	114.672	0.0000E+00	0.3119E+00	0.6881E+00	4255.	0.	42853.	167257.	-1.	-6785.
aa	55	55	161460.	106.731	0.1958E+00	0.4085E+00	0.3977E+00	33165.	72.	33165.	128223.	0.	-4800.
aa	56	56	149263.	79.375	0.1825E+00	0.7428E+00	0.7469E-01	12330.	90759.	12330.	46174.	0.	-1736.
aa	57	57	145247.	57.839	0.5358E-02	0.9754E+00	0.1925E-01	4921.	122316.	4921.	18010.	0.	-384.
aa	58	58	143134.	43.980	0.0000E+00	0.9852E+00	0.1476E-01	2262.	131791.	2512.	9081.	0.	-290.
aa	59	59	140837.	34.826	0.0000E+00	0.9878E+00	0.1216E-01	1288.	134001.	1551.	5568.	0.	-261.
aa	60	60	138198.	29.803	0.0000E+00	0.9888E+00	0.1122E-01	865.	133139.	1172.	4194.	0.	-250.
aa	61	61	244465.	128.695	0.0000E+00	0.2158E+00	0.7842E+00	0.	0.	61744.	244465.	-1.	-10672.
aa	62	62	236525.	125.615	0.0000E+00	0.2373E+00	0.7627E+00	0.	0.	59815.	236525.	-1.	-9500.
aa	63	63	228317.	124.467	0.0000E+00	0.2560E+00	0.7440E+00	0.	0.	57818.	228317.	-1.	-8648.
aa	64	64	219837.	123.246	0.0000E+00	0.2734E+00	0.7268E+00	0.	0.	55752.	219837.	-1.	-7971.
aa	65	65	211083.	121.944	0.0000E+00	0.2905E+00	0.7095E+00	0.	0.	53615.	211083.	-1.	-7390.
aa	66	66	202069.	120.556	0.0000E+00	0.3089E+00	0.6911E+00	0.	0.	51410.	202069.	-1.	-6838.
aa	67	67	192829.	119.081	0.0000E+00	0.3327E+00	0.6673E+00	0.	0.	49146.	192829.	-1.	-6217.
aa	68	68	183375.	117.510	0.0000E+00	0.3780E+00	0.6220E+00	0.	0.	46824.	183375.	-1.	-5255.
aa	69	69	174532.	109.048	0.5705E-01	0.4337E+00	0.5093E+00	35787.	0.	35787.	138745.	0.	-4377.
aa	70	70	162272.	96.622	0.1025E+00	0.8182E+00	0.7928E-01	23481.	49090.	23481.	89701.	0.	-1301.
aa	71	71	158936.	74.350	0.7221E-03	0.9801E+00	0.1915E-01	10073.	111351.	10073.	37512.	0.	-337.
aa	72	72	157046.	56.609	0.0000E+00	0.9846E+00	0.1538E-01	3289.	138762.	4649.	16995.	0.	-295.
aa	73	73	154968.	43.232	0.0000E+00	0.9878E+00	0.1242E-01	1051.	145173.	2421.	8744.	0.	-263.
aa	74	74	152607.	34.467	0.0000E+00	0.9891E+00	0.1093E-01	384.	146785.	1521.	5458.	0.	-246.
aa	75	75	149927.	29.611	0.0000E+00	0.9895E+00	0.1047E-01	144.	145835.	1159.	4148.	0.	-240.
bn	1	76	246139.	126.918	0.0000E+00	0.1638E+00	0.8362E+00	0.	0.	62150.	246139.	-2.	-14940.
bn	2	77	246540.	126.972	0.0000E+00	0.1705E+00	0.8295E+00	0.	0.	62247.	246540.	-1.	-14239.
bn	3	78	247087.	127.045	0.0000E+00	0.1735E+00	0.8265E+00	0.	0.	62380.	247087.	-1.	-13932.
bn	4	79	247736.	127.131	0.0000E+00	0.1767E+00	0.8233E+00	0.	0.	62538.	247736.	-1.	-13630.
bn	5	80	248527.	127.236	0.0000E+00	0.1931E+00	0.8069E+00	0.	0.	62729.	248527.	-1.	-12225.
bn	6	81	102294.	30.592	0.0000E+00	0.8836E+00	0.1164E+00	1177.	98729.	1225.	4388.	0.	-988.
bn	7	82	113420.	30.605	0.0000E+00	0.9724E+00	0.2760E-01	1158.	107872.	1228.	4391.	0.	-415.
bn	8	83	125057.	29.759	0.0000E+00	0.9809E+00	0.1908E-01	1097.	119777.	1169.	4183.	0.	-336.
bn	9	84	136693.	29.321	0.0000E+00	0.9889E+00	0.1110E-01	819.	131795.	1140.	4079.	0.	-249.
bn	10	85	148410.	29.142	0.0000E+00	0.9898E+00	0.1042E-01	114.	144259.	1128.	4037.	0.	-240.

Figure 25. Printed output for part 4 of problem 4 after 106.5 days of steam injection

(continued).







\*\*\*\*\* volume- and mass-balances \*\*\*\*\*

\*\*\*\*\* [kyc, iter] = [ 148, 4] \*\*\*\*\*

the time is 0.98080E+09 seconds, or 0.11120E+05 days

phase volumes in place

gas 0.24204E+02 m\*\*3; water 0.19583E+02 m\*\*3; hydrocarbon 0.85319E+00 m\*\*3

phase mass in place

gas 0.28825E+02 kg aqueous 0.19033E+05 kg liquid hydrocarbon 0.69885E+03 kg

air/water component mass in place

air 0.84984E+00 kg water vapor 0.26113E+02 kg liquid water 0.19031E+05 kg

hydrocarbon component mass in place

voc vapor 0.20059E+01 kg dissolved voc 0.20144E+01 kg liquid voc 0.69885E+03 kg total voc 0.70287E+03 kg

\*\*\*\*\*

```

no convergence at [ 147, 1] --- deltex = 0.12000E+08 max. res. = 0.16883E+01 at element aa 40* equation 3
000000 oil phase disappears at element aa 40**** sw = 0.28740E+00 %%%%%%%%% sg = 0.73803E+00
no convergence at [ 147, 2] --- deltex = 0.12000E+08 max. res. = 0.39878E+00 at element aa 41* equation 1
no convergence at [ 147, 3] --- deltex = 0.12000E+08 max. res. = 0.20509E+00 at element aa 40* equation 3
no convergence at [ 147, 4] --- deltex = 0.12000E+08 max. res. = 0.25740E-01 at element aa 25* equation 3
no convergence at [ 147, 5] --- deltex = 0.12000E+08 max. res. = 0.31805E-03 at element aa 25* equation 3
***** kyc = 147 iter = 6 st = 0.96092E+09 dt = 0.12000E+08 *****
aa 52 p = 193244. t = 119.15 so = 0.0000E+00 sg = 0.7684E+00 pcw = -9847. pco = -1. cg = 0.8200E-16 cw = 0.8468E-17
no convergence at [ 148, 1] --- deltex = 0.12000E+08 max. res. = 0.79683E+01 at element aa 40* equation 3
000000 oil phase disappears at element aa 26**** sw = 0.28718E+00 %%%%%%%%% sg = 0.74854E+00
no convergence at [ 148, 2] --- deltex = 0.12000E+08 max. res. = 0.10953E+01 at element aa 26* equation 3
no convergence at [ 148, 3] --- deltex = 0.12000E+08 max. res. = 0.58215E+00 at element aa 40* equation 3
no convergence at [ 148, 4] --- deltex = 0.12000E+08 max. res. = 0.17562E-01 at element aa 40* equation 3
***** kyc = 148 iter = 5 st = 0.98104E+09 dt = 0.12000E+08 *****
aa 52 p = 194179. t = 119.30 so = 0.0000E+00 sg = 0.7705E+00 pcw = -9958. pco = -1. cg = 0.0000E+00 cw = 0.0000E+00
no convergence at [ 149, 1] --- deltex = 0.12000E+08 max. res. = 0.57188E+01 at element aa 26* equation 3
000000 oil phase disappears at element aa 12**** sw = 0.29316E+00 %%%%%%%%% sg = 0.74773E+00
$$$$$$ hydrocarbon phase evolves at elementaa 15***** pvo = 0.16471E+04 %%%%%%%%% psato = 0.16376E+04
000000 oil phase disappears at element aa 89**** sw = 0.39552E+00 %%%%%%%%% sg = 0.62827E+00
no convergence at [ 149, 2] --- deltex = 0.12000E+08 max. res. = 0.27299E+01 at element aa 12* equation 3
$$$$$$ hydrocarbon phase evolves at elementaa 29***** pvo = 0.49587E+04 %%%%%%%%% psato = 0.28856E+04
$$$$$$ hydrocarbon phase evolves at elementaa 30***** pvo = 0.17094E+04 %%%%%%%%% psato = 0.15797E+04
$$$$$$ hydrocarbon phase evolves at elementaa 44***** pvo = 0.23690E+04 %%%%%%%%% psato = 0.21159E+04
$$$$$$ hydrocarbon phase evolves at elementaa 58***** pvo = 0.40758E+04 %%%%%%%%% psato = 0.34348E+04
$$$$$$ hydrocarbon phase evolves at elementbn 7***** pvo = 0.15044E+04 %%%%%%%%% psato = 0.14988E+04
no convergence at [ 149, 3] --- deltex = 0.12000E+08 max. res. = 0.29574E+00 at element aa 89* equation 3
000000 oil phase disappears at element aa 30**** sw = 0.96980E+00 %%%%%%%%% sg = 0.30208E-01
000000 oil phase disappears at element bn 7**** sw = 0.97242E+00 %%%%%%%%% sg = 0.27593E-01
no convergence at [ 149, 4] --- deltex = 0.12000E+08 max. res. = 0.16743E-01 at element aa 89* equation 3
no convergence at [ 149, 5] --- deltex = 0.12000E+08 max. res. = 0.37463E-04 at element aa 89* equation 3
***** kyc = 149 iter = 6 st = 0.98110E+09 dt = 0.12000E+08 *****
aa 52 p = 194739. t = 119.39 so = 0.0000E+00 sg = 0.7727E+00 pcw = -10076. pco = -1. cg = 0.4141E-17 cw = 0.4247E-18
no convergence at [ 150, 1] --- deltex = 0.12000E+08 max. res. = 0.36913E+01 at element aa 12* equation 3
no convergence at [ 150, 2] --- deltex = 0.12000E+08 max. res. = 0.20822E+01 at element aa 12* equation 3
no convergence at [ 150, 3] --- deltex = 0.12000E+08 max. res. = 0.11288E+00 at element aa 12* equation 3
no convergence at [ 150, 4] --- deltex = 0.12000E+08 max. res. = 0.10342E-02 at element aa 12* equation 3
***** kyc = 150 iter = 5 st = 0.98128E+09 dt = 0.12000E+08 *****
aa 52 p = 195711. t = 119.55 so = 0.0000E+00 sg = 0.7746E+00 pcw = -10177. pco = -1. cg = 0.2724E-15 cw = 0.2781E-16
no convergence at [ 151, 1] --- deltex = 0.12000E+08 max. res. = 0.11492E+01 at element aa 55* equation 3
000000 oil phase disappears at element aa 55**** sw = 0.30513E+00 %%%%%%%%% sg = 0.70875E+00

```

110

Figure 25. Printed output for part 4 of problem 4 after 106.5 days of steam injection (continued).



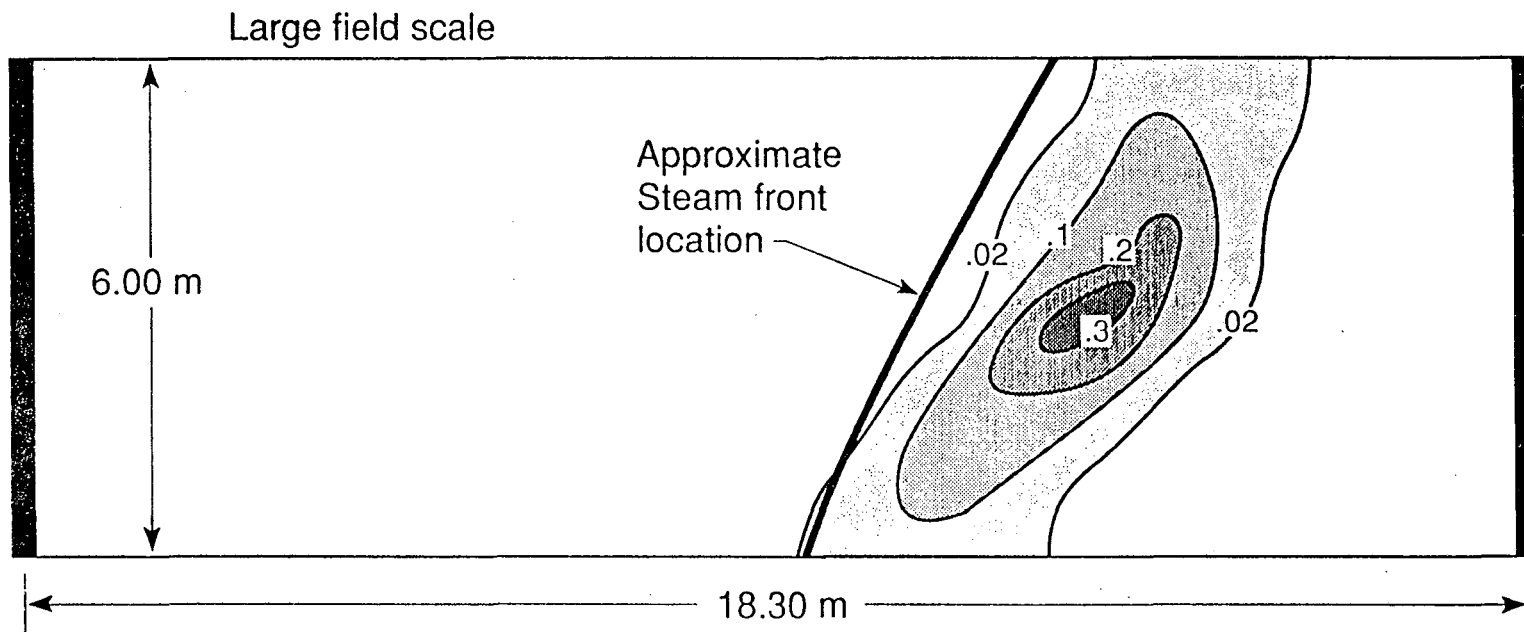


Figure 26. Separate phase xylene saturation distribution and steam front location after 106.5 days of steam injection.



elem	index	p	t	so	sw	sg	pvoc	pair	psato	psatw	pco	pcw	
		(pa)	(deg-c)				(pa)	(pa)	(pa)	(pa)	(pa)	(pa)	
aa	46	46	256767.	128.312	0.0000E+00	0.1736E+00	0.8284E+00	0.	0.	64726.	256767.	-1.	-13914.
aa	47	47	249412.	127.353	0.0000E+00	0.1750E+00	0.8250E+00	0.	0.	82944.	249412.	-1.	-13783.
aa	48	48	241837.	126.340	0.0000E+00	0.1771E+00	0.8229E+00	0.	0.	61106.	241837.	-1.	-13597.
aa	49	49	234003.	125.286	0.0000E+00	0.1795E+00	0.8205E+00	0.	0.	59202.	234003.	-1.	-13392.
aa	50	50	225868.	124.118	0.0000E+00	0.1819E+00	0.8181E+00	0.	0.	57222.	225868.	-1.	-13186.
aa	51	51	217389.	122.866	0.0000E+00	0.1844E+00	0.8156E+00	0.	0.	55155.	217389.	-1.	-12986.
aa	52	52	208526.	121.555	0.0000E+00	0.1869E+00	0.8131E+00	0.	0.	52990.	208526.	-1.	-12793.
aa	53	53	199232.	120.109	0.0000E+00	0.1893E+00	0.8107E+00	0.	0.	50715.	199232.	-1.	-12604.
aa	54	54	189451.	118.527	0.0000E+00	0.1919E+00	0.8081E+00	0.	0.	48317.	189451.	-1.	-12414.
aa	55	55	179116.	116.780	0.0000E+00	0.1947E+00	0.8053E+00	0.	0.	45776.	179116.	-1.	-12218.
aa	56	56	168141.	114.833	0.0000E+00	0.1977E+00	0.8023E+00	0.	0.	43071.	168141.	-1.	-12006.
aa	57	57	156415.	112.634	0.0000E+00	0.2012E+00	0.7988E+00	0.	0.	40173.	156415.	-1.	-11771.
aa	58	58	143792.	110.109	0.0000E+00	0.2056E+00	0.7945E+00	0.	0.	37042.	143792.	-1.	-11497.
aa	59	59	130069.	107.149	0.0000E+00	0.2117E+00	0.7883E+00	0.	0.	33625.	130069.	-1.	-11109.
aa	60	60	114911.	103.563	0.0000E+00	0.2330E+00	0.7670E+00	0.	0.	29834.	114911.	-1.	-9897.
aa	61	61	257343.	128.366	0.0000E+00	0.2043E+00	0.7957E+00	0.	0.	64866.	257343.	-1.	-11400.
aa	62	62	249880.	127.415	0.0000E+00	0.2183E+00	0.7817E+00	0.	0.	63058.	249880.	-1.	-10513.
aa	63	63	242227.	126.393	0.0000E+00	0.2301E+00	0.7699E+00	0.	0.	61200.	242227.	-1.	-9860.
aa	64	64	234336.	125.312	0.0000E+00	0.2404E+00	0.7596E+00	0.	0.	59283.	234336.	-1.	-9348.
aa	65	65	226162.	124.160	0.0000E+00	0.2498E+00	0.7504E+00	0.	0.	57293.	226162.	-1.	-8931.
aa	66	66	217656.	122.926	0.0000E+00	0.2578E+00	0.7422E+00	0.	0.	55220.	217656.	-1.	-8584.
aa	67	67	208774.	121.593	0.0000E+00	0.2653E+00	0.7347E+00	0.	0.	53051.	208774.	-1.	-8290.
aa	68	68	199466.	120.146	0.0000E+00	0.2721E+00	0.7279E+00	0.	0.	50773.	199466.	-1.	-8039.
aa	69	69	189674.	118.564	0.0000E+00	0.2784E+00	0.7218E+00	0.	0.	48371.	189674.	-1.	-7823.
aa	70	70	179330.	116.817	0.0000E+00	0.2840E+00	0.7160E+00	0.	0.	45829.	179330.	-1.	-7636.
aa	71	71	168351.	114.871	0.0000E+00	0.2893E+00	0.7107E+00	0.	0.	43123.	168351.	-1.	-7473.
aa	72	72	156629.	112.675	0.0000E+00	0.2942E+00	0.7058E+00	0.	0.	40226.	156629.	-1.	-7328.
aa	73	73	144028.	110.158	0.0000E+00	0.2989E+00	0.7011E+00	0.	0.	37101.	144028.	-1.	-7193.
aa	74	74	130359.	107.214	0.0000E+00	0.3050E+00	0.6950E+00	0.	0.	33698.	130359.	-1.	-7026.
aa	75	75	115299.	103.660	0.0000E+00	0.3254E+00	0.6746E+00	0.	0.	29931.	115299.	-1.	-6480.
bn	1	78	259148.	128.618	0.0000E+00	0.1810E+00	0.8390E+00	0.	0.	65303.	259148.	-2.	-15242.
bn	2	77	259485.	128.661	0.0000E+00	0.1871E+00	0.8329E+00	0.	0.	65385.	259485.	-2.	-14570.
bn	3	78	259945.	128.720	0.0000E+00	0.1699E+00	0.8301E+00	0.	0.	65496.	259945.	-1.	-14269.
bn	4	79	260501.	128.791	0.0000E+00	0.1730E+00	0.8270E+00	0.	0.	65630.	260501.	-1.	-13961.
bn	5	80	261194.	128.879	0.0000E+00	0.1891E+00	0.8109E+00	0.	0.	65798.	261194.	-1.	-12528.
bn	6	81	103986.	100.728	0.0000E+00	0.2125E+00	0.7875E+00	0.	0.	27088.	103986.	-1.	-11116.
bn	7	82	104434.	100.849	0.0000E+00	0.2660E+00	0.7340E+00	0.	0.	27201.	104434.	-1.	-8404.
bn	8	83	104985.	100.997	0.0000E+00	0.3136E+00	0.6864E+00	0.	0.	27340.	104985.	-1.	-6811.
bn	9	84	105639.	101.172	0.0000E+00	0.3658E+00	0.6342E+00	0.	0.	27504.	105639.	-1.	-5564.
bn	10	85	106047.	101.281	0.0000E+00	0.4494E+00	0.5506E+00	0.	0.	27607.	106047.	0.	-4185.

Figure 27. Printed output at the end of part 4 of problem 4 (continued).



	(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m**3)	(kg/m**3)	(m**2/s)	(m**2/s)	(m**2/s)	
aa 54	0.0000E+00	0.0000E+00	0.1047E+01	0.0000E+00	0.1274E-04	0.1000E+01	0.0000E+00	0.6973E+00	0.1065E-02	0.0000E+00
aa 55	0.0000E+00	0.0000E+00	0.9945E+00	0.0000E+00	0.1268E-04	0.1000E+01	0.0000E+00	0.6901E+00	0.1164E-02	0.0000E+00
aa 56	0.2018E-13	0.2363E-14	0.9383E+00	0.0000E+00	0.1266E-04	0.1000E+01	0.0000E+00	0.6822E+00	0.1280E-02	0.0000E+00
aa 57	0.1850E-13	0.2316E-14	0.8778E+00	0.0000E+00	0.1252E-04	0.1000E+01	0.0000E+00	0.6731E+00	0.1423E-02	0.0000E+00
aa 58	0.1679E-13	0.2270E-14	0.8123E+00	0.0000E+00	0.1242E-04	0.1000E+01	0.0000E+00	0.6623E+00	0.1610E-02	0.0000E+00
aa 59	0.7268E-12	0.1075E-12	0.7406E+00	0.0000E+00	0.1231E-04	0.1000E+01	0.0000E+00	0.6467E+00	0.1912E-02	0.0000E+00
aa 60	0.1118E-09	0.1954E-10	0.6604E+00	0.0000E+00	0.1217E-04	0.1000E+01	0.0000E+00	0.5951E+00	0.3226E-02	0.0000E+00
aa 61	0.1425E-17	0.1134E-18	0.1388E+01	0.0000E+00	0.1311E-04	0.1000E+01	0.0000E+00	0.8663E+00	0.1657E-02	0.0000E+00
aa 62	0.0000E+00	0.0000E+00	0.1351E+01	0.0000E+00	0.1308E-04	0.1000E+01	0.0000E+00	0.6303E+00	0.2274E-02	0.0000E+00
aa 63	0.0000E+00	0.0000E+00	0.1313E+01	0.0000E+00	0.1304E-04	0.1000E+01	0.0000E+00	0.6018E+00	0.3023E-02	0.0000E+00
aa 64	0.8630E-14	0.7394E-15	0.1273E+01	0.0000E+00	0.1300E-04	0.1000E+01	0.0000E+00	0.5777E+00	0.3798E-02	0.0000E+00
aa 65	0.8110E-14	0.7260E-15	0.1232E+01	0.0000E+00	0.1295E-04	0.1000E+01	0.0000E+00	0.5588E+00	0.4591E-02	0.0000E+00
aa 66	0.7648E-14	0.7089E-15	0.1190E+01	0.0000E+00	0.1291E-04	0.1000E+01	0.0000E+00	0.5384E+00	0.5394E-02	0.0000E+00
aa 67	0.7228E-14	0.6956E-15	0.1145E+01	0.0000E+00	0.1286E-04	0.1000E+01	0.0000E+00	0.5221E+00	0.6198E-02	0.0000E+00
aa 68	0.7408E-14	0.7434E-15	0.1098E+01	0.0000E+00	0.1280E-04	0.1000E+01	0.0000E+00	0.5075E+00	0.6998E-02	0.0000E+00
aa 69	0.6942E-14	0.7292E-15	0.1048E+01	0.0000E+00	0.1274E-04	0.1000E+01	0.0000E+00	0.4944E+00	0.7782E-02	0.0000E+00
aa 70	0.6265E-14	0.6925E-15	0.9956E+00	0.0000E+00	0.1268E-04	0.1000E+01	0.0000E+00	0.4826E+00	0.8551E-02	0.0000E+00
aa 71	0.5793E-14	0.6783E-15	0.9393E+00	0.0000E+00	0.1260E-04	0.1000E+01	0.0000E+00	0.4720E+00	0.9302E-02	0.0000E+00
aa 72	0.7827E-14	0.9786E-15	0.8789E+00	0.0000E+00	0.1252E-04	0.1000E+01	0.0000E+00	0.4622E+00	0.1004E-01	0.0000E+00
aa 73	0.7117E-14	0.9605E-15	0.8135E+00	0.0000E+00	0.1243E-04	0.1000E+01	0.0000E+00	0.4527E+00	0.1080E-01	0.0000E+00
aa 74	0.2559E-10	0.3781E-11	0.7420E+00	0.0000E+00	0.1231E-04	0.1000E+01	0.0000E+00	0.4409E+00	0.1182E-01	0.0000E+00
aa 75	0.4221E-08	0.6977E-09	0.6625E+00	0.0000E+00	0.1218E-04	0.1000E+01	0.0000E+00	0.4026E+00	0.1571E-01	0.0000E+00
bn 1	0.0000E+00	0.0000E+00	0.1396E+01	0.0000E+00	0.1312E-04	0.1000E+01	0.0000E+00	0.7818E+00	0.3108E-03	0.0000E+00
bn 2	0.0000E+00	0.0000E+00	0.1398E+01	0.0000E+00	0.1312E-04	0.1000E+01	0.0000E+00	0.7845E+00	0.4138E-03	0.0000E+00
bn 3	0.1267E-14	0.9993E-16	0.1400E+01	0.0000E+00	0.1313E-04	0.1000E+01	0.0000E+00	0.7686E+00	0.4894E-03	0.0000E+00
bn 4	0.3568E-20	0.2909E-21	0.1403E+01	0.0000E+00	0.1313E-04	0.1000E+01	0.0000E+00	0.7480E+00	0.5338E-03	0.0000E+00
bn 5	0.2102E-18	0.1651E-19	0.1407E+01	0.0000E+00	0.1313E-04	0.1000E+01	0.0000E+00	0.7047E+00	0.9698E-03	0.0000E+00
bn 6	0.0000E+00	0.0000E+00	0.6022E+00	0.0000E+00	0.1206E-04	0.1000E+01	0.0000E+00	0.6448E+00	0.1951E-02	0.0000E+00
bn 7	0.1716E-12	0.3104E-13	0.6046E+00	0.0000E+00	0.1207E-04	0.1000E+01	0.0000E+00	0.5208E+00	0.6275E-02	0.0000E+00
bn 8	0.4608E-11	0.8296E-12	0.6075E+00	0.0000E+00	0.1207E-04	0.1000E+01	0.0000E+00	0.4246E+00	0.1337E-01	0.0000E+00
bn 9	0.1144E-09	0.2949E-10	0.6110E+00	0.0000E+00	0.1208E-04	0.1000E+01	0.0000E+00	0.3338E+00	0.2577E-01	0.0000E+00
bn 10	0.4503E-08	0.8033E-09	0.6132E+00	0.0000E+00	0.1208E-04	0.1000E+01	0.0000E+00	0.2168E+00	0.5849E-01	0.0000E+00

Figure 27. Printed output at the end of part 4 of problem 4 (continued).



```

***** volume- and mass-balances *****
***** [kcyrc,iter] = [ 202, 3] ***** the time is 0.96840E+09 seconds, or 0.11185E+05 days

phase volumes in place
gas 0.38058E+02 m**3; water 0.85843E+01 m**3; hydrocarbon 0.00000E+00 m**3

phase mass in place
gas 0.38840E+02 kg aqueous 0.81081E+04 kg liquid hydrocarbon 0.00000E+00 kg

air/water component mass in place
air -0.38402E-10 kg water vapor 0.38840E+02 kg liquid water 0.81081E+04 kg

hydrocarbon component mass in place
voc vapor 0.20704E-08 kg dissolved voc 0.18714E-09 kg liquid voc 0.00000E+00 kg total voc 0.22575E-08 kg

*****

write file *save* after 202 time steps --- the time is 0.96840E+09 seconds

end of tough simulation job --- elapsed time = 1951.8301 sec
-- calculation time = 1951.1801 sec-- data input time = 0.6500 sec

```

Figure 27. Printed output at the end of part 4 of problem 4 (continued).

## APPENDIX 1: Relative Permeability Functions

Several relative permeability functions have been added for problems involving NAPL flow. Unless it is otherwise stated, the original TOUGH two phase functions have been retained. If one of the TOUGH two phase functions is chosen, the NAPL relative permeability will be assumed to be equal to zero. The notation used below is:  $k_{rw}$  - aqueous phase relative permeability;  $k_{rg}$  - gas phase relative permeability;  $k_{rn}$  - NAPL relative permeability.

IRP = 5      "All perfectly mobile"

$$k_{rw} = 1$$

$$k_{rg} = 1$$

$$k_{rn} = 1$$

no parameters.

IRP = 6      Stone's first three phase method (Stone [1970])

$$k_{rw} = [(S_w - S_{wr})/(1 - S_{wr})]^n$$

$$k_{rg} = [(S_g - S_{gr})/(1 - S_{wr})]^n$$

$$k_{rncw} = (1 - S_{wr})^n$$

$$k_{rnw} = (1 - S_w)^n$$

$$k_{rng} = (1 - S_g - S_{wr})^n$$

$$S_w^* = (S_w - S_{wr})/(1 - S_{wr} - S_{nr})$$

$$\beta_w = k_{rnw}/(k_{rncw}(1 - S_w^*))$$

$$S_g^* = S_g/(1 - S_{wr} - S_{nr})$$

$$\beta_g = k_{rng}/(k_{rncw}(1 - S_g^*))$$



$$S_n^* = (S_n - S_{nr}) / (1 - S_{wr} - S_{nr})$$

$$k_{rn} = k_{rncw} S_n^* \beta_w \beta_g$$

where  $S_{wr}$ =RP(1);  $S_{nr}$ =RP(2);  $S_{gr}$ =RP(3);  $n$ =RP(4). The value of RP(4) is rounded off to the nearest integer value.

IRP = 9      three phase functions of Parker et al. [1987]

$$m = 1 - 1/n$$

$$\bar{S}_g = S_g / (1 - S_m)$$

$$\bar{S}_w = (S_w - S_m) / (1 - S_m)$$

$$\bar{S}_i = (S_w + S_n - S_m) / (1 - S_m)$$

$$k_{rg} = (\bar{S}_g)^{-5} [1 - (\bar{S}_i)^{1/m}]^{2m}$$

$$k_{rw} = (\bar{S}_w)^{-5} [1 - (1 - (\bar{S}_w)^{1/m})^m]^2$$

$$k_{rn} = (\bar{S}_i - \bar{S}_w)^{-5} [(1 - (\bar{S}_w)^{1/m})^m - (1 - (\bar{S}_i)^{1/m})^m]^2$$

where  $k_{rw}$ ,  $k_{rg}$ , and  $k_{rn}$  are limited to values between 0 and 1, with  $S_m$ =RP(1), and  $n$ =RP(2).

IRP = 10      same as IRP = 6 except that

$$k_{rg} = 1 - \left[ \frac{S_n + S_w - S_{wr}}{1 - S_{wr}} \right]^n$$

IRP = 11      functions used by Faust [1985] for two phase Buckley-Leverett problem

$$k_{rw} = (S_w - 0.16)^2 / 0.64$$

$$k_{rg} = 0$$

$$k_{rn} = (0.8 - S_w)^2 / 0.64$$

where  $k_{rw}$  and  $k_{rn}$  are limited to values between 0 and 1, no parameters.

## APPENDIX 2: Capillary Pressure Functions

A three phase capillary pressure function has been included in STMVOC. The original TOUGH two phase functions have been retained, and if one of the TOUGH two phase functions is chosen, the gas-NAPL capillary pressure will be assumed to be equal to zero. The notation used below is:  $P_{cgn}$  = gas-NAPL capillary pressure;  $P_{cgw}$  = gas-water capillary pressure. It should be noted that the pressure between the NAPL and the aqueous phases,  $P_{cnw} = P_{cgw} - P_{cgn}$ .

IRP = 8      three phase capillary functions from Parker et al. [1987]

$$m = 1 - 1/n$$

$$\bar{S}_w = (S_w - S_m)/(1 - S_m)$$

$$\bar{S}_t = (S_w + S_n - S_m)/(1 - S_m)$$

$$P_{cgn} = -\frac{\rho_w g}{\alpha_{gn}} [(\bar{S}_t)^{-1/m} - 1]^{1/n}$$

$$P_{cgw} = -\frac{\rho_w g}{\alpha_{nw}} [(\bar{S}_w)^{-1/m} - 1]^{1/n} - \frac{\rho_w g}{\alpha_{gn}} [(\bar{S}_t)^{-1/m} - 1]^{1/n}$$

where  $S_m = \text{CP}(1)$ ;  $n = \text{CP}(2)$ ;  $\alpha_{gn} = \text{CP}(3)$ ;  $\alpha_{nw} = \text{CP}(4)$ . These functions have been modified so that at low aqueous saturations, the capillary pressures remain finite. This is done by calculating the slope of the capillary pressure functions at  $\bar{S}_w$  and  $\bar{S}_t = 0.1$ . If  $\bar{S}_w$  or  $\bar{S}_t$  is less than 0.1, the capillary pressures are calculated as linear functions in this region with slopes equal to those calculated at scaled saturations of 0.1.

IRP = 9      zero capillary pressures

$$P_{cgn} = 0$$

$$P_{cgw} = 0$$

no parameters.

## NOTATION

- $C_R$  soil grain heat capacity,  $J/kg\ K$ .
- $C_s^c$  concentration of chemical in the solid phase,  $kg/m^3$ .
- $C_\beta^K$  concentration of mass component  $K$  in phase  $\beta$ ,  $kg/m^3$ .
- $D_g^K$  molecular diffusivity of mass component  $K$  in a multicomponent gas,  $m^2/s$ .
- $F^K$  total flux of component  $K$ ; for  $K \neq h$ :  $kg/m^2s$ ; for  $K = h$ :  $J/m^2s$ .
- $F_\beta$  total mass flux in the  $\beta$  phase,  $kg/m^2s$ .
- $F_\beta^K$  flux of component  $K$  in the  $\beta$  phase; for  $K \neq h$ :  $kg/m^2s$ ; for  $K = h$ :  $J/m^2s$ .
- $f_{oc}$  fraction of organic carbon in the soil.
- $g$  magnitude of gravitational acceleration,  $m/s^2$ .
- $\mathbf{g}$  gravitational acceleration vector,  $m/s^2$ .
- $h$  specific enthalpy,  $J/kg$ .
- $h_\beta$  specific enthalpy of phase  $\beta$ ,  $J/kg$ .
- $h_g^K$  specific enthalpy of mass component  $K$  in the gas phase,  $J/kg$ .
- $H$  Dimensionless Henry's constant,  $H = C_g^c/C_w^c$ .
- $H_{gw}^K$  Henry's constant for gas-water partitioning of mass component  $K$ ,  $Pa$ .
- $J_g^K$  diffusive mass flux of component  $K$  in the gas phase,  $kg/m^2s$ .
- $K$  component index,  $K = a$ : air;  $w$ : water;  $c$ : chemical;  $h$ : heat.
- $K_D$  chemical-solid distribution coefficient,  $m^3/kg$ .
- $K_{oc}$  chemical-organic carbon partition coefficient,  $m^3/kg$ .
- $k$  porous medium permeability,  $m^2$ .
- $k_{r\beta}$  relative permeability of the  $\beta$  phase.

- $k_{rncw}$  NAPL relative permeability in the presence of an irreducible water saturation.
- $k_{rnw}$  NAPL relative permeability in a two phase NAPL-water system.
- $k_{rng}$  NAPL relative permeability in a two phase NAPL-gas system.
- $m$  exponent used in the calculation of relative permeabilities and capillary pressures.
- $M^K$  amount of component  $K$  per unit porous medium volume; for  $K \neq h$ :  $kg/m^3$ ; for  $K=h$ :  $J/m^3$ .
- $n$  exponent used in the calculation of relative permeabilities and capillary pressures.
- $\mathbf{n}$  outward unit normal vector.
- $P$  pressure,  $Pa$ .
- $P_\beta$  pressure in the  $\beta$  phase,  $Pa$ .
- $P_{cgw}$  gas-water capillary pressure,  $Pa$ .
- $P_{cgn}$  gas-NAPL capillary pressure,  $Pa$ .
- $P_{cnw}$  NAPL-water capillary pressure,  $Pa$ .
- $P_{wb}$  wellbore pressure,  $Pa$ .
- $P_{sat}^c$  saturated NAPL vapor pressure,  $Pa$ .
- $PI$  productivity index,  $m^3$ .
- $q^K$  rate of generation of component  $K$  per unit volume; for  $K \neq h$ :  $kg/m^3s$ ; for  $K=h$ :  $J/m^3s$ .
- $q_\beta$  mass rate of generation of phase  $\beta$  in a source element,  $kg/s$ .
- $\hat{q}^K$  rate of generation of component  $K$  in a source element; for  $K \neq h$ :  $kg/s$ ; for  $K=h$ :  $J/s$ .
- $R_g$  chemical gas phase retardation coefficient.
- $S_\beta$   $\beta$  phase saturation.
- $S_{\beta r}$  residual  $\beta$  phase saturation.

- $S_m$  empirical constant used in the calculation of capillary pressures.
- $S_\beta^*$  scaled  $\beta$  phase saturation defined in Appendix 1.
- $\bar{S}_\beta$  scaled  $\beta$  phase saturation defined in Appendix 1.
- $T$  temperature,  $K$ .
- $u$  specific internal energy,  $J/kg$ .
- $u_\beta$  specific internal energy of the  $\beta$  phase,  $J/kg$ .
- $u_g^K$  specific internal energy of mass component  $K$  in the gas phase,  $J/kg$ .
- $V_l$  volume of region  $l$  of porous medium,  $m^3$ .
- $\alpha_{gn}$  constant used in the calculation of the gas-NAPL capillary pressure,  $1/m$ .
- $\alpha_{gw}$  constant used in the calculation of the gas-water capillary pressure,  $1/m$ .
- $\alpha_{nw}$  constant used in the calculation of the NAPL-water capillary pressure,  $1/m$ .
- $\beta$  phase index,  $\beta = g$ : gas phase;  $w$ : water phase;  $n$ : NAPL.
- $\beta_g$  defined in Appendix 1.
- $\beta_w$  defined in Appendix 1.
- $\chi_\beta^K$  mole fraction of mass component  $K$  in the  $\beta$  phase.
- $\Gamma_l$  surface area,  $m^2$ .
- $\lambda$  overall porous medium thermal conductivity,  $W/m K$ .
- $\mu_\beta$   $\beta$  phase viscosity,  $kg/ms$ .
- $\rho$  density,  $kg/m^3$ .
- $\rho_\beta$  density of the  $\beta$  phase,  $kg/m^3$ .
- $\rho_b$  soil dry bulk density,  $kg/m^3$ .
- $\rho_R$  scale parameter defined in (B.3).

$\tau_g$  gas phase tortuosity.

$\phi$  porosity.

$\omega_\beta^K$  mass fraction of mass component  $K$  in the  $\beta$  phase.

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LAWRENCE BERKELEY LABORATORY  
UNIVERSITY OF CALIFORNIA  
INFORMATION RESOURCES DEPARTMENT  
BERKELEY, CALIFORNIA 94720