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T2VOC
User's Guide

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ABSTRACT

T2VOC is a numerical simulator for three-phase, three-component, non-isothermal flow of water, air, and a volatile organic compound (VOC) in multidimensional heterogeneous porous media. Developed at the Lawrence Berkeley Laboratory, T2VOC is an extension of the TOUGH2 general-purpose simulation program.

This report is a self-contained guide to application of T2VOC to subsurface contamination problems involving nonaqueous phase liquids (NAPLs). It gives a technical description of the T2VOC code, including a discussion of the physical processes modeled, and the mathematical and numerical methods used. Detailed instructions for preparing input data are presented along with several illustrative sample problems.

1. INTRODUCTION

T2VOC is a three dimensional numerical simulation program for modeling the transport of organic chemical contaminants in nonisothermal multiphase systems. The code was designed to simulate processes such as the migration of hazardous nonaqueous phase liquids (NAPLs) in variably saturated media, forced vacuum extraction of organic chemical vapors from the unsaturated zone (soil vapor extraction), evaporation and diffusion of chemical vapors in the unsaturated zone, air injection into the saturated zone for removal of volatile organics (air sparging), direct pumping of contaminated water and free product, and steam injection for the removal of NAPLs from contaminated soils and aquifers.

T2VOC uses a general integral finite difference formulation for multiphase, multi-component mass and energy balance equations known as MULKOM (Pruess, 1983a; 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 versions of MULKOM are the TOUGH and TOUGH2 simulators (Pruess, 1987, 1991). TOUGH (**t**ransport **o**f **u**nsaturated **g**roundwater and **h**eat) is a three dimensional code for simulating the coupled transport of water, water vapor, air, and heat in porous and fractured porous media. TOUGH2 is similar to TOUGH, in architecture as well as input and output formats, the main difference being that the flow terms in TOUGH2 are coded in general fashion for an arbitrary number of fluid components and phases. For simulating flow in multiphase multicomponent systems, TOUGH2 needs to be linked with appropriate fluid property or "EOS" ("equation-of-state") modules that describe the thermophysical properties of the fluid mixture at hand and perform appropriate phase diagnostics.

The development of T2VOC started from TOUGH. Falta (1990) added a third fluid component to TOUGH and developed a flexible fluid property package for representing volatile and slightly water-soluble organic compounds. This resulted in a code for the simulation of multiphase contamination and remediation processes involving non-aqueous phase liquids known as "STMVOC" (Falta, 1990; Falta et al., 1992a, b). STMVOC was subsequently modified to fit into the TOUGH2 environment so that (a) TOUGH2 user features and capabilities would become available for three-phase three-component flow simulations, and (b) future code maintenance and development would be facilitated by minimizing the number of free-standing offshoots of the TOUGH/MULKOM family of codes. Following alignment of STMVOC with the TOUGH2 architecture and data structure considerable enhancements of simulation capabilities were made. The code resulting from

these developments is T2VOC. It is basically a version of TOUGH2, and is to be used in conjunction with and as part of the TOUGH2 program. The T2VOC module includes a number of program units that supersede the corresponding program units in TOUGH2. It also contains additional subroutines that are not present in the standard version of TOUGH2. Table 1 shows a summary of program units used by T2VOC, as generated by the internal version control system and printed at the end of a T2VOC simulation run. Program units that were modified relative to standard TOUGH2 are identified with an exclamation after the version number in Table 1, while for T2VOC-specific program units a "V" is placed after the version number.

The T2VOC source code consists of the standard TOUGH2 program files (or modules) and an additional FORTRAN77 program file "`t2voc.f`". In this report we use the term "T2VOC" in two different but closely related meanings that will be clear from the context: (i) to denote the new program module "`t2voc.f`", and (ii) as the name of the simulation code that is obtained by linking `t2voc.f` with "standard" TOUGH2.

This report contains a description of the physical processes included in the T2VOC simulator, and a discussion of the mathematical formulation. Much of the relevant information from the TOUGH and TOUGH2 user's guides has been repeated here to make the present report self contained. Complete instructions for preparing input files are also given, along with four illustrative sample problems.

Table 1. Summary of Program Units Used in T2VOC.

SUMMARY OF PROGRAM UNITS USED

UNIT	VERSION	DATE	COMMENTS
IO	1.0	15 APRIL 1991	OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*
SECOND	1.0	11 OCTOBER 1991	DUMMY SUBROUTINE FOR CPU TIMING FUNCTION
TOUGH2	1.05 !	4 JUNE 1993	MAIN PROGRAM
INPUT	1.01 !	16 SEPTEMBER 1994	READ ALL DATA PROVIDED THROUGH FILE *INPUT*
MESHM	1.0	24 MAY 1990	EXECUTIVE ROUTINE FOR INTERNAL MESH GENERATION
GXYZ	1.0	18 MARCH 1991	GENERATE 1, 2, OR 3-D CARTESIAN MESH
PCAR	1.0	25 MARCH 1991	MAKE STRUCTURED PRINTOUT OF CARTESIAN MESH
FLOP	1.0	11 APRIL 1991	CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC
RFILE	1.0	23 APRIL 1991	INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
CYCIT	1.0	5 MARCH 1991	EXECUTIVE ROUTINE FOR MARCHING IN TIME
EOS	1.22 !	15 SEPTEMBER 1994	*EVOC* THERMOPHYSICAL PROPERTIES MODULE FOR WATER/AIR/VOC
SATO	0.5 V	1 APRIL 1993	HYDROCARBON VAPOR PRESSURE
SATW	1.1 V	1 APRIL 1993	SATURATION PRESSURE AS FUNCTION OF TEMPERATURE; PREVENT LIQUID PHASE DISSAPPEARANCE
SUPST	1.0	29 JANUARY 1990	VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
SUPSTO	0.5 V	1 APRIL 1993	DENSITY AND INTERNAL ENERGY OF HYDROCARBON VAPOR
COWATO	0.5 V	1 APRIL 1993	DENSITY AND INTERNAL ENERGY OF LIQUID HYDROCARBON
COWAT	1.0	22 JANUARY 1990	LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
VISW	1.0	22 JANUARY 1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
PCAP	1.1 !	1 APRIL 1993	CAPILLARY PRESSURE AS FUNCTION OF SATURATION (INCL 3-PHASE)
RELP	1.1 !	12 NOVEMBER 1993	RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION (INCL 3-PHASE) IRP = 6 OPTION ("STONE I") MODIFIED TO FORCE KRN --> 0 AS SN --> SNR
HCO	0.5 V	1 APRIL 1993	HENRY'S CONSTANT FOR HYDROCARBON
VISCO2	0.5 V	1 SEPTEMBER 1994	MULTICOMPONENT GAS VISCOSITY
VISCO	1.0	1 FEBRUARY 1990	CALCULATE VISCOSITY OF VAPOR-AIR MIXTURES
COVIS	1.0	1 FEBRUARY 1990	COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
VISS	1.0	22 JANUARY 1990	VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE AND PRESSURE
BALLA	1.12 !	15 SEPTEMBER 1994	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
MULTI	1.11 !	16 SEPTEMBER 1994	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS, INCLUDING SORPTION AND BIODEGRADATION
QU	1.0	22 JANUARY 1990	ASSEMBLE ALL SOURCE AND SINK TERMS
DIFFU	0.5 V	1 APRIL 1993	CALCULATE MULTICOMPONENT DIFFUSIVITY
LINEQ	1.0	22 JANUARY 1990	INTERFACE FOR THE LINEAR EQUATION SOLVER MA28
VISO	0.5 V	1 APRIL 1993	CALCULATES LIQUID HYDROCARBON VISCOSITY
CONVER	1.0	4 MARCH 1991	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
OUT	1.1 !	7 SEPTEMBER 1994	PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
WRIFI	1.0	22 JANUARY 1990	AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*

2. HARDWARE REQUIREMENTS AND CODE INSTALLATION

The T2VOC code development was carried out partly on Cray supercomputers, and partly on workstations. Like other members of the TOUGH/MULKOM family of codes, T2VOC requires 64-bit arithmetic. It is available as a FORTRAN77 program that is intrinsically single precision, and may be used on 64-bit processors, or on 32-bit processors whose compiler has an internal double-precision "switch". For example, on an IBM RS/6000 workstation with a 32-bit CPU compilation should be made with the option "`-qautodbl=dblpad`" to obtain 64-bit arithmetic; on Sun and Solbourne workstations the same effect is achieved by specifying the "`-r8`" compilation option. A version that is intrinsically double-precision is available for execution on PCs.

The standard TOUGH2 FORTRAN77 source code consists of the files `t2m.f`, `eosx.f`, `meshm.f`, `t2f.f`, and `ma28.f`, where `eosx.f` is any one of a number of different fluid property (equation-of-state) modules. To illustrate the assembly of T2VOC, we list the compilation and linking commands that would be used on an IBM RISC/6000 workstation. "Standard" TOUGH2 with the EOS3 module (water, air) would be compiled and linked into an executable called "`x3`" as follows.

```
xlf -c -qautodbl=dblpad t2m.f eos3.f meshm.f t2f.f ma28.f
xlf -o x3 t2m.o eos3.o meshm.o t2f.o ma28.o
```

The "`-qautodbl=dblpad`" instruction is required to obtain 64-bit arithmetic on a 32-bit processor. To use the T2VOC module, the FORTRAN77 program file `t2voc.f` should be compiled and linked in place of the TOUGH2 modules `t2m.f` and `eosx.f`. As T2VOC includes its own equation-of-state package no additional EOS-module is required. On an IBM RS/6000, the compilation and linking instructions for producing an executable "`xvoc`" are as follows.

```
xlf -c -qautodbl=dblpad t2voc.f meshm.f t2f.f ma28.f
xlf -o xvoc t2voc.o meshm.o t2f.o ma28.o
```

Execution of an input file `rgdif` (first sample problem, see section 12.1) would be made with the command

```
xvoc <rgdif >rgdif.out
```

where output is printed to file `rgdif.out`.

As mentioned before, T2VOC includes modified versions of some of the same program units that appear in standard TOUGH2, creating a situation of “duplicate names” during the linking process. On most computers the linker will simply use the first program unit with a given name, and will ignore subsequent program units with the same name. On some computers the presence of duplicate names during linking will create a fatal error. The simplest way of avoiding this is to change the names of the unwanted program units. For example, T2VOC includes a modified version of subroutine INPUT. If a name conflict appears during linking, the user should, prior to compilation, simply change the name of INPUT in TOUGH2 file “`t2f.f`“ to INPUX, say.

T2VOC may also be used with the preconditioned conjugate gradient module, T2CG1 (Moridis and Pruess, 1995), which makes possible the solution of large 2-D and 3-D problems with 5000 grid blocks or more. To incorporate T2CG1, simply compile and link the program file “`t2cg1.f`” in front of the other object codes. On an IBM RS/6000 the linking instruction is as follows.

```
xlf -o xvoc1 t2cg1.o t2voc.o meshm.o t2f.o ma28.o
```

Note that again duplicate names may appear, with T2CG1 containing program units that supersede some of the units in T2VOC as well as in standard TOUGH2. The default options for T2VOC are to solve NEQ = 4 balance equations for NK = 3 mass components and heat, and to treat flow of NPH = 3 phases. It is recommended to specify the dimensioning parameters in the main program of T2CG1 accordingly, i.e., MNEQ = 4, MNK = 3, and MNPH = 3.

3. PHYSICAL PROCESSES AND ASSUMPTIONS

In the T2VOC formulation, the multiphase system is assumed to be composed of three mass components: air, water, and a volatile, water-soluble organic chemical. Although air consists of several components (nitrogen, oxygen, etc.), it is here treated as a single "pseudo-component" with averaged properties. The three fluid components in T2VOC may be present in different proportions in any of the three phases, gas, aqueous, and NAPL, except that the (usually) small solubility of water in the NAPL phase has been neglected. A new aqueous-phase density model was introduced into T2VOC. This makes the code applicable not only to slightly but also to strongly water-soluble organic compounds (see section 7.1), overcoming the restriction to slightly water-soluble organic chemicals in the original STMVOC program. The phases and components considered by the T2VOC simulator are listed in Table 2, where the dominant component in each of the three phases is shown with a bold **X**.

Table 2. T2VOC Fluid Phases and Components

Phases / ***Components***	**gas**	**aqueous**	**NAPL**
water	X	**X**	---
air	**X**	X	X
VOC †	X	X	**X**

† VOC = volatile organic compound

In addition, VOC may be adsorbed by the porous medium. 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 also occurs 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 no chemical reactions are taking place other than (a) interphase mass transfer, (b) adsorption of the chemical component to the solid phase, and (c) decay of VOC by biodegradation. 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, 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 porous media thermal conductivity is calculated as a function of water and NAPL saturation, and depends on the chemical characteristics of the NAPL.

Water properties in the liquid and vapor state are calculated, within experimental accuracy, from the steam table equations given by the International Formulation Committee (1967). Thermophysical properties of the NAPL phase 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 Henry's constant for dissolution of organic chemical vapors in the aqueous phase is calculated as a function of temperature. The Henry's constants for air dissolution in aqueous and NAPL phases are small and for simplicity have been assumed to be constant.

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 formulation of T2VOC makes no

reference to a global coordinate system, and no particular dimensionality is required. The T2VOC simulator may therefore be used for one, two, or three-dimensional anisotropic, heterogenous porous or fractured systems having complex geometries. However, internal mesh generation facilities are presently limited to standard (block-centered) finite difference grids (see section 8). The porous medium porosity may be specified to be a function of pore pressure and temperature, but no stress calculations are made.

4. GOVERNING EQUATIONS

ln 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, 1991) with extensions to account for a NAPL phase and a chemical component. The balance equations for component κ (κ = w-water, a-air, c-chemical, h-heat) are written in integral form for an arbitrary flow region V_n with surface area Γ_n as follows

$$\frac{d}{dt}\int_{V_n} M^{\kappa}\, dV_n = \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n}\, d\Gamma_n + \int_{V_n} q^{\kappa} dV_n \qquad (1).$$

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

4.1 Accumulation Terms

The mass accumulation terms for water and air (κ = w, a) contain a sum over the three phases β (β = g-gas, w-aqueous, n-NAPL).

$$M^{\kappa} = \phi \sum_{\beta} S_{\beta}\, \rho_{\beta}\, X_{\beta}^{\kappa} \qquad (2)$$

Here ϕ is the porosity, S_{β} is the saturation (pore volume fraction) occupied by phase β, ρ_{β} is the β phase density, and X_{β}^{κ} is the mass fraction of component κ in phase β. The organic chemical accumulation term (κ = c) includes the effect of linear equilibrium adsorption onto the solid phase.

$$M^{c} = \rho_b\, \rho_w\, X_w^c\, K_D + \phi \sum_{\beta} S_{\beta}\, \rho_{\beta}\, X_{\beta}^{c} \qquad (3)$$

where ρ_b is the dry bulk density of the soil, X_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 on the right hand side of Eq. (3) represents the adsorbed mass of chemical per unit volume of soil, and may be written as

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

Here $C_w^c = \rho_w X_w^c$ 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. It has been found that the degree of adsorption of organic chemicals depends largely on the amount of organic carbon present in the soil. Accordingly, K_D is often written as

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

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).

It is useful to relate the above formulation for the VOC accumulation term to alternative formulations that use a retardation factor. Extracting a factor $\phi S_g \rho_g X_g^c$ from Eq. (3), which is the standard form of the gas phase accumulation term for single-phase conditions and no sorption, we can write

$$M^c = \phi S_g \rho_g X_g^c R_g^c \qquad (6).$$

Here, R_g^c is the retardation factor for gas phase transport of the organic chemical which for two-phase gas-aqueous conditions (no NAPL present) is given by

$$R_g^c = 1 + \frac{S_w C_w^c}{S_g C_g^c} + \frac{\rho_b K_D C_w^c}{\phi S_g C_g^c} \qquad (7).$$

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

$$M^h = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta u_\beta \qquad (8),$$

where ρ_R is the soil grain density, C_R is the heat capacity of the soil grains, T is the temperature, and u_β is the specific internal energy of phase β. 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 as

$$u_g = \sum_{\kappa=w,a,c} X_g^\kappa u_g^\kappa \tag{9}$$

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

4.2 Flux Terms

The mass flux terms of the three components water, air, and chemical include a sum of contributions from the three phases, β = gas, aqueous, and NAPL.

$$\mathbf{F}^\kappa = \sum_\beta \mathbf{F}_\beta^\kappa \tag{10}$$

For aqueous and NAPL phases we have $\mathbf{F}_\beta^\kappa = X_\beta^\kappa \mathbf{F}_\beta$, where the phase fluxes $\mathbf{F}_\beta$ are given by a multiphase extension of Darcy's law,

$$\mathbf{F}_\beta = -k \frac{k_{r\beta} \rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \tag{11}.$$

Here k is the absolute permeability, $k_{r\beta}$ is the relative permeability of phase β, μ_β is the β phase dynamic viscosity, P_β is the fluid pressure in phase β, and $\mathbf{g}$ is the gravitational acceleration vector. Aqueous and gas phase pressures are related by

$$P_w = P_g + P_{cgw} \tag{12}$$

where $P_{cgw} < 0$ is the gas-water capillary pressure. The NAPL phase pressure is related to the gas phase pressure by

$$P_n = P_g + P_{cgn} \tag{13}$$

where $P_{cgn} < 0$ is the gas-NAPL capillary pressure. For most geologic materials, the wettability order is (1) aqueous phase, (2) NAPL phase, (3) gas phase; accordingly, the gas-water capillary pressure is usually stronger (more negative) than the gas-NAPL capillary pressure. The NAPL-water capillary pressure, P_{cnw} is, from Eqs. (12, 13),

$$P_{cnw} = P_{cgw} - P_{cgn} = P_w - P_n \tag{14}.$$

Mass flux in the gas phase includes advection as well as diffusion of each component.

$$\mathbf{F}_g^\kappa = -k_o \left(1 + \frac{b}{P_g}\right) \frac{k_{rg}\rho_g}{\mu_g} X_g^\kappa (\nabla P_g - \rho_g \mathbf{g}) + \mathbf{J}_g^\kappa \tag{15}$$

Here k_o is the absolute permeability at large gas pressure, which is equal to the single-phase liquid permeability, and b is the Klinkenberg b-factor (Klinkenberg, 1941), which accounts for gas slippage that effectively increases gas permeability at low pressures. $\mathbf{J}_g^\kappa$ is the diffusive mass flux of component κ in the gas phase. The diffusive mass fluxes of water vapor and organic chemical vapor, $\mathbf{J}_g^w$, and $\mathbf{J}_g^c$ are calculated by

$$\mathbf{J}_g^\kappa = -\phi S_g \tau_g D_g^\kappa \rho_g \nabla X_g^\kappa \tag{16}$$

where D_g^κ is the multicomponent molecular diffusion coefficient of component κ in the gas phase when no porous medium is present. τ_g is the gas phase tortuosity computed from the Millington and Quirk (1961) model

$$\tau_g = \phi^{1/3} S_g^{7/3} \tag{17}$$

The use of (17) to predict the gas phase tortuosity does not account for possible enhancements to the diffusive flow of condensible 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 (16), the air diffusive mass flux, $\mathbf{J}_g^a$ is determined from the requirement that

$$\mathbf{J}_g^a + \mathbf{J}_g^w + \mathbf{J}_g^c = 0 \qquad (18)$$

The use of (18) 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 heat flux includes both conduction and convection

$$\mathbf{F}^h = -K\nabla T + \sum_\beta h_\beta \mathbf{F}_\beta \qquad (19)$$

where K is the overall porous medium thermal conductivity, h_β is the β phase specific enthalpy, and $\mathbf{F}_\beta$ is the total β 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

$$h_g = \sum_{\kappa=w,a,c} X_g^\kappa h_g^\kappa \qquad (21)$$

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).

4.3 Sink and Source Terms

T2VOC includes an optional sink term that permits a simple approximate representation of biodegradation of VOCs. It is assumed that VOC dissolved in the aqueous phase may decay according to the standard exponential decay law

$$dM_w^c = -\lambda M_w^c \, dt \qquad (22),$$

where the rate constant λ is related to the half-life $T_{1/2}$ as $\lambda = \ln 2/T_{1/2}$. This decay process is represented by incorporating a sink term ($q^c < 0$) into Eq. (1).

$$q^c = -\lambda M_w^c = -\lambda \phi S_w \rho_w X_w^c \tag{23}$$

Several sink and source term options are available in the T2VOC simulator for specifying the production ($q < 0$) or injection ($q > 0$) of fluids and heat. Any of the three mass components (water, air, chemical) may be injected in an element at a constant or time-dependent rate. 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 may be handled by prescribing a constant or time-dependent mass rate. In this case, the phase composition of the produced fluid may be determined by the relative phase mobilities in the source element. Alternatively, the produced phase composition may be specified to be the same as the phase composition in the producing element. In either case, the mass fractions of the components in the produced phases are determined by the corresponding component mass fractions in the producing element.

Another production option involves 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 β from a grid block with phase pressure $P_\beta > P_{wb}$ is

$$q_\beta = \frac{k_{r\beta}}{\mu_\beta} \rho_\beta \cdot PI \cdot (P_\beta - P_{wb}) \tag{24}$$

For steady radial flow the productivity index is given by (Coats, 1977; Thomas, 1982)

$$(PI)_l = \frac{2\pi\left(k\,\Delta z_l\right)}{\ln\left(r_e/r_w\right) + s - 1/2} \tag{25}$$

Here, Δz_l denotes the layer thickness, $(k\ \Delta z)_l$ is the permeability-thickness product in layer l, r_e is the grid block radius, r_w is the well radius, and s is the skin factor. If the well is producing from a grid block which does not have cylindrical shape, an approximate PI can be computed by using an effective radius

$$r_e = \sqrt{A/\pi} \tag{26}$$

where A is the grid block area; e.g., $A = \Delta x \bullet \Delta y$ for an areal Cartesian grid. More accurate expressions for specific well patterns and grid block shapes have been given in the literature (e.g., Peaceman, 1978, 1982; Coats and Ramesh, 1982).

The rate at which each mass component ($\kappa \neq h$) is produced is

$$\hat{q}^{\kappa} = \sum_{\beta} X_{\beta}^{\kappa} q_{\beta} \tag{27}$$

For wells which are screened in more than one layer (element), the flowing wellbore pressure P_{wb} can be corrected to approximately account for gravity effects according to the depth-dependent flowing density in the wellbore. Assume that the open interval extends from layer $l = 1$ at the bottom to $l = L$ at the top. The flowing wellbore pressure in layer l, $P_{wb,l}$, is obtained from the wellbore pressure in layer $l + 1$ immediately above it by means of the following recursion formula

$$P_{wb,l} = P_{wb,l+1} + \frac{g}{2}\left(\rho_l^f \Delta z_l + \rho_{l+1}^f \Delta z_{l+1}\right) \tag{28}$$

Here, g is acceleration of gravity, and ρ_l^f is the flowing density in the tubing opposite layer l. Flowing densities are computed using a procedure given by Coats (private communication, 1982). If wellbore pressure were zero, we would obtain the following volumetric production rate of phase β from layer l.

$$r_{l,\beta} = \left(\frac{k_{r\beta}}{\mu_\beta}\right)_l (PI)_l \, P_{l,\beta} \tag{29}$$

The total volumetric flow rate of phase β opposite layer l is, for zero wellbore pressure

$$r_{l,\beta}^T = \sum_{m=1}^{l} r_{m,\beta} \tag{30}$$

From this we obtain an approximate expression for flowing density opposite layer l which can be used in Eq. (28).

$$\rho_l^f = \frac{\sum_\beta \rho_{l,\beta}\, r_{l,\beta}^T}{\sum_\beta r_{l,\beta}^T} \tag{31}$$

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

$$\hat{q}^h = \sum_\beta q_\beta\, h_\beta \tag{32}$$

where h_β is the specific enthalpy of phase β.

For numerical solution, the nonlinear coupled balance Eqs. (1) must be discretized in space and time. Space is discretized with the integral finite difference method (Narasimhan and Witherspoon, 1976), which for regular grid systems is mathematically equivalent to conventional finite differences but offers added geometric flexibility. Time differencing is made fully implicitly, using first-order backward finite differences. For a flow system with N grid blocks and NEQ balance equations per block, discretization results in a system of N * NEQ coupled non-linear algebraic equations which is solved by Newton-Raphson iteration. The linear equations arising at each iteration step are solved either by sparse direct matrix methods (Duff, 1977) or by means of iterative pre-conditioned conjugate gradient techniques (Moridis and Pruess, 1995). A more detailed description of discretization procedure and solution technique is given in Appendix A. Appendix B describes double and multiple-porosity techniques that are available in T2VOC for modeling flow in fractured media, or in heterogeneous media with embedded low-permeability regions such as silt or clay lenses.

5. INITIAL AND BOUNDARY CONDITIONS

Flow systems are initialized by assigning a complete set of primary thermodynamic variables to each grid block. Various options are available and are described in section 6. Default conditions can be assigned to the entire flow domain. These defaults can be overwritten by assigning specific conditions to certain domains, which in turn may be superseded by assigning specific thermodynamic conditions to individual grid blocks. The primary variables depend on the fluid phase composition and will generally be different in different grid blocks. A summary of primary variables used in T2VOC is given in Table 3, below.

Simulation of environmental contamination and remediation problems will usually proceed in several steps. A first step often involves preparation of a "natural" state, prior to the contamination, for the flow system under study. This state may correspond to gravity-capillary equilibrium, with or without water infiltration, or it may be a dynamic state of regional flow. Such a model of a "natural" state may be simulated by assigning more or less arbitrary initial conditions, then imposing appropriate boundary conditions (see below), and running the flow system to a state of static or dynamic equilibrium. Pre-contamination conditions can be efficiently simulated by running T2VOC in "two-component mode", with only water and air present. The thermodynamic conditions calculated for this state consist of a complete list of all primary thermodynamic variables for all grid blocks, which is written out as a disk file called "SAVE" at the end of a T2VOC simulation run. This data may be provided as initial conditions for a subsequent second simulation run which models the release and spreading of contaminant. The thermodynamic conditions calculated in this second simulation step may be provided as initial conditions to a third step in which different remediation operations are modeled that involve injection and extraction of fluids and heat.

Boundary conditions are basically of two types, Neumann (prescribed fluxes) or Dirichlet (prescribed thermodynamic variables, such as pressure, temperature, etc.). "No flux" boundary conditions are implemented simply by not introducing any interface that could carry flow at the desired "no flux" boundary. More general Neumann boundary conditions are specified by introducing appropriate sinks or sources in the flow domain, which are placed in grid blocks adjacent to the desired flux boundary.

Dirichlet conditions can be implemented by assigning very large volumes (e.g., $V = 10^{50}$ m^3) to grid blocks adjacent to the boundary so that their thermodynamic conditions do

not change at all from fluid or heat exchange with “finite-size” blocks in the flow domain. In addition, a “small” value should be specified for the nodal distance of such blocks, so that boundary conditions are maintained at the surface where they are desired and not at some distance from it. Time-dependent Neumann conditions can be specified by making sink and source rates time dependent. Time-dependent Dirichlet conditions can also be implemented; these are realized by placing appropriate sinks or sources in the “boundary blocks” (for an example, see Moridis and Pruess, 1992).

T2VOC offers an alternative and more elegant means for implementing Dirichlet conditions, which provides savings in computational work along with added user conveniences in running simulation problems. This is accomplished with the simple device of "active" and "inactive" elements. By convention, elements encountered in data block "ELEME" (or in geometry files "MESH" or "MINC") are taken to be "active" until the first element entry with a zero or negative volume is encountered. The first element with volume less than or equal to zero, and all subsequent elements, are by convention taken to be "inactive." For the inactive elements no mass or energy balance equations are set up, and their primary thermodynamic variables are not included in the list of unknowns. Otherwise, however, inactive elements can appear in flow connections and initial condition specifications like all other elements. This feature can be conveniently used to specify Dirichlet boundary conditions, by gathering all elements beyond the desired flow domain boundary at the end of the ELEME-block, and inserting a "dummy" volume element of zero volume in front of them. Because the thermodynamic state variables of the inactive elements are not included in the list of unknowns, the thermodynamic conditions in these elements will not change and be rigorously maintained during a simulation run. The computational overhead of inactive elements is small because they do not increase the number of equations to be solved in a flow problem.

6. PRIMARY VARIABLES AND VARIABLE SWITCHING

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 parameters" is needed for the solution of the four coupled balance equations. These secondary parameters include thermodynamic and transport properties such as enthalpies, densities, relative permeabilities, viscosities, and mass fractions. The four primary variables must be chosen to be independent so that the entire set of secondary parameters may be calculated as functions of the primary variables.

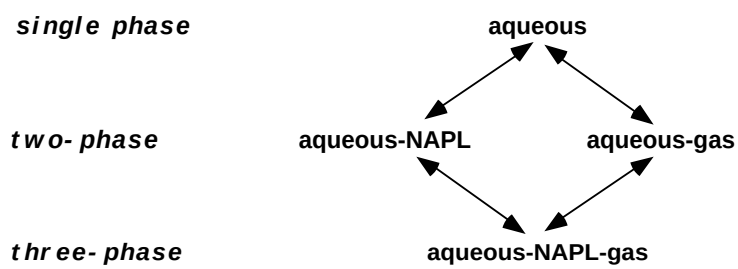
In multiphase flow problems involving phase transitions (ie. appearance or disappearance of a phase), the number of possible phase combinations may become large. In a system in which a maximum of three fluid phases may be present, there are seven possible phase combinations. These combinations include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

Ideally, different sets of primary variables should be used for different phase combinations. During phase transitions the primary variables then need to be switched so that thermodynamic conditions in all grid blocks are always fully defined 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 different sets of primary variables and would be cumbersome to code. An alternative method is to prohibit complete phase transitions and maintain some finite (small) saturation of each phase in each element. Phases can be 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 may be quite 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 T2VOC simulator, a compromise is made between the robustness and elegance of the variable substitution method, and the simplicity of the minimum saturation method. The number of phase combinations is reduced to four by assuming that the aqueous phase never totally disappears, although the aqueous phase saturation may be quite small ($\approx 10^{-4}$). The initial conditions for T2VOC simulations must always include at least a small amount of aqueous phase ($S_w > 10^{-4}$). Figure 1 shows the phase conditions that may be described with T2VOC. Arrows indicate appearance or disappearance of phases.

Figure 1. Fluid Phase Conditions in T2VOC.



The different primary variables used for single, two and three-phase conditions are summarized in Table 3.

Table 3. Choice of Primary Variables in T2VOC.

Phases	Primary Variables			
	X1	X2	X3	X4
1 aqueous	P	Xaw+50	Xmolow	T
2 aq., NAPL	P	Sw	Xaw+50	T
2 aq., gas	P	Sw	Xmolog	T
3 aq., gas, NAPL	P	Sw	Sg+10	T

The variables are P - pressure, Xaw - mass fraction of air in aqueous phase, Xmolow - mole fraction of VOC in aqueous phase, T - temperature, Sw - water saturation, Xmolog - mole fraction of VOC in gas phase, and Sg - gas saturation. The increments

(adding 10, 50) and place changes for some of the primary variables have been chosen so as to enable the fluid property module to recognize fluid phase compositions from the numerical values of the primary variables present.

In the course of a T2VOC simulation run, phase conditions in different grid blocks may change, and primary variables must be switched accordingly. After each Newton-Raphson iteration the primary variables are updated in all grid blocks, and subsequently the EOS subroutine is called to diagnose phase conditions, and calculate all secondary parameters (see below). In order to describe phase change diagnostics and associated variable switching in T2VOC let us consider a grid block that is in single-phase aqueous conditions. After each iterative updating of the primary variables the possible appearance of a NAPL or a gas phase must be tested. Appearance of a NAPL phase is examined by comparing dissolved mole fraction in the aqueous phase, Xmolow, with the VOC mole fraction that would be present at the solubility limit at prevailing temperature. If Xmolow exceeds the solubility limit a NAPL phase will appear, and primary variables are switched as shown in Table 3. Specifically, the primary variable # 2 in single-phase aqueous conditions, Xaw + 50, is made variable # 3, and variable # 2, which now denotes water saturation Sw, is initialized as $Sw = 1 - 10^{-6}$, to allow for evolution of a small amount of NAPL phase at saturation $Sn = 1 - Sw = 10^{-6}$. If no NAPL phase is found to appear, the possible appearance of a gas phase is checked by comparing the “bubble” (or total gas phase) pressure, $P_{bub} = P_{vap} + P_{air} + P_{VOC}$, with total pressure P. If $P_{bub} > P$ a gas phase evolves. The second primary variable is again switched to become water saturation and is initialized as $Sw = 1 - 10^{-6}$, while the third primary variable is converted from VOC mole fraction in the aqueous phase to VOC mole fraction in the gas phase.

Analogous tests are made to evaluate whether two-phase points (aqueous-NAPL or aqueous-gas) evolve a third phase; if so, the third primary variable becomes Sg + 10. Gas saturation is initialized as $Sg = 10^{-6}$ if the preceding two-phase conditions were aqueous-NAPL; if the preceding two-phase conditions were aqueous-gas, gas saturation is reduced from Sg to $Sg' = Sg \times (1 - 10^{-6})$, to initialize a small NAPL saturation $Sn = 1 - Sw - Sg' = Sg \times 10^{-6}$.

Disappearance of phases is recognized very easily by monitoring saturations. In 3-phase conditions, gas phase disappears when $Sg < 0$, and NAPL-phase disappears when $Sw + Sg > 1$. In two-phase conditions, the second phase (gas or NAPL) disappears when $Sw > 1$. For any change in phase composition, primary variables are switched as shown in

Table 3. Needless to say, the phase diagnostic and variable switching must be performed after each iterative change in primary variables, one grid block at a time, for all of the grid blocks in the flow domain.

T2VOC optionally offers the capability to solve only 2 mass balance equations, for water and air, omitting the VOC mass balance (through input data block **MULTI**, see below). This feature is useful for preparing "natural states" in saturated or unsaturated flow systems, prior to release of contaminant. Possible phase compositions are either single-phase aqueous, or two-phase aqueous-gas. When only two mass balances are set up, the third primary variable is omitted, and (P, Xaw+50, T) is used for single phase conditions, (P, Sw, T) is used for two-phase aqueous-gas conditions. 3-component simulation runs (water, air, VOC) can be initialized from 2-component (water, air) initial conditions by appropriate specification of parameter MOP(19) in record PARAM.1, see section 9.

T2VOC can also be run in isothermal mode (see **MULTI** input, below), which reduces the number of balance equations per grid block by one and provides considerable savings in computational work. When running isothermally the user must still provide temperature assignments just as for non-iosthermal calculations; however, no heat balance equation will be solved and temperatures will automatically be maintained constant during a simulation.

7. SECONDARY PARAMETERS

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 parameters from the primary variables is of considerable importance. ln the formulation of T2VOC an effort has been made to include all of the parametric dependencies which significantly contribute to the nonlinearity of the problem. A complete list of all secondary parameters along with their dependence on the primary variables is given in Table 4. The dependence of the secondary parameters on

Table 4. Secondary Variables and Functional Dependence

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

specific primary variables may change under different phase conditions due to the primary variable switching. In Table 4, 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.

7.1 Aqueous Phase Density

The solubility of VOCs in the aqueous phase is usually small, typically of the order of a few hundred ppm. It may appear, then, that the presence of such a small amount of VOC in the aqueous phase would have negligible impact on the aqueous phase density, and that sufficient accuracy would be attained by taking the aqueous phase density equal to that of pure water, regardless of how much VOC may be dissolved. A closer examination of the issue reveals, however, that neglecting the impact of dissolved VOC on the aqueous phase density may result in unacceptably large spurious pressure excursions. Consider the dissolution of TCE with a density of 1462 kg/m^3 at ambient conditions in water with an ambient density of 998 kg/m^3. If TCE were permitted to dissolve in the aqueous phase without any density change of the latter, then the dissolution process would be accompanied by an increase in total fluid volume. If fluid volume were held constant an increase in fluid pressure would result which can be estimated as follows. At the solubility limit a mass fraction of approximately 10^{-3} of TCE is present in the aqueous phase. Dissolving this amount of NAPL in an aqueous phase of constant density, at constant pressure, would cause a relative increase in the volume of the water-NAPL two-phase mixture of $\Delta V/V \approx 0.068$ %. If fluid volume were held constant, a pressure increase of $\Delta P = (\Delta V/V)/c_w \approx 1.36\text{x}10^6$ Pa would result, which is so surprisingly large because of the small compressibility of liquid water, $c_w \approx 5\text{x}10^{-10}$ Pa^{-1} at ambient conditions.

These estimates were confirmed by means of numerical dissolution experiments, and subsequently a better density model was implemented for the aqueous phase that avoids these problems. The basic assumption we make is that, when NAPL dissolves in water, both total fluid mass and total fluid volume are conserved. Denoting water and NAPL phase volumes by V_w and V_n, respectively, the volume of the aqueous phase after NAPL dissolution is given by

$$V_{aq} = V_w + V_n \tag{30}$$

Similarly, the mass of the aqueous phase is

$$M_{aq} = M^w + M^n \tag{31}$$

Dividing Eq. (31) by (30) and inserting the mass fractions $X^w = M^w/M_{aq}$ of water and $X^n = M^n/M_{aq}$ of dissolved VOC, we obtain for the aqueous phase density $\rho_{aq} = M_{aq}/V_{aq}$.

$$\frac{1}{\rho_{aq}} = \frac{V_{aq}}{M_{aq}} = \frac{X^w}{\rho_w} + \frac{X^n}{\rho_n} \tag{32}$$

7.2 Gas Phase Density and Mass Fractions

By assuming that all components of the gas phase obey the ideal gas law, and that the total pressure is equal to the sum of the partial pressures, the gas density is calculated as the sum of the component gas concentrations. The partial pressure of water in the gas phase, P_g^w, is equal to the saturated vapor pressure of water at the local temperature, P_{sat}^w. This value is calculated using steam table equations given by the International Formulation Committee (1967). From the ideal gas law, the concentration of water in the gas phase (i.e., the vapor density), C_g^w,

$$C_g^w = \frac{P_g^w \, M_{wt}^w}{R\,T} \tag{33}$$

where M_{wt}^w is the molecular weight of water, and R is the universal gas constant. Next, the partial pressure of the organic chemical is calculated. If the NAPL phase is not present, then

$$P_g^c = \chi_g^c \, P_g \tag{34}$$

where χ_g^c is the chemical mole fraction in the gas phase, and P_g is the gas phase pressure. If the NAPL phase is present, then P_g^c is set equal to the saturated vapor pressure of the chemical which is calculated as a function of temperature by the Wagner equation (Reid et al., 1987)

$$P_{sat}^c = P_{crit} \exp\left(\frac{ax + bx^{1.5} + cx^3 + dx^6}{1 - x}\right) \tag{35}$$

$$x = 1 - \frac{T}{T_{crit}} \tag{36}$$

Here, P_{crit} and T_{crit} are the critical pressure and critical temperature of the organic compound, and a, b, c, and d are empirically determined constants. Values of these constants for about 500 compounds are given by Reid et al. (1987). Using the ideal gas law for the chemical concentration results in

$$C_g^c = \frac{P_g^c \, M_{wt}^c}{R \, T} \tag{37}$$

where M_{wt}^c is the molecular weight of the chemical.

Given the total gas phase pressure, and the water and chemical partial pressures, the air partial pressure is calculated by

$$P_g^a = P_g - P_g^w - P_g^c \tag{38}$$

$$C_g^a = \frac{P_g^a \, M_{wt}^a}{R \, T} \tag{39}$$

where M_{wt}^a is the mixture molecular weight of air. The gas density is then calculated as the sum of the component concentrations

$$\rho_g = C_g^a + C_g^w + C_g^c \tag{40}$$

and the gas phase mass fractions are simply

$$X_g^a = \frac{C_g^a}{\rho_g} \tag{41}$$

$$X_g^w = \frac{C_g^w}{\rho_g} \tag{42}$$

$$X_g^c = \frac{C_g^c}{\rho_g} \tag{43}$$

The use of the ideal gas law for calculating the gas density and mass fractions is a reasonable approximation as long as the total pressure is less than about two or three atmospheres. For instance, the error in the calculated water vapor density at a pressure of five atmospheres using the ideal gas law is less than five percent. In cases where the pressure is very high, as in petroleum reservoirs, the real gas law should be used instead of the ideal gas law.

7.3 Gas Phase Viscosity

The gas viscosity is computed as a function of temperature, pressure, and composition. In areas where only air and water vapor are present, the gas viscosity is calculated using a modified version of the kinetic gas theory formulation given by Hirschfelder et al. (1954) in which the water vapor viscosity is calculated from steam table equations (Pruess, 1987).

In areas where the chemical vapor is present, the viscosity is calculated from a modified version of the Wilke semi-empirical method for multicomponent gas viscosity (Bird et al., 1960).

$$\mu_g = \frac{\mu_g^c}{1 + \Phi_{c,aw}\left[\chi_g^{aw} / \chi_g^c\right]} + \frac{\mu_g^{aw}}{1 + \Phi_{aw,c}\left[\chi_g^c / \chi_g^{aw}\right]} \tag{44}$$

In (43), μ_g^{aw} is the air-water vapor viscosity calculated from the modified kinetic gas theory formulation (Hirschfelder et al., 1954), μ_g^c is the viscosity of pure chemical vapor (see Appendix E), χ_g^{aw} is the sum of the air and water vapor mole fractions, and χ_g^c is the chemical vapor mole fraction. The interaction parameters, $\Phi_{c,aw}$ and $\Phi_{aw,c}$ are

$$\Phi_{c,aw} = \frac{\left[1 + \left(\mu_g^c / \mu_g^{aw}\right)^{1/2} \left(M_{wt}^{aw} / M_{wt}^c\right)^{1/4}\right]^2}{\left[8\left(1 + M_{wt}^c / M_{wt}^{aw}\right)\right]^{1/2}} \tag{45}$$

and

$$\Phi_{aw,c} = \frac{\left[1+\left(\mu_g^{aw}/\mu_g^c\right)^{1/2}\left(M_{wt}^{aw}/M_{wt}^c\right)^{1/4}\right]^2}{\left[8\left(1+M_{wt}^{aw}/M_{wt}^c\right)\right]^{1/2}} \tag{46}$$

in which M_{wt}^c is the chemical molecular weight, and M_{wt}^{aw} is the air-water vapor mixture molecular weight. The chemical vapor viscosity (μ_g^c in Eq. 44) is computed from the corresponding states method (Reid et al., 1987). Details of this method are given in Appendix E.

The method of calculating the gas phase viscosity described above is expected to give good accuracy over the entire range of composition. As the mole fraction of chemical vapor tends towards zero, (44) reduces to the air-water viscosity calculated by the kinetic gas theory model. Comparisons with experimental data over the range of air-water composition and at temperatures up to 150 ^oC have shown this model to be accurate to within four percent. As the mole fraction of chemical vapor tends towards one, the formulation reduces to the corresponding states method for the chemical vapor viscosity which has an average error of about three percent (Reid et al., 1987). For intermediate compositions, Bird et al. (1960) report that the use of (44) results in an average error of about two percent given accurate values for the individual viscosities.

7.4 NAPL Phase Density and NAPL and Aqueous Phase Viscosities

Due to the low solubility of most organic liquids in water, and to the low solubility of water and air in organic liquids, variations of aqueous and NAPL viscosities, and NAPL density with composition are neglected. The aqueous and NAPL viscosities are calculated as a function of temperature. The viscosity of liquid water is calculated from steam table equations given by the International Formulation Committee (1967).

The variation of NAPL density with temperature is computed using the Modified Rackett technique (Reid et al., 1987)

$$\rho_{ns} = \rho_{nsR}\, Z_{RA}^{\left[(1-T_{rR})^{2/7}-(1-T_r)^{2/7}\right]} \tag{47}$$

where

$$Z_{RA} = 0.29056 - 0.08775\omega$$

$$T_{rR} = T_R / T_{crit}$$

$$T_r = T / T_{crit}$$

In (47), ρ_{nsR} is a known NAPL density at a temperature of T_R and a pressure equal to the NAPL saturation pressure, and ω is the Pitzer acentric factor for the chemical. The NAPL density calculated by (47), ρ_{ns}, is the density at a pressure equal to the NAPL saturation pressure at the prevailing temperature.

The NAPL viscosity is calculated using one of two semi-empirical methods suggested by Reid et al. (1987). When sufficient experimental data is available, the viscosity may be accurately calculated by

$$\mu_n = \exp\left(a + b/T + cT + dT^2\right) \tag{48}$$

where a, b, c, and d are empirically determined constants. Values of these constants for about 350 organic liquids are given by Reid et al. (1987). If only one viscosity data point is available, the viscosity in units of centipoise is calculated from

$$\mu_n = \left(\mu_{nR}^{-0.2661} + \frac{T - T_R}{233}\right)^{-3.758} \tag{49}$$

where μ_{nR} is the viscosity (in cP) at a temperature of T_R. This expression is only approximate, and errors in the calculated viscosity may be as high as 15 percent in some cases (Reid et al., 1987).

7.5 Specific Enthalpies

The specific enthalpy of the water and NAPL phases is assumed to be independent of compositional effects, and is calculated as a function of temperature and pressure only. The liquid water specific enthalpy is computed from steam table equations given by the International Formulation Committee (1967). The specific enthalpy of the NAPL is calculated from

$$h_n = \int_{T_{ref}}^{T} C_{pn}\, d\zeta \tag{50}$$

where T_{ref} is the temperature at which the enthalpy is zero (enthalpy and internal energy are relative quantities). The reference temperature is normally chosen to be 0 ^{o}C, but the choice of T_{ref} is not important as long as a consistent value is used in all of the other heat calculations. The heat capacity of the NAPL, C_{pn}, is calculated in two stages. First, the ideal gas molar heat capacity is computed using the method of Joback (Reid et al., 1987)

$$C_{pn}^{0} = a + bT + cT^{2} + dT^{3} \tag{51}$$

where a, b, c, and d are empirically determined constants provided by Reid (1987) for about 500 organic compounds. The liquid heat capacity is calculated from the ideal gas heat capacity by the Rowlinson-Bondi method (Reid et al., 1987)

$$\begin{aligned} C_{pn} = \frac{1}{M_{wt}^{c}} \Bigg\{ C_{pn}^{0} + R \Bigg[& 1.45 + 0.45\left(1 - T_r\right)^{-1} \\ & + 0.25\omega \Big\langle 17.11 + 25.2\left(1 - T_r\right)^{1/3} T_r^{-1} \\ & + 1.742\left(1 - T_r\right)^{-1} \Big\rangle \Bigg] \Bigg\} \end{aligned} \tag{52}$$

where $T_r = (T/T_{crit})$ is the reduced temperature, R is the universal gas constant, and ω is Pitzer's acentric factor. In (52), C_{pn} has units of kJ/kgK. Because the heat capacity of a liquid is only a weak function of temperature, the integral in (50) is numerically evaluated using the two-point Gaussian quadrature method (Burden et al., 1981).

The specific enthalpy of the gas phase is a very strong function of composition. The gas enthalpy is calculated as the mass fraction weighted sum of the component enthalpies. As with the previously discussed water thermophysical properties, the water vapor specific enthalpy is calculated from steam table equations provided by the International Formulation Committee (1967). The specific enthalpy of the chemical vapor is calculated as the sum of the liquid enthalpy and the latent heat of vaporization

$$h_g^{c} = h_n + h_{vap}^{c} \tag{53}$$

where h_n is given by (50). The latent heat of vaporization of the chemical is calculated in two parts. First, the heat of vaporization at the normal boiling point is computed by the Chen method (Reid et al., 1987)

$$h^c_{vap,b} = \frac{R\,T_{crit}\,T_{br}}{M^c_{wt}} \left[\frac{3.978\,T_{br} - 3.958 + 1.555 \ln\left(P_{crit}\right)}{1.07 - T_{br}} \right] \qquad (54)$$

where T_{br} is equal to the normal boiling temperature of the chemical, T_b, divided by the critical temperature, and $h^c_{vap,b}$ has units of kJ/kg. The heat of vaporization is then calculated as a function of temperature by the Watson relation (Reid et al., 1987)

$$h^c_{vap} = h^c_{vap,b} \left(\frac{1-T_r}{1-T_{br}} \right)^{.375} \qquad (55)$$

The specific enthalpy of the air (a noncondensible gas) is

$$h^a_g = C_{va}\,T + \frac{P^a_g}{C^a_g} \qquad (56)$$

In (56), the temperature dependence of the air heat capacity, C_{va}, is neglected. It should be noted that this formulation corresponds to the air internal energy, $u^a_g = C_{va}\,T$, being normalized to zero at $T = 0\ ^oC$.

The overall gas specific enthalpy is then calculated to be

$$h_g = X^a_g\,h^a_g + X^w_g\,h^w_g + X^c_g\,h^c_g \qquad (57)$$

It is interesting to note that the specific gas enthalpy of most organic compounds is smaller than that of water by a factor of roughly five. This is mainly due to the smaller latent heat of vaporization of the organic liquids.

7.6 Henry's Constants and Water and NAPL Phase Mass Fractions

Under conditions of local chemical equilibrium, the concentration of a compound in a phase is related to the concentration in another phase by a constant. Strictly speaking, this

constant is a function of both temperature and concentration. In situations where the compound is only slightly soluble in one or more of the phases, the equilibrium constant is often independent of concentration.

The equilibrium expression for the gas-liquid distribution of a dilute compound is known as Henry's law, and may be written for the air and chemical components in a gas-water system as

$$P_g^\kappa = H_{gw}^\kappa \chi_w^\kappa \qquad (\kappa = a, c) \tag{58}$$

where P_g^κ is the partial pressure of component κ in the gas phase, χ_w^κ is the mole fraction of κ in the aqueous phase, and H_{gw}^κ is Henry's constant for κ, a function of temperature. In this context, Henry's constant has units of pressure. If Henry's constant is assumed to be independent of concentration, and κ is a slightly soluble organic compound, Henry's constant may be determined by

$$H_{gw}^c = \frac{P_{vap}^c}{\overline{\chi}_w^c} \tag{59}$$

where P_{vap}^c is the saturated vapor pressure of the organic chemical given as a function of temperature by (35), and $\overline{\chi}_w^c$ is the solubility of the chemical in water (mole fraction). The solubility of a chemical in water is a complex function of temperature which may increase or decrease with increasing temperature (see e.g. API, 1977). As a general rule, the solubility of organic liquids tends to increase with increasing temperature, while the solubility of noncondensible gases tends to decrease with increasing temperature. In some cases, the solubility of organic liquids decreases with temperature to some minimum value and then increases with temperature (API, 1977). If data for the chemical solubility are available, the solubility may be approximated by

$$\overline{\chi}_w^c = a + bT + cT^2 + dT^3 \tag{60}$$

where a, b, c, and d are determined by fitting the data. Unfortunately, data for the solubility of most organic chemicals are only available for a narrow temperature range. Estimation methods are available for computing aqueous solubilities (see e.g. Prausnitz et al., 1986; Reid et al., 1987), but these methods are complex and do not always give accurate results.

In the present work, if experimental solubility data are only available at one temperature, then the solubility is assumed to be constant, and b, c, d in (60) are set equal to zero.

The gas-water distribution of the air component is calculated using (58) with a constant value for Henry's constant of 10^{10} Pa. Although the variation of H^a_{gw} with temperature is neglected, this value is accurate to within 10 percent at temperatures ranging from 40 to 100 ^oC (Loomis, 1928). The solubilities of air and water in the NAPL are assumed to be very small, and independent of temperature. The air mole fraction in the NAPL, χ^a_n, is calculated using an equation similar to (58) with H^a_{gn} equal to an experimentally determined constant (normally assumed to equal the air-water value). The water mole fraction in the NAPL is included in the formulation, but is normally assumed to be equal to zero. In most instances, the mole fractions of air and water in the NAPL are very small, and $\chi^c_n \approx 1$.

Given the dissolved mole fractions in the water and NAPL phases, the remaining mole fractions are determined from the requirement that the sum of the mole fractions in all phases is equal to one.

$$\sum_{\kappa = a, w, c} \chi^\kappa_\beta = 1 \tag{61}$$

From the mole fractions, the mass fractions in the water and NAPL phases are calculated by

$$X^\kappa_\beta = \frac{\chi^\kappa_\beta M^\kappa_{wt}}{\sum_{\kappa = a, w, c} \chi^\kappa_\beta M^\kappa_{wt}} \tag{62}$$

7.7 Capillary Pressures and Relative Permeabilities

Of the various secondary variables, the multiphase capillary pressures and relative permeabilities are among the most important parameters affecting the multiphase flow. Unfortunately, these parameters are also very difficult to predict in a general fashion due to the variability of the pore space geometry in natural media, and the complexity of the different fluid interactions. Further compounding the situation is the fact that it is very difficult to experimentally measure capillary pressures and relative permeabilities under three phase conditions. For these reasons, it is a common practice to develop three-phase

capillary pressure and relative permeability functions from two-phase relationships (Leverett, 1941; Leverett and Lewis, 1941; Stone, 1970; Stone, 1973; Aziz and Settari, 1979; Parker et al., 1987).

In the T2VOC code, several three-phase relative permeability and capillary pressure models are available. These are summarized in Appendices C and D, respectively, and should be considered preliminary. T2VOC users are encouraged to follow ongoing research into three-phase relative permeabilities and capillary pressures reported in the literature, and to add suitable formulations to subroutines RELP and PCAP, respectively.

7.8 Other Secondary Variables

Additional secondary variables include the porous medium thermal conductivity, gas phase multicomponent molecular diffusivities, and the porosity.

The thermal conductivity of the porous medium, λ, is a function of the rock grain thermal conductivity, λ_r, the water thermal conductivity, λ_w, the NAPL thermal conductivity, λ_n, the porosity and pore geometry, and the water and NAPL saturations. In general, λ is a complex function of these parameters, and researchers have developed theoretical (Walsh and Decker, 1966; Beck, 1976; Zimmerman, 1989) and empirical (Somerton, 1958; Sugawara and Yoshizawa, 1962; Somerton et al., 1973; 1974) methods for predicting λ. One method for estimating the overall thermal conductivity is known as the parallel model (Bejan, 1984). With this model, the overall thermal conductivity is a combination of the individual conductivities

$$\lambda = \lambda_r (1-\phi) + \lambda_w \phi S_w + \lambda_n \phi S_n \tag{63}$$

where λ_r is usually measured experimentally, λ_w is about 0.61 W/(m K), and λ_n is calculated by the method of Sato and Riedel (Reid et al., 1987)

$$\lambda_n = \frac{\left(1.11/M_{wt}^c\right)^{1/2}\left[3 + 20\left(1 - T_r\right)^{2/3}\right]}{3 + 20\left(1 - T_{br}\right)^{2/3}} \tag{64}$$

where $T_r = (T/T_{crit})$ is the reduced temperature, and $T_{br} = (T_b/T_{crit})$ is the reduced NAPL boiling temperature. The first term in (63) is usually several times larger than the second and third terms. Additionally, because the thermal conductivity of water is about four times

larger than the thermal conductivity of most organic liquids, the last term in (63) is usually small compared to the second term.

The multicomponent diffusivities for water and chemical vapor in the gas phase are calculated from the three sets of binary diffusivities by the Wilke method [API, 1977]

$$D_g^w = \frac{1-\chi_g^w}{\dfrac{\chi_g^a}{D_g^{aw}} + \dfrac{\chi_g^c}{D_g^{cw}}} \tag{65}$$

and

$$D_g^c = \frac{1-\chi_g^c}{\dfrac{\chi_g^w}{D_g^{cw}} + \dfrac{\chi_g^a}{D_g^{ac}}} \tag{66}$$

where D_g^{aw} is the binary air-water vapor diffusivity, D_g^{cw} is the binary chemical-water vapor diffusivity, and D_g^{ac} is the binary air-chemical vapor diffusivity. Due to the condition specified by (18), it is not necessary to calculate the multicomponent air diffusivity, D_g^a. The binary air-water and air-chemical diffusivities are calculated as functions of temperature and pressure by (Vargaftik, 1975; Walker et al., 1981).

$$D_g^{ij} = D_g^{ijR}\left(P_R/P_g\right)\left(T/T_R\right)^{\theta_{ij}} \tag{67}$$

where D_g^{ijR} is the experimentally determined i-j binary diffusivity at a temperature of T_R and a pressure of P_R, and θ_{ij} is an experimentally determined constant. For air-water diffusion, θ_{aw} has a value of 1.80 (Vargaftik, 1975). For the diffusion of organic compounds in air, the value of θ_{ca} is typically about 1.6 (Vargaftik, 1975). Because direct experimental data for the water-chemical vapor diffusivity are not usually available, the diffusivity is calculated using the Wilke and Lee empirical correlation (Reid et al., 1987). Details of this method are given in Appendix F.

8. SPECIFICATION OF FLOW GEOMETRY

Handling of flow geometry data in T2VOC is upward compatible with TOUGH input formats and data handling. As in other "integral finite difference" codes (Edwards, 1972; Narasimhan and Witherspoon, 1976), flow geometry is defined by means of a list of volume elements ("grid blocks"), and a list of flow connections between them. This formulation can cope with regular and irregular flow geometries in one, two, and three dimensions. Single- and multiple-porosity systems (porous and fractured media) can be specified, and higher order methods, such as seven- and nine-point differencing, can be implemented by means of appropriate specification of geometric data (Pruess and Bodvarsson, 1983).

Volume elements in T2VOC are identified by five-character names, such as "`ELE10`". Flow connections are specified as ordered pairs of elements, such as "(`ELE10`,`ELEll`)." A variety of options and facilities are available for entering and processing the corresponding geometric data. As in TOUGH, element volumes and domain identification can be provided by means of a data block **ELEME** in the INPUT file, while a data block **CONNE** can be used to supply connection data, including interface area, nodal distances from the interface, and orientation of the nodal line relative to the vertical. These data are internally written to a disk file MESH, which in turn initializes the geometry data arrays used during the flow simulation. The data formats on file MESH are identical with the format specifications for data blocks **ELEME** and **CONNE**.

T2VOC offers additional avenues for defining flow system geometry. By means of the keyword **MESHM**AKER in the INPUT file, a special program module can be invoked to perform a number of mesh generation and processing operations. The MESHMAKER module itself has a modular structure; present sub-modules include **RZ2D** for generating two-dimensional radially symmetric (R-Z) meshes, and **XYZ** for one-, two-, and three-dimensional rectilinear (Cartesian) grids. Multiple-porosity processing for simulation of flow in naturally fractured reservoirs can be invoked by means of a keyword **MINC**, which stands for "multiple interacting continua" (Pruess and Narasimhan, 1982, 1985; Pruess, 1983b; see Appendix B). The MINC-process operates on the data of the "primary" (porous medium) mesh as provided on disk file "MESH," and generates a "secondary" mesh containing fracture and matrix elements with identical data formats on file "MINC." (The file MESH used in this process can be either directly supplied by the user, or it can have been internally generated either from data in INPUT blocks **ELEME** and **CONNE**, or from **RZ2D** or **XYZ** mesh-making.) As a convenience for users desiring graphical

display of data, the internal mesh generation process will also write nodal point coordinates on file MESH. These data are written in 3E10.4 format into columns 51-80 of each grid block entry in data block **ELEME**. At the present time, no internal use whatsoever is made of nodal point coordinates in T2VOC .

In T2VOC elements are referenced by names consisting of a string of five characters, '`12345`.' These are arbitrary, except that the last two characters (#4 and 5) must be numbers. Specific naming conventions have been adopted in the internal mesh generation process. For **RZ2D**, the last two characters directly number the radial grid blocks, from 1 through 99. Character #3 is blank for the first 99 radial blocks, and then runs through the sequence 1, 2, ..., 9, A, B, ..., Z for a maximum total of 3599 radial blocks. The second character counts up to 35 grid layers as 1, 2, ..., 9, A, B, ..., Z. The first character is 'A' for the first 35 layers, and is incremented to B, C, ..., Z, 1, 2, ..., 9 for subsequent groups of 35 layers.

For rectilinear meshes generated by **XYZ**, characters 4 and 5 together number the grid blocks in X-direction, while character #3 = 1, 2, ..., 9, A, B, ..., Z numbers Y direction grid blocks, and character #2, running through the same sequence as #3, numbers grid blocks in Z direction. "Overflows" in any of these (more than 99 X-blocks, more than 35 Y- or Z-blocks) advance character #l through the sequence A, B, C, ..., Z. Both **RZ2D** and **XYZ** assign all grid blocks to domain #l (first entry in block **ROCKS**); a user desiring changes in domain assignments must do so "by hand," either through editing of the MESH file, or by appropriate source code changes in subroutines WRZ2D and GXYZ. T2VOC runs that involve **RZ2D** or **XYZ** mesh generation will produce a special printout, showing element names arranged in their actual geometric pattern. An example is given in Fig. 18.

The naming conventions for the **MINC** process are somewhat different from those originally adopted in the GMINC program (Pruess, 1983b), and are as follows. For a primary grid block with name '`12345`,' the corresponding fracture subelement in the secondary mesh is named '`  2345`' (character #1 replaced with a blank for easy recognition). The successive matrix continua are labeled by running character #1 through 2, ..., 9, A, B, ..., Z. The domain assignment is incremented by 1 for the fracture grid blocks, and by 2 for the matrix grid blocks. Thus, domain assignments in data block **ROCKS** should be provided in the following order: the first entry is the single (effective)

porous medium (POMED), then follows the effective fracture continuum (FRACT), and then the rock matrix (MATRX).

Users should beware that the MINC process may lead to ambiguous element names when the "inactive" element device (see below) is used to keep a portion of the primary mesh as unprocessed porous medium.

Mesh generation and/or MINC processing can be performed as part of a simulation run. Alternatively, by closing the INPUT file with the keyword **ENDFI** (instead of **ENDCY**), it is possible to skip the flow simulation and only execute the MESHMAKER module to generate a MESH or MINC file. These files can then be used, with additional user-modifications "by hand" if desired, in subsequent flow simulations. MESHMAKER input formats are described in Section 10, and examples of practical applications are given in the sample problems. Execution of MESHMAKER produces printed output which is self-explanatory.

9. T2VOC INPUT FORMATS

The input data for T2VOC are read in a format which is nearly identical to that used by the TOUGH and TOUGH2 codes (Pruess, 1987, 1991). The data are organized in blocks which are defined by keywords. The blocks **ROCKS**, **ELEME**, **CONNE**, **GENER**, **INCON** and **MESHM**aker can have a variable number of records, depending upon how many items the user wishes to specify. The end of these variable-length blocks is indicated with a blank record. (For **CONNE**, **GENER**, and **INCON** it is possible to have, instead of the blank record, a record with "+++" typed in columns 1-3, followed by some element and source cross-referencing information in the case of **CONNE** and **GENER**, and followed by restart information in the case of **INCON**; see below.)†

Much of the data handling in T2VOC is accomplished by means of several disk files, which are written in a format of 80 characters per record, so that they can be edited and modified with any normal text editor. Table 5 summarizes the disk files other than (default) INPUT and OUTPUT used in T2VOC, all of which are identical to those used in TOUGH2. The initialization of the arrays for geometry, generation, and initial condition data is always made from the disk files MESH (or MINC), GENER, and INCON. A user can either provide these files at execution time, or they can be written from T2VOC input data during the initialization phase of the program.

In comparison to standard TOUGH2, T2VOC has an additional data block CHEMP which supplies all of the information for a given volatile organic compound that is needed to compute the various thermophysical properties. All T2VOC input except for the CHEMP-data is in standard metric (SI) units, such as meters, seconds, Newtons, kilograms, Joules, and the corresponding derived units, such as Pascal = N/m^2 for pressure. We shall now explain the records and variables in detail. Keywords are shown bold-face; they are to be entered as character variables in A5 format. A summary of T2VOC input data is given in Fig. 2; clarifying examples will be given in section 12.

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†If the number of grid blocks exceeds 9999, FORMAT statements # 1505 in subroutine RFILE in `t2f.f` and in subroutine INPUT in `t2voc.f` must be changed from 20I4 to 16I5.

Table 5. T2VOC Disk Files

File	Use
MESH	written in subroutine INPUT from ELEME and CONNE data, or in module MESHMAKER from mesh specification data; read in RFILE to initialize all geometry data arrays used to define the discretized flow problem
GENER	written in subroutine INPUT from GENER data; read in RFILE to define nature, strength, and time-dependence of sinks and sources
INCON	written in subroutine INPUT from INCON data; read in RFILE to provide a complete specification of thermodynamic conditions
SAVE	written in subroutine WRIFI to record thermodynamic conditions at the end of a T2VOC simulation run; compatible with formats of file or data block INCON for initializing a continuation run
MINC	written in module MESHMAKER with MESH-compatible specifications, to provide all geometry data for a fractured-porous medium mesh (double porosity, dual permeability, etc.); read (optionally) in subroutine RFILE to initialize geometry data for a fractured-porous system
LINEQ	written during linear equation solution, to provide informative messages on linear equation solution
TABLE	not used by T2VOC
VERS	written in all T2VOC program units with informational message on version number, date, and function; read in main program and printed to default OUTPUT at the conclusion of a T2VOC simulation run; printing of version information is suppressed when keyword 'NOVER' is present in INPUT file

Figure 2.

T2VOC INPUT FORMATS

TITLE

ROCKS

MAT	NAD	DROK	POR	PER (1)	PER (2)	PER (3)	CWET	SPHT
COM		EXPAN	CDRY	TORTX	GK	FOC		
IRP		RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)
ICP		CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)

CHEMP

TCRIT	PCRIT	ZCRIT	OMEGA	DIPOLM
TBOIL	VPA	VPB	VPC	VPD
AMO	CPA	CPB	CPC	CPD
RHOREF	TDENRF	DIFV0	TDIFRF	TEXPO
VLOA	VLOB	VLOC	VLOD	VOLCRT
SOLA	SOLB	SOLC	SOLD	
OCK	FOX	ALAM		

(optional)

MULTI

NK	NEQ	NPH	NB

(optional)

START

MOP: 123456789012345678901234

PARAM

NOITE → MCYC, MSEC, MCYPR, MOP (I), I=1, 24, DIFF0, TEXP

KDATA →

TSTART	TIMAX	DELTEN or -NDLT	DELTMX	ELST	GF	REDLT	SCALE
DLT (1)	DLT (2)	DLT (3)					
					DLT (M)	(M≤8*NDLT)	
RE1	RE2	U	WUP	WNR	DFAC		
DEP (1)		DEP (2)		DEP (3)			

(optional)

RPCAP

IRP		RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)
ICP		CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)

(optional)

TIMES

ITI	ITE	DELAF	TINTER		
TIS(1)		TIS (2)	TIS (3)	TIS (ITI)	

(optional)

ELEME

EL	NE	NSEQ	NADD	MA1	MA2	VOLX			X	Y	Z

(optional)

CONNE

EL1	NE1	EL2	NE2	NSEQ	NAD1	NAD2	ISOT	D1	D2	AREAX	BETAX

Figure 2.

T2VOC INPUT FORMATS (continued)

GENER (optional)

1	2	3	4	5	6	7	8
EL, NE, SL, NS, NSEQ	NADD, NADS	LTAB	TYPE (ITAB)	GX	EX	HG	
F1(1)	F1(2)	F1(LTAB)					
F2(1)	F2(2)	F2(LTAB)					
F3(1)	F3(2)	F3(LTAB)					

INCON (optional)

1	2	3	4	5	6	7	8
EL, NE, NSEQ, NADD	PORX						
X1	X2	X3	X4				

NOVER (optional)

INDOM (optional)

MAT

1	2	3	4	5	6	7	8
X1	X2	X3	X4				

MESHM (optional)

ENDFI (optional)

ENDCY

TITLE is the first record of the input file, containing a header of up to 80 characters, to be printed on output. This can be used to identify a problem. If no title is desired, leave this record blank.

MESHM introduces parameters for internal mesh generation and processing. The MESHMaker input has a modular structure which is organized by keywords. Detailed instructions for preparing MESHMaker input are given in section 10, below.

Record MESHM.1

Format(A5)
WORD

WORD enter one of several keywords, such as **RZ2D**, **RZ2DL**, **XYZ**, **MINC**, to generate different kinds of computational meshes.

Record MESHM.2 A blank record closes the MESHM data block.

ENDFI is a keyword that can be used to close a T2VOC input file when no flow simulation is desired. This will often be used for a mesh generation run when some “hand-editing” of the mesh will be needed before the actual flow simulation.

ROCKS introduces material parameters for up to 27 different reservoir domains.

Record ROCKS.1

Format (A5, I5, 7E10.4)
MAT, NAD, DROK, POR, (PER (I), I = 1,3), CWET, SPHT

MAT material name (rock type).

NAD if zero or negative, defaults will take effect for a number of parameters (see below);

≥1: will read another data record to override defaults.

≥2: will read two more records with domain-specific parameters for relative permeability and capillary pressure functions.

DROK rock grain density (kg/m^3)

POR default porosity (void fraction) for all elements belonging to domain "MAT" for which no other porosity has been specified in block INCON. Option "START" is necessary for using default porosity.

PER(I), I = 1,3 absolute permeabilities along the three principal axes, as specified by ISOT in block CONNE.

CWET formation heat conductivity under fully liquid-saturated conditions (W/m ˚C).

SPHT rock grain specific heat (J/kg ˚C). Domains with SPHT > 10^4 J/kg ˚ C will not be included in global material balances. This provision is useful for boundary nodes, which are given very large volumes so that their thermodynamic state remains constant. Because of the large volume, inclusion of such nodes in global material balances would make the balances useless.

<u>Record ROCKS.1.1</u> (optional, NAD ≥ 1 only)

Format (6E10.4)
COM, EXPAN, CDRY, TORTX, GK, FOC

COM compressiblity (Pa^{-1}), $(1/\phi)(\partial\phi/\partial P)_T$ (default is 0)

EXPAN expansivity (1/ ˚C), $(1/\phi)(\partial\phi/\partial T)_P$ (default is 0)

CDRY formation heat conductivity under desaturated conditions (W/m ˚C). (default is CWET)

TORTX tortuosity factor for binary diffusion. If TORTX = 0, a porosity and saturation-dependent tortuosity will be calculated internally from the Millington and Quirk (1961) model.

GK Klinkenberg parameter b for enhancing gas phase permeability according to the relationship $k_{gas} = k_{liq} * (1 + b/P)$; units are Pa^{-1}.

FOC fraction of organic carbon present in domain; used for calculating amount of VOC adsorbed.

<u>Record ROCKS.1.2</u> (optional, NAD ≥ 2 only)

Format (I5, 5X,7E10.4)
IRP, (RP(I), I= 1,7)

IRP integer parameter to choose type of relative permeability function (see Appendix C).

RP(I), I = 1, ..., 7 parameters for relative permeability function.

<u>Record ROCKS.1.3</u> (optional, NAD ≥ 2 only)

Format (I5, 5X,7E10.4)
ICP, (CP(I), I = 1,7)

ICP integer parameter to choose type of capillary pressure function (see Appendix D).

CP(I) I = 1, ..., 7 parameters for capillary pressure function.

Repeat records 1, 1.1, 1.2, and 1.3 for up to 27 reservoir domains.

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 can be taken 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. (1992a).

Record CHEMP.1

Format (5E10.4)
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 (5E10.4)
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 (5El0.4)
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 (5El0.4)
RHOREF, TDENRF, DIFV0, TDIFRF, TEXPO

RHOREF reference NAPL (liquid) density, kg/m^3.

TDENRF reference temperature for NAPL density, K.

DIFV0 reference binary diffusivity of VOC in air, m^2/s.

TDIFRF reference temperature for gas diffusivity, K.

TEXPO exponent for calculation of chemical diffusivity.

Record CHEMP.5 introduces data for NAPL viscosity.

Format (5El0.4)
VLOA, VLOB, VLOC, VLOD, VOLCRT

Two options are available for calculating the NAPL liquid viscosity. The liquid viscosity constants VLOA - VLOD for the desired NAPL may be assigned data given in Table 9-8 of Reid et al. (1987), and the viscosity will be calculated using a polynomial fit to actual viscosity data. Alternatively, VLOA and VLOB may be set equal to 0, and VLOC and VLOD are assigned equal to a reference viscosity and a reference temperature, respectively. In this case, the viscosity is calculated from a more general (and less accurate) empirical relationship.

VLOA liquid NAPL viscosity constant from Reid et al. (1987).

VLOB liquid NAPI viscosity constant from Reid et al. (1987).

VLOC liquid NAPL viscosity constant from Reid et al. (1987).
If VLOA and VLOB = 0, VLOC is reference NAPL viscosity, cP.

VLOD liquid NAPL viscosity constant from Reid et al. (1987).
If VLOA and VLOB = 0, VLOD is reference temperature for NAPL viscosity, K.

VOLCRT chemical critical volume, cm^3/mole.

Record CHEMP.6 introduces data for chemical solubility.

Fomat (4E10.4)
SOLA, SOLB, SOLC, SOLD

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 should be calculated from a polynomial fit of the data. If such 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.

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^2.

SOLD constant for chemical solubility in water, mole fraction/K^3.

Record CHEMP.7

Fomat (3El0.4)
OCK, FOX, ALAM

OCK chemical organic carbon partition coefficient K_{oc} (see Eq. 5), m^3/kg.

FOX default value for fraction of organic carbon in soil, used for all domains for which no specific value is provided in record ROCKS.1.1.

ALAM decay constant for biodegradation of VOC, s^{-1}. Biodegradation is assumed to take place only in the aqueous phase, and to follow a first order decay law, $M_{VOC}(t) = M_{VOC,0} * \exp(-\lambda t)$. The decay constant λ = ALAM is expressed in terms of the half life $T_{1/2}$ of the VOC as follows: $\lambda = (\ln 2) / T_{1/2}$. Default is ALAM = 0.

MULTI permits the user to select the number and nature of balance equations that will be solved. The keyword MULTI is followed by a single data record.

Record MULTI. l

Format (4I5)
NK, NEQ, NPH, NB

NK number of mass components. Available options are NK = 2, for solving water and air mass balances only, and NK = 3 (default), for solving three mass balances for water, air, and VOC.

NEQ number of balance equations per grid block. Available options are NEQ = NK, for solving NK mass balance equations, and NEQ = NK + 1, for solving NK mass and one energy balance. Default is NEQ = 4.

NPH number of phases that can be present (NPH = 3 is only available option).

NB number of secondary parameters in PAR-array other than component mass fractions (NB = 6 is only available option).

Note that when NK = 2 is specified only 3 primary variables are used, namely, (X1, X2, X4), where X1 is pressure, X4 is temperature, and X2 depends on the phase composition. X2 is water saturation (0 < X2 < 1) for 2-phase water-gas conditions, it is (50 + dissolved air mass fraction) for single phase (aqueous) conditions.

START (optional)

A record with START typed in columns 1-5 allows a more flexible initialization. More specifically, when START is present, INCON data can be in arbitrary order, and need not be present for all grid blocks (in which case defaults will be used). Without START, there must be a one-to-one correspondence between the data in blocks ELEME and INCON.

PARAM introduces computation parameters.

Record PARAM.1

Format (2I2, 3I4, 24I1, 2E10.4).
NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), DIFF0, TEXP

NOITE specifies the maximum number of Newtonian iterations per time step (default value is 8)

KDATA specifies amount of printout (default = 1).

0 or 1: print a selection of the most important variables.

2: in addition print mass and heat fluxes and flow velocities.

3: in addition print primary variables and their changes.

If the above values for KDATA are increased by 10, printout will occur after each iteration (not just after convergence).

MCYC maximum number of time steps to be calculated.

MSEC maximum duration, in machine seconds, of the simulation (default is infinite).

MCYPR printout will occur for every multiple of MCYPR steps (default is 1).

MOP(I), I = 1,24 allows choice of various options, which are documented in printed output from a T2VOC run.

MOP(1) if unequal 0, a short printout for non-convergent iterations will be generated.

MOP(2) through MOP(6) generate additional printout in various subroutines, if set ≠ 0. This feature should not be needed in "normal" applications, but it may be convenient when a user suspects a bug and wishes to examine the inner workings of the code. The amount of printout increases with MOP(I) (consult source code listings for details).

MOP(2) CYCIT (main subroutine).

MOP(3) MULTI (flow- and accumulation-terms).

MOP(4) QU (sinks/sources).

MOP(5) EOS (equation of state).

MOP(6) LINEQ (linear equations).

MOP(7) if unequal 0, a printout of input data will be provided.

Calculational choices are as follows:

MOP(9) determines the composition of produced fluid with the MASS option (see GENER, below). The relative amounts of phases are determined as follows:

0: according to relative mobilities in the source element.

1: source fluid has the same phase composition as the producing element.

MOP(10) chooses the interpolation formula for heat conductivity as a function of liquid saturation (Sl)

0: $C(S_l) = CDRY + SQRT(S_l * [CWET - CDRY])$

1: $C(S_l) = CDRY + S_l * (CWET - CDRY)$

MOP(11) determines evaluation of mobility and permeability at interfaces.

0: mobilities are upstream weighted with WUP (default is WUP = 1), permeability is upstream weighted.

1: mobilities are averaged between adjacent elements, permeability is upstream weighted.

2: mobilities are upstream weighted, permeability is harmonic weighted.

3: mobilities are averaged between adjacent elements, permeability is harmonic weighted.

4: mobility and permeability are both harmonic weighted.

MOP(12) determines interpolation procedure for time-dependent generation data.

0: triple linear interpolation.

1: step function option.

MOP(14) determines handling of pivot failures in matrix decomposition (MA28 only).

0: perform new matrix decomposition when encountering a pivot failure.

≠0: ignore pivot failures.

MOP(16) provides automatic time step control. Time step size will be doubled if convergence occurs within ITER ≤ MOP(16) iterations.

MOP(17) permits to choose a scaling-option for preconditioning the Jacobian matrix (MA28 only).

0: no scaling.

7: do perform scaling.

MOP(18) allows to select handling of interface density.

0: perform upstream weighting for interface density.

>0: average interface density between the two grid blocks. However, when one of the two phase saturations is zero, upstream weighting will be performed.

MOP(19) allows conversion of primary variables when initializing a three-component run (water, air, VOC; default NK = 3 specified in block **MULTI**) from NK = 2 data (only water and air components present). This is useful when initial conditions such as gravity-capillary equilibrium prior to a NAPL spill, obtained from a simulation run with NK = 2, are to be used in subsequent simulations of NAPL contamination and remediation. An illustrative example of the use of MOP(19) is given in sample problem 4, section 12.4.

0: primary variables will be initialized exactly as input by the user.

1: user-specified primary variables are (X1, X2, X4), where X1 is pressure, X4 is temperature, and X2 depends on the phase composition. X2 is water saturation (0 < X2 < 1) for 2-phase water-gas conditions, it is (50 + dissolved air mass fraction) for single phase (aqueous) conditions; see Table 3.During initialization these user-specified variables are

converted to (X1, X2, X3=0, X4), where X3 is VOC mole fraction in the aqueous phase (single-phase aqueous conditions), or VOC mole fraction in the gas phase (2-phase water-gas conditions).

MOP(21) permits to select the linear equation solver (available only when the preconditioned conjugate gradient module T2CG1 is used).

0: defaults to MOP(21) = 3, DSLUCS, Lanczos-type preconditioned bi-conjugate gradient solver.

1: MA28 sparse direct solver.

2: DSLUBC, bi-conjugate gradient solver.

3: DSLUCS (see MOP(21) = 0).

4: DSLUGM, generalized minimum residual preconditioned conjugate gradient solvers.

All conjugate gradient solvers use incomplete LU-factorization as a preconditioner.

DIFF0 strength parameter for air-vapor diffusion at standard conditions of T = 0 ˚C, P = 1 bar; DIFF0 = 2.13e-5 m2/s. DIFF0 = 0 results in no gas diffusion-calculation.

TEXP parameter for temperature dependence of vapor-air diffusion coefficient. Default value is TEXP = 1.80.

<u>Record PARAM.2</u>

Format (4E10.4, A5, 5X,3E10.4)
TSTART, TIMAX, DELTEN, DELTMX, ELST, GF, REDLT, SCALE

TSTART starting time of simulation in seconds (default is 0).

TIMAX time in seconds at which simulation should stop (default is infinite).

DELTEN length of time steps in seconds. If DELTEN is a negative integer, DELTEN = -NDLT, the program will proceed to read NDLT records with time step information. Note that - NDLT must be provided as a floating point number, with decimal point.

DELTMX upper limit for time step size in seconds (default = ∞)

ELST set equal to the name of one element to obtain a short printout after each time step.

GF magnitude (m/sec^2) of the gravitational acceleration vector. Blank or zero gives "no gravity" calculation.

REDLT factor by which time step is reduced in case of convergence failure or other problems (default is 4).

SCALE scale factor to change the size of the mesh (default = 1.0).

Record PARAM.2.1, 2.2, etc.

Format (8E10.4)
(DLT(I), I = 1, 100)

DLT(I) Length (in seconds) of time step I.

This set of records is optional for DELTEN = - NDLT, a negative integer. Up to 13 records can be read, each containing 8 time step data. If the number of simulated time steps exceeds the number of DLT(I), the simulation will continue with time steps equal to the last non-zero DLT(I) encountered (except for automatic time step reductions when problems are encountered, or time step increases when automatic time step control is chosen with MOP(16) $\neq$ 0)

Record PARAM.3

Format (6E10.4)
RE1, RE2, U, WUP, WNR, DFAC

RE1 convergence criterion for relative error (default= 1.E-5).

RE2 convergence criterion for absolute error (default= 1).

U pivoting parameter for linear equation solution with the MA28 direct solver. U must be in the range $0 \leq U < 1$, and the default is U = 0.1. Increased value for U will make criterion for pivot selection more stringent, resulting in better numerical stability at the expense of increased computing time for matrix decomposition.

WUP upstream weighting factor for mobilities and enthalpies at interfaces (default = 1.0 is recommended). $0 \leq WUP \leq 1$.

WNR weighting factor for increments in Newton/Raphson - iteration (default = 1.0 is recommended). $0 < WNR \leq 1$.

DFAC increment factor for numerically computing derivatives (default value is DFAC = $10^{-k/2}$, where k, evaluated internally, is the number of significant digits of the floating point processor used; for 64-bit arithmetic, DFAC $\approx 10^{-8}$).

Record PARAM.4 introduces a set of primary variables (see Table 3) which are used as default initial conditions for all elements not specified in block INCON. Option START is necessary to use default INCON.

Format (3E20.14)
DEP(I), I = 1,4

DEP(1) pressure (Pa).

DEP(2) < 1: aqueous phase saturation (two and three-phase conditions).

≥ 50: (dissolved air mass fraction + 50) (single-phase aqueous conditions).

DEP(3) < 1: mole fraction of VOC in aqueous phase (single-phase aqueous conditons), or mole fraction of VOC in gas phase (two-phase aqueous-gas conditions).

10 < DEP(3) < 11: (gas saturation + 10) (three-phase conditions).

> 50: (air mass fraction in aqueous phase + 50) (two-phase aqueous-NAPL conditions).

DEP(4) temperature (^{o}C).

Note: When NK = 2 is specified in data block MULTI, the third primary variable is omitted and DEP(4), temperature, appears in slot # 3.

NOVERSION (optional)

One record with 'NOVER' typed in columns 1-5 will suppress printing of a summary of versions and dates of the program units used in a T2VOC run.

INDOM introduces domain-specific initial conditions. Option START is needed to use INDOM conditions.

Record INDOM. l

Format(A5)
MAT

MAT name of a reservoir domain, as specified in data block ROCKS.

Record INDOM.2

Format(4E20.13)
Xl, X2, X3, X4

A set of primary variables assigned to all grid blocks in the domain specified in record INDOM. l. See data block PARAM.4 and Table 3 for an explanation of the primary variables.

Record INDOM.3

A blank record closes the INDOM data block. Repeat records INDOM. l and INDOM.2 for as many domains as desired. The ordering is arbitrary and need not be the same as in block ROCKS.

RPCAP introduces information on relative permeability and capillary pressure functions, which will be applied for all flow domains for which no data were specified in records ROCKS.1.2 and ROCKS.1.3. A catalog of relative permeability and capillary pressure functions is presented in Appendix C and Appendix D, respectively.

Record RPCAP.1

Format (I5,5X,7E10.4)
IRP, (RP(I),I = 1, 7)

IRP integer parameter to choose type of relative permeability function (see Appendix C).

RP(I), I = 1, ..., 7 parameters for relative permeability function.

Record RPCAP.2

Format (I5,5X,7E10.4)
ICP, (CP(I), I = 1, 7)

ICP integer parameter to choose type of capillary pressure function (see appendix D).

CP(I) I = 1, ..., 7 parameters for capillary pressure function.

TIMES permits the user to obtain printout at specified times (optional). This printout will occur in addition to printout specified in record PARAM.1.

Record TIMES.1

Format (2I5,2E10.4)
ITI, ITE, DELAF, TINTER

ITI number of times provided on records TIMES.2, TIMES.3, etc., (see below; restriction: ITI ≤ 100).

ITE total number of times desired (ITI ≤ ITE ≤ 100; default is ITE = ITI).

DELAF maximum time step size after any of the prescribed times have been reached (default is ∞).

TINTER time increment for times with index ITI, ITI+1, ..., ITE.

Record TIMES.2, TIMES.3, etc.

Format (8E10.4)
(TIS(I), I = l, ITI)

TIS(I) list of times (in ascending order) at which printout is desired.

ELEME introduces element information.

Record ELEME.1

Format (A3, I2, 2I5, A3, A2, E10.4,20X,3E10.4)
EL, NE, NSEQ, NADD, MA1, MA2, VOLX, X, Y, Z

EL, NE 5-character code name of an element. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional elements having the same volume and belonging to the same reservoir domain.

NADD increment between the code numbers of two successive elements. (Note: the maximum permissible code number NE + NSEQ * NADD is ≤ 99.).

MA1, MA2 a five character material identifier corresponding to one of the reservoir domains as specified in block ROCKS. If the first three characters are blanks and the last two characters are numbers then they indicate the sequence number of the domain as entered in ROCKS. If both MA1 and MA2 are left blank the element is by default assigned to the first domain in block ROCKS.

VOLX element volume (m^3).

X, Y, Z Cartesian coordinates of grid block centers. These data are not used in T2VOC; they may be included in the ELEME data to make subsequent plotting of results more convenient.

Repeat record ELEME.1 for the number of elements desired.

Record ELEME.2 A blank record closes the ELEME data block.

CONNE introduces information for the connections (interfaces) between elements.

Record CONNE.1

Format (A3, I2, A3, I2, 4I5, 4E10.4)
EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

EL1, NE1 code name of the first element.

EL2, NE2 code name of the second element.

NSEQ number of additional connections in the sequence.

NAD1 increment of the code number of the first element between two successive connections.

NAD2 increment of the code number of the second element between two successive connections.

ISOT set equal to 1, 2, or 3; specifies absolute permeability to be PER(ISOT) for the materials in elements (EL1, NE1) and (EL2, NE2), where PER is read in block ROCKS. This allows assignment of different permeabilities, e.g., in the horizontal and vertical direction.

D1 } distance (m) from center of first and second element, respectively,
D2 } to their common interface.

AREAX interface area (m^2).

BETAX cosine of the angle between the gravitational acceleration vector and the line between the two elements. GF * BETAX > 0 (<0) corresponds to first element being above (below) the second element.

Repeat record CONNE.1 for the number of connections desired.

Record CONNE.2 A blank record closes the CONNE data block. Alternatively, connection information may terminate on a record with '+++' typed in the first three columns, followed by element cross-referencing information. This is the termination used when generating a MESH file with T2VOC.

GENER introduces sinks and/or sources.

Record GENER.1

Format (A3, I2, A3, I2, 4I5, 5X,A4, A1,3E10.4)
EL, NE, SL, NS, NSEQ, NADD, NADS, LTAB, TYPE, ITAB, GX, EX, HG

EL, NE code name of the element containing the sink/source.

SL, NS code name of the sink/source. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional sinks/sources with the same injection/production rate (not applicable for TYPE = DELV).

NADD increment between the code numbers of two successive elements with identical sink/source.

NADS increment between the code numbers of two successive sinks/sources.

LTAB number of points in table of generation rate versus time. Set 0 or 1 for constant generation rate. For wells on deliverability, LTAB denotes the number of open layers, to be specified only for the bottommost layer.

TYPE HEAT - heat sink/source.

COMl	}}	- component 1 (water).	injection
WATE	}}		
COM2	}}	- component 2 (air).	only
AIR	}}		
COM3	}}	- component 3 (VOC)	

MASS - mass production rate specified.

DELV - well on deliverability, i.e. production occurs against specified wellbore pressure. If well is completed in more than one layer, bottommost layer must be specified first, with number of layers given in LTAB. Subsequent layers must be given sequentially for a total number of LTAB layers.

ITAB unless left blank, table of specific enthalpies will be read (LTAB > 1 only).

GX constant generation rate; positive for injection, negative for production; GX is mass rate (kg/sec) for generation types COMl, WATE, COM2, AIR, COM3, and MASS; it is energy rate (J/s) for a HEAT sink/source. For wells on deliverability, GX is productivity index PI (m^3).

EX fixed specific enthalpy (J/kg) of the fluid for mass injection (GX>0). For wells on deliverability, EX is bottomhole pressure P_{wb} (Pa), at the center of the topmost producing layer in which the well is open.

HG thickness of layer (m; wells on deliverability only).

<u>Record GENER.l.l</u> (optional, LTAB > l only)

Format (4E14.7)
Fl(L), L=l, LTAB

F1 generation times

Record GENER.1.2 (optional, LTAB > 1 only)

Format (4E14.7)
F2(L), L=1, LTAB

F2 generation rates.

Record GENER.1.3 (optional, LTAB > 1 and ITAB non-blank only)

Format (4E14.7)
F3(L), L=1, LTAB

F3 specific enthalpy of produced or injected fluid.

Repeat records GENER.1, 1.1, 1.2, and 1.3 for up to 100 sinks/sources.

Record GENER.2 A blank record closes the GENER data block. Alternatively, generation information may terminate on a record with '+++' typed in the first three columns, followed by element cross-referencing information.

INCON introduces element-specific initial conditions.

Record INCON.1

Format (A3, I2, 2I5, E15.9)
EL, NE, NSEQ, NADD, PORX

EL, NE code name of element.

NSEQ number of additional elements with the same initial conditions.

NADD increment between the code numbers of two successive elements with identical initial conditions.

PORX porosity (void fraction); if zero or blank, porosity will be taken as specified in block ROCKS if option START is used.

Record INCON.2 specifies primary variables (see Table 3).

Format (4E20.14)
X1, X2, X3, X4

Set of primary variables for the element specified in record INCON.1.

X1 pressure (Pa).

X2 < 1: aqueous phase saturation (two and three-phase conditions).

≥ 50: (dissolved air mass fraction + 50) (single-phase aqueous conditions).

X3 < 1: mole fraction of VOC in aqueous phase (single-phase aqueous conditons), or mole fraction of VOC in gas phase (two-phase aqueous-gas conditions).

10 < X3 < 11: (gas saturation + 10) (three-phase conditions).

> 50: (air mass fraction in aqueous phase + 50) (two-phase aqueous-NAPL conditions).

X4 temperature (^{o}C).

Note: When NK = 2 is specified in data block MULTI, the third primary variable is omitted and X4, temperature, appears in slot # 3.

Record INCON.3 A blank record closes the INCON data block. Alternatively, initial condition information may terminate on a record with '+++' typed in the first three columns, followed by time stepping information. This feature is used for a continuation run from a previous T2VOC simulation.

ENDCY closes the T2VOC input file and initiates the simulation.

Note on closure of blocks CONNE, GENER, and INCON

The "ordinary" way to indicate the end of any of the above data blocks is by means of a blank record. There is an alternative available if the user makes up an input file from files MESH, GENER, or SAVE, which have been generated by a previous T2VOC run. These files are written exactly according to the specifications of data blocks ELEME and CONNE (file MESH), GENER (file GENER), and INCON (file SAVE), except that the CONNE, GENER, and INCON data terminate on a record with "+++" in columns 1-3, followed by some cross-referencing and restart information. T2VOC will accept this type of input, and in this case there is no blank record at the end of the indicated data blocks.

10. INPUT FORMATS FOR MESHMAKER

The keyword **MESHM**AKER introduces parameters for internal mesh generation and processing. The MESHMAKER input has a modular structure and a variable number of records; its end is indicated by a blank record.

At the present time there are three sub-modules available in MESHMAKER**:** keywords **RZ2D** or **RZ2DL** invoke generation of a one or two-dimensional radially symmetric R-Z mesh; **XYZ** initiates generation of a one, two, or three dimensional Cartesian X-Y-Z mesh; and **MINC** calls a modified version of the "GMINC" program (Pruess, 1983b) to sub-partition a "primary" porous medium mesh into a "secondary" mesh for fractured media, using the method of "multiple interacting continua" (Pruess and Narasimhan, 1982, 1985). The meshes generated under keyword **RZ2D** or **XYZ** are internally written to file MESH. The **MINC** processing operates on the data in file MESH, so that invoking the **RZ2D** or **XYZ** options, or assignment of **ELEME** and **CONNE** blocks in the INPUT file must precede the **MESHM**AKER/**MINC** data. We shall now separately describe the preparation of input data for the three MESHMAKER sub-modules.

10.1 Generation of radially symmetric grids

Keyword **RZ2D** (or **RZ2DL**) invokes generation of a radially symmetric mesh. Values for the radii to which the grid blocks extend can be provided by the user or can be generated internally (see below). Nodal points will be placed half-way between neighboring radial interfaces. When **RZ2D** is specified, the mesh will be generated "by columns;" i.e., in the **ELEME** block we will first have the grid blocks at smallest radius for all layers, then the next largest radius for all layers, and so on. With keyword **RZ2DL** the mesh will be generated "by layers;" i.e., in the **ELEME** block we will first have all grid blocks for the first (top) layer from smallest to largest radius, then all grid blocks for the second layer, and so on. Apart from the different ordering of elements, the two meshes for **RZ2D** and **RZ2DL** are identical. The reason for providing the two alternatives is as a convenience to users in implementing boundary conditions by way of "inactive" elements (see Section 5). Assignment of inactive elements would be made by using a text editor on the RZ2D-generated "MESH" file, and moving groups of elements towards the end of the **ELEME** block, past a "dummy" element with zero volume. **RZ2D** makes it easy to declare a vertical column inactive, facilitating assignment of boundary conditions in the vertical, such as a gravitationally equilibrated pressure gradient. **RZ2DL** on the other hand facilitates implementation of "areal" (top and bottom layer) boundary conditions.

RADII is the first keyword following **RZ2D**; it introduces data for defining a set of interfaces (grid block boundaries) in the radial direction.

Record RADII.l

Format(I5)
NRAD

NRAD number of radius data that will be read. At least one radius must be provided, indicating the inner boundary of the mesh.

Record RADII.2

Format(8E10.4)
RC(I), I = 1, NRAD

RC(I) a set of radii in ascending order.

EQUIDISTANT introduces data on a set of equal radial increments.

Record EQUID. l

Format(I5, 5X, E10.4)
NEQU, DR

NEQU number of desired radial increments.
DR magnitude of radial increment.

Note: At least one radius must have been defined via block **RADII** before **EQUID** can be invoked.

LOGARITHMIC introduces data on radial increments that increase from one to the next by the same factor ($\Delta R_{n+l} = f \bullet \Delta R_n$).

Record LOGAR. l

Format(A5, 5X, 2E10.4)
NLOG, RLOG, DR

NLOG number of additional interface radii desired.
RLOG desired radius of the last (largest) of these radii.
DR reference radial increment: the first ΔR generated will be equal to f • DR, with f internally determined such that the last increment will bring total radius to RLOG. f < 1 for decreasing radial increments is permissible. If DR is set equal to zero, or left blank, the last increment DR generated before keyword **LOGAR** will be used as default.)

Additional blocks **RADII**, **EQUID**, and **LOGAR** can be specified in arbitrary order.

Note: At least one radius must have been defined before **LOGAR** can be invoked. If DR = 0, at least two radii must have been defined.

LAYER introduces information on horizontal layers, and signals closure of **RZ2D** input data.

Record LAYER. l

Format(I5)
NLAY

NLAY number of horizontal grid layers.

Record LAYER.2

Format(8E10.4)
H(I), I = 1, NLAY

H(I) a set of layer thicknesses, from top layer downward. By default, zero or blank entries for layer thickness will result in assignment of the last preceding non-zero entry. Assignment of a zero layer thickness, as needed for inactive layers, can be accomplished by specifying a negative value.

The **LAYER** data close the **RZ2D** data block. Note that one blank record must follow to indicate termination of the **MESHM** data block. Alternatively, keyword **MINC** can appear to invoke MINC-processing for fractured media (see below).

10.2 Generation of rectilinear grids

XYZ invokes generation of a Cartesian (rectilinear) mesh.

Record XYZ.l

Format(E10.4)
DEG

DEG angle (in degrees) between the Y-axis and the horizontal. If gravitational acceleration (parameter GF in record PARAM.2) is specified positive, -90° < DEG < 90° corresponds to grid layers going from top down. Grids can be specified from bottom layer up by setting GF or BETA negative. Default (DEG = 0) corresponds to horizontal Y- and vertical Z-axis. X-axis is always horizontal.

Record XYZ.2

Format(A2, 3X, I5, E10.4)
NTYPE, NO, DEL

NTYPE set equal to **NX**, **NY** or **NZ** for specifying grid increments in X, Y, or Z direction.

NO number of grid increments desired.

DEL constant grid increment for NO grid blocks, if set to a non zero value.

Record XYZ.3 (optional, DEL = 0. or blank only)

Format(8E10.4)
DEL(I), I = 1, NO

DEL(I) a set of grid increments in the direction specified by NTYPE in record XYZ.2. Additional records with formats as XYZ.2 and XYZ.3 can be provided, with X, Y, and Z-data in arbitrary order.

Record XYZ.4 a blank record closes the XYZ data block.

Note that the end of block **MESHM**AKER is also marked by a blank record. Thus, when **MESHM**AKER/**XYZ** is used, there will be two blank records at the end of the corresponding input data block.

10.3 MINC processing for fractured media

MINC invokes postprocessing of a primary porous medium mesh from file MESH. The input formats in data block **MINC** are identical to those of the GMINC program (Pruess, 1983b), with two enhancements: there is an additional facility for specifying global matrix-matrix connections ("dual permeability"); further, only "active" elements will be subjected to MINC-processing, the remainder of the MESH remaining unaltered as porous medium grid blocks. See Appendix B for further discussion.

PART is the first keyword following **MINC**; it introduces information on the nature of fracture distributions and matrix-matrix connections.

Format(2A5, 5X, A5)
PART, TYPE, DUAL

PART identifier of data block with partitioning parameters for secondary mesh.

TYPE a five-character word for selecting one of the six different proximity functions provided in MINC (Pruess, 1983b).

ONE-D: a set of plane parallel infinite fractures with matrix block thickness between neighboring fractures equal to PAR(l).

TWO-D: two sets of plane parallel infinite fractures, with arbitrary angle between them. Matrix block thickness is PAR(l) for the first set, and PAR(2) for the second set. If PAR(2) is not specified explicitly, it will be set equal to PAR(l).

THRED: three sets of plane parallel infinite fractures at right angles, with matrix block dimensions of PAR(l), PAR(2), and PAR(3), respectively. If PAR(2) and/or PAR(3) are not explicitly specified, they will be set equal to PAR(l) and/or PAR(2), respectively.

STANA: average proximity function for rock loading of Stanford large reservoir model (Lam et al., 1988).

STANB: proximity function for the five bottom layers of Stanford large reservoir model.

STANT: proximity function for top layer of Stanford large reservoir model.

Note: a user wishing to employ a different proximity function than provided in **MINC** needs to replace the function subprogram PROX(x) with a routine of the form:

```
FUNCTION PROX(x)
PROX = (arithmetic expression in x)
RETURN
END
```

It is necessary that PROX(x) is defined even when x exceeds the maximum possible distance from the fractures, and that PROX = 1 in this case. Also, when the user supplies his/her own proximity function subprogram, the parameter TYPE has to be chosen equal to **ONE-D**, **TWO-D**, or **THRED**, depending on the dimensionality of the proximity function. This will assure proper definition of innermost nodal distance (Pruess, 1983b).

DUAL is a five-character word for selecting the treatment of global matrix matrix flow.

blank: (default) global flow occurs only through the fracture continuum, while rock matrix and fractures interact locally by means of "interporosity" flow ("double-porosity" model).

MMVER: global matrix-matrix flow is permitted only in the vertical; otherwise like the double-porosity model; for internal consistency this choice should only be made for flow systems with one or two predominantly vertical fracture sets.

MMALL: global matrix-matrix flow in all directions; for internal consistency only two continua, representing matrix and fractures, should be specified ("dual-permeability").

<u>Record PART.l</u>

Format (2I3, A4, 7E10.4)
J, NVOL, WHERE, (PAR(I), I = 1, 7)

J total number of multiple interacting continua (J < 36).

NVOL total number of explicitly provided volume fractions (NVOL < J). If NVOL < J, the volume fractions with indices NVOL+l, ..., J will be internally generated; all being equal and chosen such as to yield proper normalization to 1.

WHERE specifies whether the sequentially specified volume fractions begin with the fractures (WHERE = ‘OUT ‘) or in the interior of the matrix blocks (WHERE = 'IN ').

PAR(I), I = 1, 7 holds parameters for fracture spacing (see above).

Record PART.2.1, 2.2, etc.

Format (8E10.4)
(VOL(I), I = 1, NVOL)

VOL(I) volume fraction (between 0 and 1) of continuum with index I (for WHERE = ‘OUT ‘) or index J+ l - I (for WHERE = ‘IN ‘). NVOL volume fractions will be read. For WHERE = ‘OUT ‘, I = 1 is the fracture continuum, I = 2 is the matrix continuum closest to the fractures, I = 3 is the matrix continuum adjacent to I = 2, etc. The sum of all volume fractions must not exceed 1.

11. T2VOC OUTPUT

The output produced by T2VOC occurs at times specified by the user (as in TOUGH2), and includes a listing of the conditions in all elements at that time. The T2VOC output lists each element twice in order to give a more complete description of the conditions present. The quantities printed on output are listed in tables 6 and 7.

Table 6. Output Parameters (first list).

notation	meaning
P	gas phase pressure, Pa.
T	temperature, ° C .
SO	NAPL phase saturation.
SW	aqueous phase saturation.
SG	gas phase saturation.
PVOC	VOC vapor pressure, Pa.
PAIR	air partial pressure, Pa.
PSATO	VOC saturated vapor pressure, Pa.
PSATW	water saturated vapor pressure, Pa.
PCO	gas-NAPL capillary pressure, Pa.
PCW	gas-water capillary pressure, Pa.

Table 7. Output Parameters (second list).

notation	meaning
CVOCGAS	VOC concentration in the gas phase, kg/m^3.
CVOCAQ.	VOC concentration in the aqueous phase, kg/m^3.
DGAS	gas phase density, kg/m^3.
DNAPL	NAPL density, kg/m^3.
VISGAS	gas phase viscosity, kg/m s.
VISNAPL	NAPL viscosity, kg/m s.
DIFFO	VOC vapor diffusivity, m^2/s.
DIFFW	water vapor diffusivity, m^2/s.
KRGAS	gas phase relative permeability.
KRAQ.	aqueous phase relative permeability.
KRNAPL	NAPL relative permeability.

Additional optional printed output is available for fluid and heat flow rates, (pore) velocities of the phases, primary thermodynamic variables and their increments, and specific phase enthalpies.

12. SAMPLE PROBLEMS

The following problems were run on an IBM RS/6000 workstation using double precision (64-bit) arithmetic by means of the compiler option "`-qautodbl=dblpad`". These problems are intended to illustrate T2VOC capabilities and preparation of input data; they can also serve as benchmarks to verify proper code installation on different machines.

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

In this problem, chlorobenzene vapor diffuses through two initially clean one dimensional columns. The two columns are separate and constitute two independent flow problems, except that being simulated together they must go through the same time steps. Phase partitioning of the vapor into an immobile aqueous phase and the solid phase (adsorption) is included. Initially, the columns do 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 3. We take advantage of the isothermal nature of the problem and specify NEQ = 3 in block **MULTI**, to solve just 3 mass balances and no energy equation. The mesh for each column consists of 100 elements which are connected to an inactive element (`BN 1`, with zero volume) that supplies the VOC vapor pressure boundary condition. For the first 5 m, the mesh spacing is 0.1 m. After 5 m, the mesh spacing is increased to 0.2 m for 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 assigning the default value for fraction of organic carbon in the soil to f_{oc} = .005. This value is used in domain `DIRT1` (first column, with elements `AA 1`, `AA 2`, etc.), while in domain `DIRT2` (second column, elements `aa 1`, `aa 2`, etc.) a value of f_{oc} = .0025 is specified. Due to the relatively high aqueous solubility and organic carbon partition coefficient of chlorobenzene, the chlorobenzene vapor diffusion is strongly retarded. Calculating the gas phase retardation coefficient from Eq. (7) we find R_g^c = 67.8 for f_{oc} = .005, and R_g^c = 37.0 for f_{oc} = .0025. For users who may be familiar with the STMVOC code, STMVOC-type primary variables are included in the input file after the ENDCY statement.

The initial time step size is set equal to 1 second, and is allowed to grow to a maximum value of 5 days. The simulation is terminated after one year, which is reached after 91 time steps. A partial printout of the T2VOC simulation results after one year is given in Figure 4. A comparison with an analytical solution for transient gas diffusion with

phase partitioning (Baehr, 1987) is shown in Figure 5. The numerical solution calculated using T2VOC 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 Fick's law during evaporation of the NAPL, and no density driven (buoyant) 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 T2VOC simulator. For a discussion of deviations from Fick's second law of diffusion from evaporation effects, 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 μg/l, the value of RE1 in record PARAM.3 should be reduced from the default value of $1x10^{-5}$ to a value of $1x10^{-7}$ or less. This will result in an increased number of iterations for a given problem, but will increase the accuracy of the simulation for very low concentrations.

Figure 3. T2VOC input file for problem 1.

```
*rgdif* ... 1D GAS DIFFUSION OF CHLOROBENZENE WITH PHASE PARTITIONING **********
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1         2650.0      .400   1.0E-14   1.0E-14   1.0E-14       3.1    1000.0
DIRT2    1    2650.0      .400   1.0E-14   1.0E-14   1.0E-14       3.1    1000.0
                                                        .0025

CHEMP----1----*--Chlorobenzene data----4----*----5----*----6----*----7----*----8
     632.4      45.2     0.265     0.249       1.6
     404.9    -7.587   2.26551  -4.09418   0.17038
   112.559   -33.890     .5631 -4.522E-4  1.426E-7
    1106.0     293.0    8.0E-6    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        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1 350     35010000000000000400000000   2.13E-5
            3.1558E7       1.0    4.32E5AA  1         9.8060
     1.E-5     1.E00
          1.01325e5                0.25                0.00                10.0
RPCAP----1---------2---------3---------4---------5---------6---------7---------8
    6            0.4       0.1     0.001        1.
    9
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
AA  1   49    1DIRT1     0.100
BB  1   49    1DIRT1     0.200
aa  1   49    1DIRT2     0.100
bb  1   49    1DIRT2     0.200
BN  1    1    1DIRT1

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
BN  1AA  1                  1     .0001     .0500      1.00       0.0
AA  1AA  2   48    1    1    1     .0500     .0500      1.00       0.0
AA 50BB  1                  1     .0500     .1000      1.00       0.0
BB  1BB  2   48    1    1    1     .1000     .1000      1.00       0.0
BB 50BN  2                  1     .1000     .0001      1.00       0.0
BN  1aa  1                  1     .0001     .0500      1.00       0.0
aa  1aa  2   48    1    1    1     .0500     .0500      1.00       0.0
aa 50bb  1                  1     .0500     .1000      1.00       0.0
bb  1bb  2   48    1    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
          1.01325e5                0.20               10.75                10.0

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
c.... initialization data for STMVOC-type primary variables.
BN  1                     .4
          101325.00               0.750                10.0               0.200
          101325.00               10.00                 0.0               .2500
```

Figure 4. Printed output for problem 1.

```
*rgdif* ... 1D GAS DIFFUSION OF CHLOROBENZENE WITH PHASE PARTITIONING **********

         OUTPUT DATA AFTER (  91,  2)-2-TIME STEPS                                                    THE TIME IS   .36525E+03 DAYS

@@@
```

Figure 4. (continued)

ELEM	INDEX		P (Pa)	T (deg.C)	SO	SW	SG	PVOC (Pa)	PAIR (Pa)	PSATO (Pa)	PSATW (Pa)	PCO (Pa)	PCW (Pa)
aa	1	101	101324.	10.000	.0000E+00	.2501E+00	.7499E+00	662.	99435.	674.	1227.	0.	0.
aa	2	102	101323.	10.000	.0000E+00	.2501E+00	.7499E+00	638.	99458.	674.	1227.	0.	0.
aa	3	103	101322.	10.000	.0000E+00	.2501E+00	.7499E+00	614.	99481.	674.	1227.	0.	0.
aa	4	104	101321.	10.000	.0000E+00	.2501E+00	.7499E+00	591.	99503.	674.	1227.	0.	0.
aa	5	105	101320.	10.000	.0000E+00	.2501E+00	.7499E+00	567.	99526.	674.	1227.	0.	0.
aa	6	106	101319.	10.000	.0000E+00	.2501E+00	.7499E+00	544.	99548.	674.	1227.	0.	0.
aa	7	107	101318.	10.000	.0000E+00	.2501E+00	.7499E+00	521.	99570.	674.	1227.	0.	0.
aa	8	108	101317.	10.000	.0000E+00	.2501E+00	.7499E+00	498.	99591.	674.	1227.	0.	0.
aa	9	109	101316.	10.000	.0000E+00	.2501E+00	.7499E+00	476.	99613.	674.	1227.	0.	0.
aa	10	110	101314.	10.000	.0000E+00	.2501E+00	.7499E+00	454.	99633.	674.	1227.	0.	0.
aa	11	111	101313.	10.000	.0000E+00	.2501E+00	.7499E+00	432.	99654.	674.	1227.	0.	0.
aa	12	112	101312.	10.000	.0000E+00	.2501E+00	.7499E+00	411.	99674.	674.	1227.	0.	0.
aa	13	113	101312.	10.000	.0000E+00	.2501E+00	.7499E+00	391.	99694.	674.	1227.	0.	0.
aa	14	114	101311.	10.000	.0000E+00	.2501E+00	.7499E+00	370.	99713.	674.	1227.	0.	0.
aa	15	115	101310.	10.000	.0000E+00	.2501E+00	.7499E+00	351.	99732.	674.	1227.	0.	0.
aa	16	116	101309.	10.000	.0000E+00	.2501E+00	.7499E+00	332.	99750.	674.	1227.	0.	0.
aa	17	117	101308.	10.000	.0000E+00	.2501E+00	.7499E+00	313.	99768.	674.	1227.	0.	0.
aa	18	118	101307.	10.000	.0000E+00	.2501E+00	.7499E+00	295.	99785.	674.	1227.	0.	0.
aa	19	119	101306.	10.000	.0000E+00	.2500E+00	.7500E+00	278.	99801.	674.	1227.	0.	0.
aa	20	120	101306.	10.000	.0000E+00	.2500E+00	.7500E+00	261.	99817.	674.	1227.	0.	0.
aa	21	121	101305.	10.000	.0000E+00	.2500E+00	.7500E+00	245.	99833.	674.	1227.	0.	0.
aa	22	122	101304.	10.000	.0000E+00	.2500E+00	.7500E+00	230.	99847.	674.	1227.	0.	0.
aa	23	123	101304.	10.000	.0000E+00	.2500E+00	.7500E+00	215.	99862.	674.	1227.	0.	0.
aa	24	124	101303.	10.000	.0000E+00	.2500E+00	.7500E+00	201.	99875.	674.	1227.	0.	0.
aa	25	125	101303.	10.000	.0000E+00	.2500E+00	.7500E+00	187.	99888.	674.	1227.	0.	0.
aa	26	126	101302.	10.000	.0000E+00	.2500E+00	.7500E+00	175.	99900.	674.	1227.	0.	0.
aa	27	127	101302.	10.000	.0000E+00	.2500E+00	.7500E+00	162.	99912.	674.	1227.	0.	0.
aa	28	128	101301.	10.000	.0000E+00	.2500E+00	.7500E+00	151.	99923.	674.	1227.	0.	0.
aa	29	129	101301.	10.000	.0000E+00	.2500E+00	.7500E+00	140.	99934.	674.	1227.	0.	0.
aa	30	130	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	129.	99944.	674.	1227.	0.	0.
aa	31	131	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	120.	99953.	674.	1227.	0.	0.
aa	32	132	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	110.	99962.	674.	1227.	0.	0.
aa	33	133	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	102.	99971.	674.	1227.	0.	0.
aa	34	134	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	94.	99979.	674.	1227.	0.	0.
aa	35	135	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	86.	99986.	674.	1227.	0.	0.
aa	36	136	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	79.	99993.	674.	1227.	0.	0.
aa	37	137	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	72.	100000.	674.	1227.	0.	0.
aa	38	138	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	66.	100006.	674.	1227.	0.	0.
aa	39	139	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	60.	100011.	674.	1227.	0.	0.
aa	40	140	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	55.	100017.	674.	1227.	0.	0.
aa	41	141	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	50.	100022.	674.	1227.	0.	0.
aa	42	142	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	45.	100026.	674.	1227.	0.	0.
aa	43	143	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	41.	100030.	674.	1227.	0.	0.
aa	44	144	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	37.	100034.	674.	1227.	0.	0.
aa	45	145	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	34.	100038.	674.	1227.	0.	0.
aa	46	146	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	30.	100041.	674.	1227.	0.	0.
aa	47	147	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	27.	100044.	674.	1227.	0.	0.
aa	48	148	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	25.	100047.	674.	1227.	0.	0.
aa	49	149	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	22.	100050.	674.	1227.	0.	0.
aa	50	150	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	20.	100052.	674.	1227.	0.	0.
bb	1	151	101299.	10.000	.0000E+00	.2500E+00	.7500E+00	17.	100056.	674.	1227.	0.	0.
bb	2	152	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	13.	100059.	674.	1227.	0.	0.
bb	3	153	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	11.	100063.	674.	1227.	0.	0.
bb	4	154	101300.	10.000	.0000E+00	.2500E+00	.7500E+00	8.	100065.	674.	1227.	0.	0.
bb	5	155	101301.	10.000	.0000E+00	.2500E+00	.7500E+00	6.	100067.	674.	1227.	0.	0.
bb	6	156	101301.	10.000	.0000E+00	.2500E+00	.7500E+00	5.	100069.	674.	1227.	0.	0.

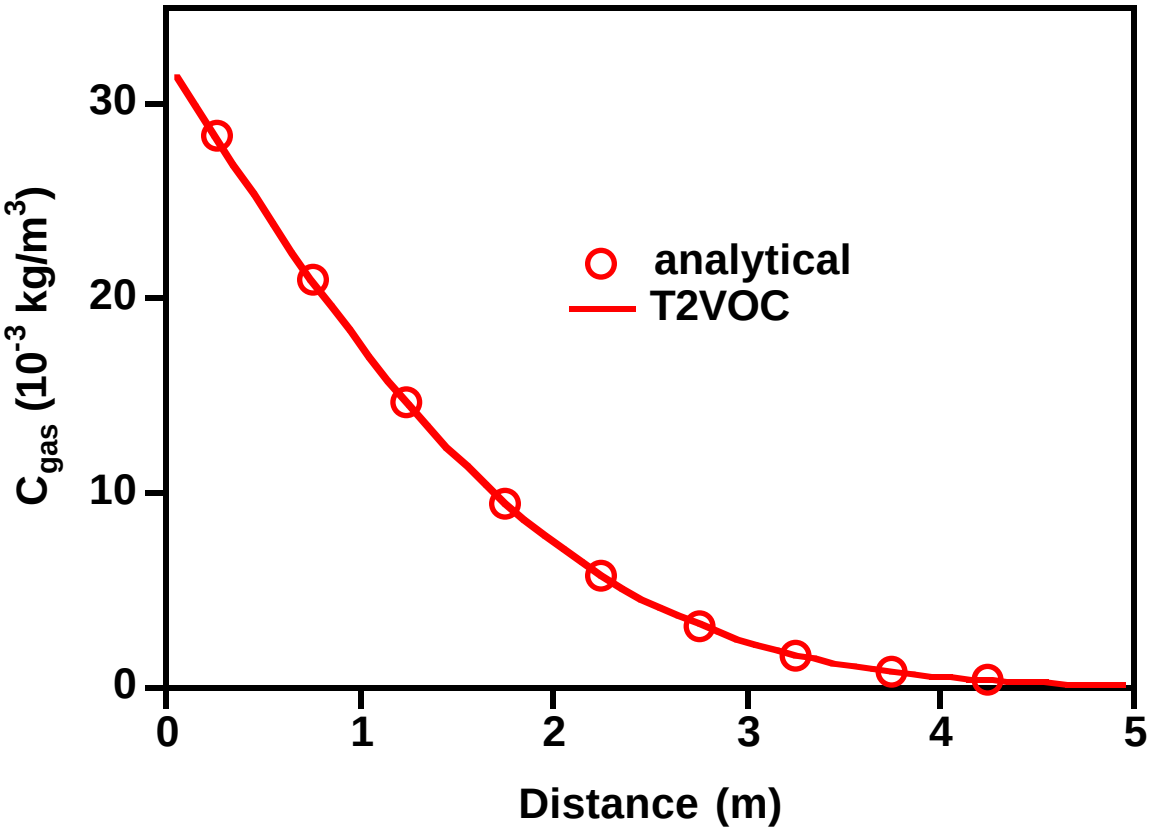
Figure 4. (continued)

rgdif ... 1D GAS DIFFUSION OF CHLOROBENZENE WITH PHASE PARTITIONING **********

KCYC = 91 - ITER = 2 - TIME = .31558E+08

ELEM	INDEX		CvocGAS (kg/m**3)	CvocAq. (kg/m**3)	DGAS (kg/m**3)	DNAPL (kg/m**3)	VISGAS (kg/m*s)	VISNAPL (kg/m*s)	DIFFO (m**2/s)	DIFFW (m**2/s)	KrGAS	KrAq.	KrNAPL
AA	1	1	.3145E-01	.4873E+00	.1264E+01	.0000E+00	.1752E-04	.1000E+01	.7979E-05	.2237E-04	.1000E+01	.0000E+00	.0000E+00
AA	2	2	.2991E-01	.4634E+00	.1263E+01	.0000E+00	.1753E-04	.1000E+01	.7979E-05	.2238E-04	.1000E+01	.0000E+00	.0000E+00
AA	3	3	.2838E-01	.4397E+00	.1262E+01	.0000E+00	.1754E-04	.1000E+01	.7979E-05	.2240E-04	.1000E+01	.0000E+00	.0000E+00
AA	4	4	.2686E-01	.4162E+00	.1261E+01	.0000E+00	.1755E-04	.1000E+01	.7980E-05	.2242E-04	.1000E+01	.0000E+00	.0000E+00
AA	5	5	.2536E-01	.3930E+00	.1259E+01	.0000E+00	.1756E-04	.1000E+01	.7980E-05	.2244E-04	.1000E+01	.0000E+00	.0000E+00
AA	6	6	.2389E-01	.3702E+00	.1258E+01	.0000E+00	.1757E-04	.1000E+01	.7980E-05	.2245E-04	.1000E+01	.0000E+00	.0000E+00
AA	7	7	.2244E-01	.3478E+00	.1257E+01	.0000E+00	.1758E-04	.1000E+01	.7980E-05	.2247E-04	.1000E+01	.0000E+00	.0000E+00
AA	8	8	.2103E-01	.3260E+00	.1256E+01	.0000E+00	.1760E-04	.1000E+01	.7980E-05	.2248E-04	.1000E+01	.0000E+00	.0000E+00
AA	9	9	.1966E-01	.3047E+00	.1255E+01	.0000E+00	.1761E-04	.1000E+01	.7980E-05	.2250E-04	.1000E+01	.0000E+00	.0000E+00
AA	10	10	.1833E-01	.2840E+00	.1254E+01	.0000E+00	.1762E-04	.1000E+01	.7980E-05	.2252E-04	.1000E+01	.0000E+00	.0000E+00
AA	11	11	.1704E-01	.2641E+00	.1253E+01	.0000E+00	.1763E-04	.1000E+01	.7980E-05	.2253E-04	.1000E+01	.0000E+00	.0000E+00
AA	12	12	.1580E-01	.2449E+00	.1252E+01	.0000E+00	.1763E-04	.1000E+01	.7981E-05	.2254E-04	.1000E+01	.0000E+00	.0000E+00
AA	13	13	.1461E-01	.2265E+00	.1251E+01	.0000E+00	.1764E-04	.1000E+01	.7981E-05	.2256E-04	.1000E+01	.0000E+00	.0000E+00
AA	14	14	.1348E-01	.2089E+00	.1250E+01	.0000E+00	.1765E-04	.1000E+01	.7981E-05	.2257E-04	.1000E+01	.0000E+00	.0000E+00
AA	15	15	.1240E-01	.1921E+00	.1250E+01	.0000E+00	.1766E-04	.1000E+01	.7981E-05	.2258E-04	.1000E+01	.0000E+00	.0000E+00
AA	16	16	.1137E-01	.1762E+00	.1249E+01	.0000E+00	.1767E-04	.1000E+01	.7981E-05	.2259E-04	.1000E+01	.0000E+00	.0000E+00
AA	17	17	.1040E-01	.1612E+00	.1248E+01	.0000E+00	.1768E-04	.1000E+01	.7981E-05	.2261E-04	.1000E+01	.0000E+00	.0000E+00
AA	18	18	.9485E-02	.1470E+00	.1247E+01	.0000E+00	.1768E-04	.1000E+01	.7981E-05	.2262E-04	.1000E+01	.0000E+00	.0000E+00
AA	19	19	.8627E-02	.1337E+00	.1247E+01	.0000E+00	.1769E-04	.1000E+01	.7981E-05	.2263E-04	.1000E+01	.0000E+00	.0000E+00
AA	20	20	.7824E-02	.1213E+00	.1246E+01	.0000E+00	.1770E-04	.1000E+01	.7981E-05	.2264E-04	.1000E+01	.0000E+00	.0000E+00
AA	21	21	.7076E-02	.1097E+00	.1246E+01	.0000E+00	.1770E-04	.1000E+01	.7981E-05	.2264E-04	.1000E+01	.0000E+00	.0000E+00
AA	22	22	.6381E-02	.9891E-01	.1245E+01	.0000E+00	.1771E-04	.1000E+01	.7981E-05	.2265E-04	.1000E+01	.0000E+00	.0000E+00
AA	23	23	.5738E-02	.8894E-01	.1245E+01	.0000E+00	.1771E-04	.1000E+01	.7981E-05	.2266E-04	.1000E+01	.0000E+00	.0000E+00
AA	24	24	.5144E-02	.7974E-01	.1244E+01	.0000E+00	.1772E-04	.1000E+01	.7981E-05	.2267E-04	.1000E+01	.0000E+00	.0000E+00
AA	25	25	.4599E-02	.7129E-01	.1244E+01	.0000E+00	.1772E-04	.1000E+01	.7981E-05	.2267E-04	.1000E+01	.0000E+00	.0000E+00
AA	26	26	.4100E-02	.6355E-01	.1243E+01	.0000E+00	.1772E-04	.1000E+01	.7981E-05	.2268E-04	.1000E+01	.0000E+00	.0000E+00
AA	27	27	.3644E-02	.5649E-01	.1243E+01	.0000E+00	.1773E-04	.1000E+01	.7981E-05	.2268E-04	.1000E+01	.0000E+00	.0000E+00
AA	28	28	.3230E-02	.5007E-01	.1243E+01	.0000E+00	.1773E-04	.1000E+01	.7982E-05	.2269E-04	.1000E+01	.0000E+00	.0000E+00
AA	29	29	.2854E-02	.4425E-01	.1242E+01	.0000E+00	.1773E-04	.1000E+01	.7982E-05	.2269E-04	.1000E+01	.0000E+00	.0000E+00
AA	30	30	.2515E-02	.3899E-01	.1242E+01	.0000E+00	.1774E-04	.1000E+01	.7982E-05	.2270E-04	.1000E+01	.0000E+00	.0000E+00
AA	31	31	.2210E-02	.3425E-01	.1242E+01	.0000E+00	.1774E-04	.1000E+01	.7982E-05	.2270E-04	.1000E+01	.0000E+00	.0000E+00
AA	32	32	.1936E-02	.3001E-01	.1242E+01	.0000E+00	.1774E-04	.1000E+01	.7982E-05	.2270E-04	.1000E+01	.0000E+00	.0000E+00
AA	33	33	.1691E-02	.2621E-01	.1242E+01	.0000E+00	.1774E-04	.1000E+01	.7982E-05	.2271E-04	.1000E+01	.0000E+00	.0000E+00
AA	34	34	.1473E-02	.2283E-01	.1241E+01	.0000E+00	.1774E-04	.1000E+01	.7982E-05	.2271E-04	.1000E+01	.0000E+00	.0000E+00
AA	35	35	.1279E-02	.1983E-01	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2271E-04	.1000E+01	.0000E+00	.0000E+00
AA	36	36	.1108E-02	.1717E-01	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2271E-04	.1000E+01	.0000E+00	.0000E+00
AA	37	37	.9565E-03	.1483E-01	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2271E-04	.1000E+01	.0000E+00	.0000E+00
AA	38	38	.8236E-03	.1277E-01	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	39	39	.7071E-03	.1096E-01	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	40	40	.6053E-03	.9384E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	41	41	.5168E-03	.8011E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7982E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	42	42	.4399E-03	.6819E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	43	43	.3734E-03	.5789E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	44	44	.3161E-03	.4900E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	45	45	.2669E-03	.4137E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	46	46	.2247E-03	.3483E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	47	47	.1887E-03	.2925E-02	.1241E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	48	48	.1580E-03	.2449E-02	.1240E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	49	49	.1320E-03	.2046E-02	.1240E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
AA	50	50	.1100E-03	.1706E-02	.1240E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
BB	1	51	.8224E-04	.1275E-02	.1240E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00
BB	2	52	.5610E-04	.8697E-03	.1240E+01	.0000E+00	.1775E-04	.1000E+01	.7981E-05	.2272E-04	.1000E+01	.0000E+00	.0000E+00

Figure 5. Comparison of T2VOC results with analytical solution of Baehr (1987) for transient diffusion with phase partitioning.



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

This problem consists of water injection into a porous medium filled with NAPL and water. As water is injected, NAPL is displaced, and a shock front develops at the leading edge of the invading water. Details of the problem specification are given by Faust (1985), and may be read off the input file for the T2VOC simulation which is given in Figure 6. The **MESHM**aker facility is used to generate a simple 1-D mesh of 40 equidistant grid blocks, terminated with an inactive block. Water is injected at constant rate of 150×10^{-6} kg/s. The two-phase relative permeability curves used for this problem (IRP = 11 in record RPCAP.I) are described in Appendix C. By setting ICP = 9 in record RPCAP.2 capillary pressure effects are neglected. A small formation compressibility (10^{-8} Pa^{-1}) is also specified.

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 from the previous problem are used (rather arbitrarily). However, for this problem, the NAPL density is 998.3 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 setting VLOA and VLOB in record CHEMP.5 equal to 0, by taking 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. Again we specify NEQ = 3 in **MULTI** to ensure that isothermal conditions prevail. A temperature of 19 °C is chosen so that the water viscosity will be equal to 1.0 cP (with a density of 998.3 kg/m^3).

The problem is initialized in two-phase (aqueous-NAPL) conditions with a water saturation of S_w = .159, just below the irreducible saturation of S_{wr} = .16. Constant 10 day time steps are prescribed, and the simulation is run to 1500 days. A printout from the T2VOC simulation for the first few time steps, and for the results after 1500 days is given in Figure 7. These results are compared with the Buckley-Leverett analytical solution (Buckley and Leverett, 1942) in Figure 8. The numerical results match the analytical solution well although some smearing of the sharp front is evident.

Figure 6. T2VOC input file for problem 2.

```
*rblev* ... Buckley/Leverett problem: inject water into chlorobenzene
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX      40      7.62
NX       1
       0.0
NY       1       1.0
NZ       1       1.0


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1    1.E+20       .20  2.96E-13  2.96E-13  2.96E-13       3.1     1000.
     1.e-8

*****************************************************************************
*************** Data block 'CHEMP' for VOC chemical parameters *****************
*****************************************************************************
--TCRIT--1--PCRIT--2--ZCRIT--3--OMEGA--4--DIPOLM-5
--TBOIL--1---VPA---2---VPB---3---VPC---4---VPD---5
---AMO---1---CPA---2---CPB---3---CPC---4---CPD---5
--RHOREF-1--TDENRF-2--DIFV0--3--TDIFRF-4--TEXPO--5
---VLOA--1---VLOB--2---VLOC--3---VLOD--4--VOLCRT-5
---SOLA--1---SOLB--2---SOLC--3---SOLD--4
---OCK---1---FOX---2---ALAM--3
************************** End of data block 'CHEMP' ***************************
CHEMP----1----*-Modified Chlorobenzene data-*----5----*----6----*----7----*----8
     632.4      45.2     0.265     0.249       1.6
     404.9    -7.587   2.26551  -4.09418   0.17038
   112.559    -33.89     .5631 -4.522E-4  1.426E-7
     998.3    292.15    8.0E-6    273.15      1.00
        0.        0.       1.0    292.15      308.
    1.0E-7        0.        0.        0.
        0.        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 200     200100000000 00000300002000   0.00E-5
             1.296E+8       -1.   8.64E+5              9.8060
      1.e3
     1.E-5     1.E00
             6.895E5                .159                50.0                19.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   11
    9
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1INJ 1                        WATE   150.6e-6  8.496E+4

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1141                       .2
             6.895E5                0.80                50.0                19.0

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 7. Printed output for problem 2.

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [   0,  0] *****                                THE TIME IS   .00000E+00 SECONDS, OR   .00000E+00 DAYS

                          PHASES PRESENT                                                  COMPONENT MASS IN PLACE (KG)
*************************************************************                  *************************************************************
 PHASES        *      GAS          AQUEOUS         NAPL                       COMPONENTS    *     WATER           AIR            VOC
*************************************************************                  *************************************************************
               *                                                               PHASES        *
 VOLUME (M^3) *  .00000000E+00  .96926400E+01  .51267360E+02                   GAS PHASE     *  .00000000E+00  .00000000E+00  .00000000E+00
 MASS   (KG)  *  .00000000E+00  .96809337E+04  .51180205E+05                   AQUEOUS       *  .96809277E+04  .00000000E+00  .60483773E-02
*************************************************************                  NAPL          *  .00000000E+00  .00000000E+00  .51180205E+05
                                                                               ADSORBED      *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                               TOTAL         *  .96809277E+04  .00000000E+00  .51180212E+05
                                                                              *************************************************************

*****************************************************************************************************************************

...ITERATING...  AT [   1,  1] --- DELTEX =  .100000E+04   MAX. RES. =  .622254E-03  AT ELEMENT A11 1  EQUATION   1
A1116(   1,  2) ST =  .100000E+04 DT =  .100000E+04 DX1= -.459539E+02 DX2=  .763978E-07 T =  19.000 P =   689454. S =  .000000E+00
...ITERATING...  AT [   2,  1] --- DELTEX =  .200000E+04   MAX. RES. =  .124373E-02  AT ELEMENT A11 1  EQUATION   1
A11 1(   2,  2) ST =  .300000E+04 DT =  .200000E+04 DX1=  .606513E+04 DX2=  .187777E-03 T =  19.000 P =   700820. S =  .000000E+00
...ITERATING...  AT [   3,  1] --- DELTEX =  .400000E+04   MAX. RES. =  .248438E-02  AT ELEMENT A11 1  EQUATION   1
A11 1(   3,  2) ST =  .700000E+04 DT =  .400000E+04 DX1=  .768572E+04 DX2=  .382907E-03 T =  19.000 P =   708506. S =  .000000E+00
...ITERATING...  AT [   4,  1] --- DELTEX =  .800000E+04   MAX. RES. =  .495644E-02  AT ELEMENT A11 1  EQUATION   1
A11 1(   4,  2) ST =  .150000E+05 DT =  .800000E+04 DX1=  .103134E+05 DX2=  .774134E-03 T =  19.000 P =   718819. S =  .000000E+00
...ITERATING...  AT [   5,  1] --- DELTEX =  .160000E+05   MAX. RES. =  .986399E-02  AT ELEMENT A11 1  EQUATION   1
A11 1(   5,  2) ST =  .310000E+05 DT =  .160000E+05 DX1=  .142293E+05 DX2=  .155866E-02 T =  19.000 P =   733049. S =  .000000E+00
...ITERATING...  AT [   6,  1] --- DELTEX =  .320000E+05   MAX. RES. =  .195351E-01  AT ELEMENT A11 1  EQUATION   1
A11 1(   6,  2) ST =  .630000E+05 DT =  .320000E+05 DX1=  .198891E+05 DX2=  .313079E-02 T =  19.000 P =   752938. S =  .000000E+00
...ITERATING...  AT [   7,  1] --- DELTEX =  .640000E+05   MAX. RES. =  .383195E-01  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [   7,  2] --- DELTEX =  .640000E+05   MAX. RES. =  .148518E-04  AT ELEMENT A11 1  EQUATION   1
A11 1(   7,  3) ST =  .127000E+06 DT =  .640000E+05 DX1=  .278418E+05 DX2=  .627603E-02 T =  19.000 P =   780780. S =  .000000E+00
...ITERATING...  AT [   8,  1] --- DELTEX =  .128000E+06   MAX. RES. =  .737931E-01  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [   8,  2] --- DELTEX =  .128000E+06   MAX. RES. =  .604817E-04  AT ELEMENT A11 1  EQUATION   1
A11 1(   8,  3) ST =  .255000E+06 DT =  .128000E+06 DX1=  .375419E+05 DX2=  .125618E-01 T =  19.000 P =   818321. S =  .000000E+00
...ITERATING...  AT [   9,  1] --- DELTEX =  .256000E+06   MAX. RES. =  .137300E+00  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [   9,  2] --- DELTEX =  .256000E+06   MAX. RES. =  .335028E-03  AT ELEMENT A11 1  EQUATION   1
A11 1(   9,  3) ST =  .511000E+06 DT =  .256000E+06 DX1=  .439442E+05 DX2=  .250328E-01 T =  19.000 P =   862266. S =  .000000E+00
...ITERATING...  AT [  10,  1] --- DELTEX =  .512000E+06   MAX. RES. =  .240363E+00  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [  10,  2] --- DELTEX =  .512000E+06   MAX. RES. =  .314054E-02  AT ELEMENT A11 2  EQUATION   1
A11 2(  10,  3) ST =  .102300E+07 DT =  .512000E+06 DX1=  .375558E+05 DX2=  .148271E-02 T =  19.000 P =   892881. S =  .000000E+00
...ITERATING...  AT [  11,  1] --- DELTEX =  .864000E+06   MAX. RES. =  .320604E+00  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [  11,  2] --- DELTEX =  .864000E+06   MAX. RES. =  .186811E-01  AT ELEMENT A11 2  EQUATION   1
...ITERATING...  AT [  11,  3] --- DELTEX =  .864000E+06   MAX. RES. =  .111063E-04  AT ELEMENT A11 1  EQUATION   1
A11 2(  11,  4) ST =  .188700E+07 DT =  .864000E+06 DX1=  .201590E+05 DX2=  .998652E-02 T =  19.000 P =   913040. S =  .000000E+00
...ITERATING...  AT [  12,  1] --- DELTEX =  .864000E+06   MAX. RES. =  .225867E+00  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [  12,  2] --- DELTEX =  .864000E+06   MAX. RES. =  .166327E-01  AT ELEMENT A11 2  EQUATION   1
...ITERATING...  AT [  12,  3] --- DELTEX =  .864000E+06   MAX. RES. =  .450873E-04  AT ELEMENT A11 2  EQUATION   1
A11 2(  12,  4) ST =  .275100E+07 DT =  .864000E+06 DX1=  .674272E+04 DX2=  .212099E-01 T =  19.000 P =   919783. S =  .000000E+00
...ITERATING...  AT [  13,  1] --- DELTEX =  .864000E+06   MAX. RES. =  .160816E+00  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [  13,  2] --- DELTEX =  .864000E+06   MAX. RES. =  .856127E-02  AT ELEMENT A11 2  EQUATION   1
...ITERATING...  AT [  13,  3] --- DELTEX =  .864000E+06   MAX. RES. =  .262367E-04  AT ELEMENT A11 2  EQUATION   1
A11 3(  13,  4) ST =  .361500E+07 DT =  .864000E+06 DX1=  .201006E+04 DX2=  .102014E-02 T =  19.000 P =   915112. S =  .000000E+00
...ITERATING...  AT [  14,  1] --- DELTEX =  .864000E+06   MAX. RES. =  .145886E+00  AT ELEMENT A11 2  EQUATION   1
...ITERATING...  AT [  14,  2] --- DELTEX =  .864000E+06   MAX. RES. =  .411084E-02  AT ELEMENT A11 3  EQUATION   1
A11 2(  14,  3) ST =  .447900E+07 DT =  .864000E+06 DX1=  .166542E+04 DX2=  .413719E-01 T =  19.000 P =   924176. S =  .000000E+00
```

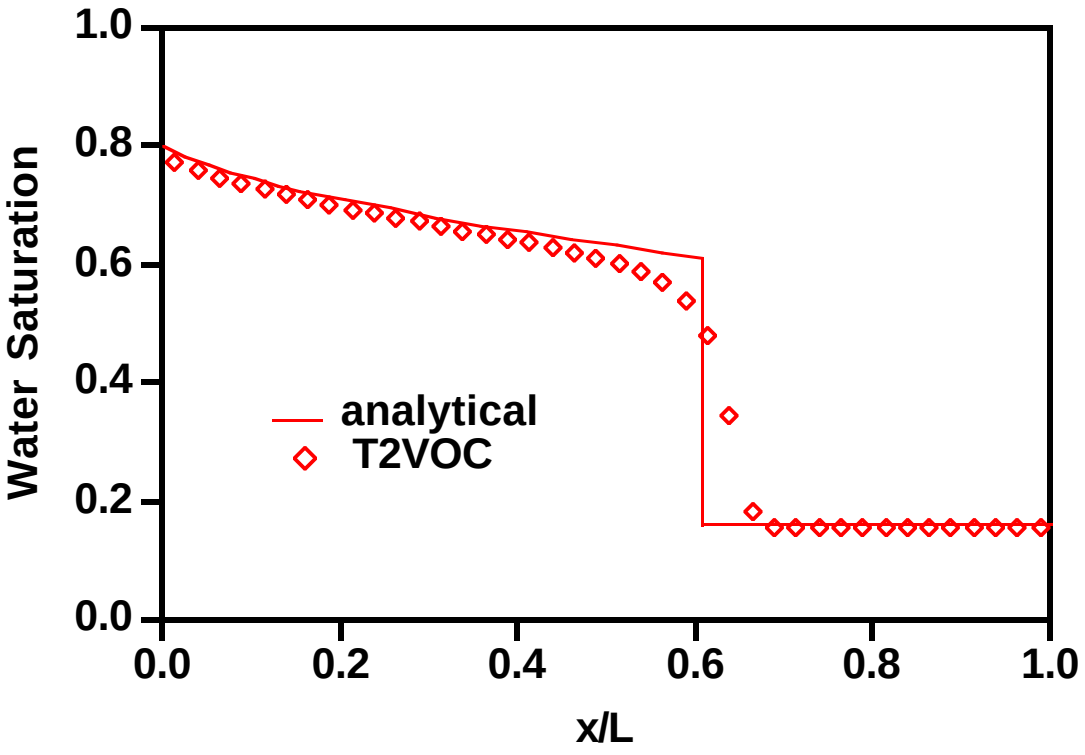
Figure 7. (continued)

rblev ... Buckley/Leverett problem: inject water into chlorobenzene

OUTPUT DATA AFTER (159, 3)-2-TIME STEPS THE TIME IS .15000E+04 DAYS

@@@

Figure 8. Comparison of T2VOC results with analytical solution for two phase flow.



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

This simulation consists of three parts and 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. (1992b). The present problem has been simplified somewhat, but captures the essential features of the original validation simulation for steam displacement of trichloroethylene (TCE) 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 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 with no air or VOC present. The initial temperature in the column is 22 °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 15th element by choosing the `COM3` 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 °C. Because the TCE injection is run in isothermal mode this enthalpy specification is not really necessary. 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 9. 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 C and D, respectively.

Trichloroethylene is injected into the column for a period of 120 s, with an initial time step size of 2 seconds. A partial printout of the T2VOC simulation results is given in Figure 10, and the liquid trichloroethylene (NAPL) phase saturation profile after 120 s is shown graphically in Figure 11.

The second part of this simulation consists of injecting cold water (22 °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 was placed into the input file, shown (partly) in Figure 12. This file is otherwise similar to the previous input file (Figure 9), 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 water (`COM1`) injection. Water with a specific enthalpy of 9.2332 x 10^4 J/kg is injected at a rate of 3.5395 x 10^{-4} kg/s (a Darcy velocity of 15 m/day) for a period of 17,880 s with an initial time step size of 2 s. The simulation is run to a total time of 18,000 s (120 s + 17,880 s), and a partial printout of results is given in Figure 13. The NAPL plume has migrated downstream and spread, see Figure 11, but has not reached the outlet. The aqueous phase downstream from the plume contains VOC at the solubility limit of 1.098 kg/m^3. 24.6 % of the original VOC has been removed by dissolution in the aqueous phase and subsequent extraction from well `PRO 1`.

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 was placed in the input file as block **INCON** (Fig. 14). During this final part of the simulation, steam with an enthalpy of 1.562x10^6 J/kg is injected at a rate of 3.5341x10^{-5} kg/s for a period of 9000 s. Parameter NEQ in **MULTI** is increased to 4, to include an energy balance equation, and printout is specified after 5000 s of steam injection (a total time of 23,000 s) using data block TIMES.

Part of the output after 5,000 s of steam injection is shown in Figure 15. These results are shown graphically in Figure 16 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 (see Figure 15).

Figure 9. T2VOC input file for part 1 of problem 3.

```
*rtce1*  STMVOC problem 3: INJECTION OF TRICHLOROETHYLENE INTO A COLUMN
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.      .385   1.6E-11   1.6E-11   1.6E-11       3.1     1000.
     0.e-8        0.      2.85       0.0

*******************************************************************************
*************** Data block 'CHEMP' for VOC chemical parameters *****************
*******************************************************************************
--TCRIT--1--PCRIT--2--ZCRIT--3--OMEGA--4--DIPOLM-5
--TBOIL--1---VPA---2---VPB---3---VPC---4---VPD---5
---AMO---1---CPA---2---CPB---3---CPC---4---CPD---5
--RHOREF-1--TDENRF-2--DIFV0--3--TDIFRF-4--TEXPO--5
---VLOA--1---VLOB--2---VLOC--3---VLOD--4--VOLCRT-5
---SOLA--1---SOLB--2---SOLC--3---SOLD--4
---OCK---1---FOX---2---ALAM--3
************************** End of data block 'CHEMP' ***************************
CHEMP----1----*--TCE data----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    30.170     .2287-2.229E-04 8.244E-08
     1462.     293.0   8.0E-06     273.0      1.60
        0.        0.      0.59    293.15     256.0
1.50954E-4        0.        0.        0.
        0.        0.        0.
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  20      20100030 0010002 4 0000000   0.00E-5
              120.00        2.      120.              9.8060
     1.E-5     1.E00
            1.0133e5                50.0                 0.0                22.0
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

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                        COM3 2.1900E-04 2.2100E+4

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 10. Portion of printed output for part 1 of problem 3.

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [   0,  0] *****                                THE TIME IS   .00000E+00 SECONDS, OR   .00000E+00 DAYS

                          PHASES PRESENT                                                COMPONENT MASS IN PLACE (KG)
 ************************************************************          ************************************************************
  PHASES       *      GAS          AQUEOUS         NAPL               COMPONENTS    *     WATER           AIR            VOC
 ************************************************************          ************************************************************
               *                                                        PHASES        *
  VOLUME (M^3) *  .00000000E+00  .71571500E-03  .00000000E+00          GAS PHASE     *  .00000000E+00  .00000000E+00  .00000000E+00
  MASS   (KG)  *  .00000000E+00  .71420419E+00  .00000000E+00          AQUEOUS       *  .71420419E+00  .00000000E+00  .00000000E+00
 ************************************************************          NAPL          *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                       ADSORBED      *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                       TOTAL         *  .71420419E+00  .00000000E+00  .00000000E+00
                                                                      ************************************************************

 ******************************************************************************************************************************


 ...ITERATING...  AT [   1,  1] --- DELTEX =  .200000E+01   MAX. RES. =  .117805E+02  AT ELEMENT AA 15  EQUATION   3
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 15 ****** PVO =  .221758E+06    PSATO =  .796165E+04  XMOLOW =  .420457E-02
 ...ITERATING...  AT [   1,  2] --- DELTEX =  .200000E+01   MAX. RES. =  .487511E+03  AT ELEMENT AA  1  EQUATION   1
 ...ITERATING...  AT [   1,  3] --- DELTEX =  .200000E+01   MAX. RES. =  .250530E+00  AT ELEMENT AA  1  EQUATION   1
 ...ITERATING...  AT [   1,  4] --- DELTEX =  .200000E+01   MAX. RES. =  .788522E-02  AT ELEMENT AA 15  EQUATION   3
 AA 14(   1,  5) ST =  .200000E+01 DT =  .200000E+01 DX1=  .834103E+03 DX2= -.300833E-31 T =  22.000 P =   102164. S =  .000000E+00
 ...ITERATING...  AT [   2,  1] --- DELTEX =  .200000E+01   MAX. RES. =  .100000E+01  AT ELEMENT AA 15  EQUATION   3
 ...ITERATING...  AT [   2,  2] --- DELTEX =  .200000E+01   MAX. RES. =  .627797E-02  AT ELEMENT AA 15  EQUATION   1
 AA 15(   2,  3) ST =  .400000E+01 DT =  .200000E+01 DX1=  .876680E+02 DX2= -.209785E-01 T =  22.000 P =   102479. S =  .000000E+00
 ...ITERATING...  AT [   3,  1] --- DELTEX =  .400000E+01   MAX. RES. =  .100000E+01  AT ELEMENT AA 15  EQUATION   3
 ...ITERATING...  AT [   3,  2] --- DELTEX =  .400000E+01   MAX. RES. =  .113998E+00  AT ELEMENT AA 14  EQUATION   3
 ...ITERATING...  AT [   3,  3] --- DELTEX =  .400000E+01   MAX. RES. =  .719068E-04  AT ELEMENT AA 14  EQUATION   3
 AA 16(   3,  4) ST =  .800000E+01 DT =  .400000E+01 DX1=  .448176E+01 DX2= -.128958E-30 T =  22.000 P =   102207. S =  .000000E+00
 ...ITERATING...  AT [   4,  1] --- DELTEX =  .800000E+01   MAX. RES. =  .995710E+00  AT ELEMENT AA 15  EQUATION   3
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 14 ****** PVO =  .195402E+05    PSATO =  .796165E+04  XMOLOW =  .370484E-03
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 16 ****** PVO =  .179044E+05    PSATO =  .796165E+04  XMOLOW =  .339471E-03
 ...ITERATING...  AT [   4,  2] --- DELTEX =  .800000E+01   MAX. RES. =  .223841E+01  AT ELEMENT AA 14  EQUATION   3
 ...ITERATING...  AT [   4,  3] --- DELTEX =  .800000E+01   MAX. RES. =  .988627E-01  AT ELEMENT AA 14  EQUATION   1
 ...ITERATING...  AT [   4,  4] --- DELTEX =  .800000E+01   MAX. RES. =  .247151E-01  AT ELEMENT AA 14  EQUATION   3
 AA 14(   4,  5) ST =  .160000E+02 DT =  .800000E+01 DX1=  .552556E+02 DX2= -.490032E+02 T =  22.000 P =   102217. S =  .000000E+00
 ...ITERATING...  AT [   5,  1] --- DELTEX =  .800000E+01   MAX. RES. =  .947768E+00  AT ELEMENT AA 16  EQUATION   3
 ...ITERATING...  AT [   5,  2] --- DELTEX =  .800000E+01   MAX. RES. =  .836890E+00  AT ELEMENT AA 14  EQUATION   3
 ...ITERATING...  AT [   5,  3] --- DELTEX =  .800000E+01   MAX. RES. =  .463528E-02  AT ELEMENT AA 16  EQUATION   3
 AA 16(   5,  4) ST =  .240000E+02 DT =  .800000E+01 DX1=  .891541E+02 DX2= -.104002E-01 T =  22.000 P =   102362. S =  .000000E+00
 ...ITERATING...  AT [   6,  1] --- DELTEX =  .160000E+02   MAX. RES. =  .148983E+01  AT ELEMENT AA 16  EQUATION   3
 ...ITERATING...  AT [   6,  2] --- DELTEX =  .160000E+02   MAX. RES. =  .541168E+00  AT ELEMENT AA 14  EQUATION   3
 ...ITERATING...  AT [   6,  3] --- DELTEX =  .160000E+02   MAX. RES. =  .663503E-02  AT ELEMENT AA 16  EQUATION   1
 ...ITERATING...  AT [   6,  4] --- DELTEX =  .160000E+02   MAX. RES. =  .350219E-04  AT ELEMENT AA 16  EQUATION   3
 AA 17(   6,  5) ST =  .400000E+02 DT =  .160000E+02 DX1=  .204320E+02 DX2= -.672072E-30 T =  22.000 P =   102227. S =  .000000E+00
 ...ITERATING...  AT [   7,  1] --- DELTEX =  .160000E+02   MAX. RES. =  .770240E+00  AT ELEMENT AA 14  EQUATION   3
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 13 ****** PVO =  .198452E+05    PSATO =  .796165E+04  XMOLOW =  .376267E-03
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 17 ****** PVO =  .126612E+05    PSATO =  .796165E+04  XMOLOW =  .240058E-03
 ...ITERATING...  AT [   7,  2] --- DELTEX =  .160000E+02   MAX. RES. =  .218973E+01  AT ELEMENT AA 13  EQUATION   3
 ...ITERATING...  AT [   7,  3] --- DELTEX =  .160000E+02   MAX. RES. =  .211732E+00  AT ELEMENT AA 13  EQUATION   1
 ...ITERATING...  AT [   7,  4] --- DELTEX =  .160000E+02   MAX. RES. =  .408578E-01  AT ELEMENT AA 13  EQUATION   3
 ...ITERATING...  AT [   7,  5] --- DELTEX =  .160000E+02   MAX. RES. =  .120437E-04  AT ELEMENT AA 13  EQUATION   1
 AA 13(   7,  6) ST =  .560000E+02 DT =  .160000E+02 DX1=  .557809E+02 DX2= -.490032E+02 T =  22.000 P =   102145. S =  .000000E+00
 ...ITERATING...  AT [   8,  1] --- DELTEX =  .160000E+02   MAX. RES. =  .892989E+00  AT ELEMENT AA 17  EQUATION   3
 ...ITERATING...  AT [   8,  2] --- DELTEX =  .160000E+02   MAX. RES. =  .119382E+01  AT ELEMENT AA 17  EQUATION   3
 ...ITERATING...  AT [   8,  3] --- DELTEX =  .160000E+02   MAX. RES. =  .390859E-02  AT ELEMENT AA 17  EQUATION   1
 AA 17(   8,  4) ST =  .720000E+02 DT =  .160000E+02 DX1=  .869068E+02 DX2= -.888393E-02 T =  22.000 P =   102368. S =  .000000E+00
 ...ITERATING...  AT [   9,  1] --- DELTEX =  .320000E+02   MAX. RES. =  .155425E+01  AT ELEMENT AA 17  EQUATION   3
 ...ITERATING...  AT [   9,  2] --- DELTEX =  .320000E+02   MAX. RES. =  .132101E+01  AT ELEMENT AA 17  EQUATION   3
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 12 ****** PVO =  .216986E+05    PSATO =  .796165E+04  XMOLOW =  .411408E-03
 ...ITERATING...  AT [   9,  3] --- DELTEX =  .320000E+02   MAX. RES. =  .905158E+00  AT ELEMENT AA 12  EQUATION   3
 ...ITERATING...  AT [   9,  4] --- DELTEX =  .320000E+02   MAX. RES. =  .282432E+00  AT ELEMENT AA 12  EQUATION   1
 ...ITERATING...  AT [   9,  5] --- DELTEX =  .320000E+02   MAX. RES. =  .567560E-03  AT ELEMENT AA 12  EQUATION   3
 AA 12(   9,  6) ST =  .104000E+03 DT =  .320000E+02 DX1=  .281030E+02 DX2= -.490014E+02 T =  22.000 P =   102054. S =  .000000E+00
 ...ITERATING...  AT [  10,  1] --- DELTEX =  .160000E+02   MAX. RES. =  .455924E+00  AT ELEMENT AA 12  EQUATION   3
$$$$$$$$ (7) NAPL EVOLVES AT ELEMENT AA 18 ****** PVO =  .171932E+05    PSATO =  .796165E+04  XMOLOW =  .325985E-03
 ...ITERATING...  AT [  10,  2] --- DELTEX =  .160000E+02   MAX. RES. =  .869736E+00  AT ELEMENT AA 18  EQUATION   3
 ...ITERATING...  AT [  10,  3] --- DELTEX =  .160000E+02   MAX. RES. =  .136553E+00  AT ELEMENT AA 18  EQUATION   1
 ...ITERATING...  AT [  10,  4] --- DELTEX =  .160000E+02   MAX. RES. =  .196900E-01  AT ELEMENT AA 18  EQUATION   3
 ...ITERATING...  AT [  10,  5] --- DELTEX =  .160000E+02   MAX. RES. =  .103139E-04  AT ELEMENT AA 18  EQUATION   1
 AA 18(  10,  6) ST =  .120000E+03 DT =  .160000E+02 DX1=  .506526E+02 DX2= -.490014E+02 T =  22.000 P =   102303. S =  .000000E+00
```

Figure 10. (continued)

```
*rtce1*  STMVOC problem 3: INJECTION OF TRICHLOROETHYLENE INTO A COLUMN

         OUTPUT DATA AFTER (  10,  6)-2-TIME STEPS                                                    THE TIME IS   .13889E-02 DAYS

@@@
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Figure 10. (continued)

rtce1 STMVOC problem 3: INJECTION OF TRICHLOROETHYLENE INTO A COLUMN

KCYC = 10 - ITER = 6 - TIME = .12000E+03

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
AA 1	1	.0000E+00	.3457E-07	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 2	2	.0000E+00	.1860E-06	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 3	3	.0000E+00	.9962E-06	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 4	4	.0000E+00	.5299E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 5	5	.0000E+00	.2792E-04	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 6	6	.0000E+00	.1452E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 7	7	.0000E+00	.7415E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 8	8	.0000E+00	.3690E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 9	9	.0000E+00	.1770E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 10	10	.0000E+00	.8031E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 11	11	.0000E+00	.3310E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 12	12	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.9806E+00	.0000E+00
AA 13	13	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.5873E+00	.2200E-02
AA 14	14	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.2573E+00	.2469E-01
AA 15	15	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.1439E+00	.5521E-01
AA 16	16	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.2847E+00	.2051E-01
AA 17	17	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.6760E+00	.9380E-03
AA 18	18	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.9950E+00	.0000E+00
AA 19	19	.0000E+00	.1673E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 20	20	.0000E+00	.2043E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 21	21	.0000E+00	.2281E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 22	22	.0000E+00	.2434E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 23	23	.0000E+00	.2528E-04	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 24	24	.0000E+00	.2584E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 25	25	.0000E+00	.2613E-06	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 26	26	.0000E+00	.2625E-07	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 27	27	.0000E+00	.2626E-08	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 28	28	.0000E+00	.2620E-09	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 29	29	.0000E+00	.2609E-10	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 30	30	.0000E+00	.2595E-11	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 31	31	.0000E+00	.2580E-12	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 32	32	.0000E+00	.2564E-13	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 33	33	.0000E+00	.2547E-14	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 34	34	.0000E+00	.2530E-15	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 35	35	.0000E+00	.2513E-16	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 36	36	.0000E+00	.2496E-17	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 37	37	.0000E+00	.2479E-18	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 38	38	.0000E+00	.2462E-19	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 39	39	.0000E+00	.2445E-20	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 40	40	.0000E+00	.2429E-21	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 41	41	.0000E+00	.2412E-22	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 42	42	.0000E+00	.2395E-23	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 43	43	.0000E+00	.2379E-24	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 44	44	.0000E+00	.2362E-25	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 45	45	.0000E+00	.2346E-26	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 46	46	.0000E+00	.2330E-27	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 47	47	.0000E+00	.2314E-28	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 48	48	.0000E+00	.2298E-29	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 49	49	.0000E+00	.2282E-30	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 50	50	.0000E+00	.2267E-31	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00

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Figure 10. (continued)

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        *rtce1*  STMVOC problem 3: INJECTION OF TRICHLOROETHYLENE INTO A COLUMN

                                                                                                KCYC =   10  -  ITER =    6  -  TIME =  .12000E+03

ELEMENT SOURCE INDEX  GENERATION RATE    ENTHALPY      FF(GAS)      FF(AQ. )     FF(NAPL)     FF(VOCG)    FF(VOCAQ)      P(WB)
                       (KG/S) OR (W)      (J/KG)                                                                            (PA)

 AA  1   INJ 1    1       -.99834E-04    .92317E+05   .00000E+00   .10000E+01   .00000E+00   .00000E+00   .34644E-10   .10140E+06
 AA 50   PRO 1    2       -.49995E-04    .92317E+05   .00000E+00   .10000E+01   .00000E+00   .00000E+00   .22713E-34   .10140E+06
 AA 15   INO 1    3        .21900E-03    .22100E+05

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```

Figure 11. NAPL phase saturation distribution after trichloroethylene injection, and after waterflood.

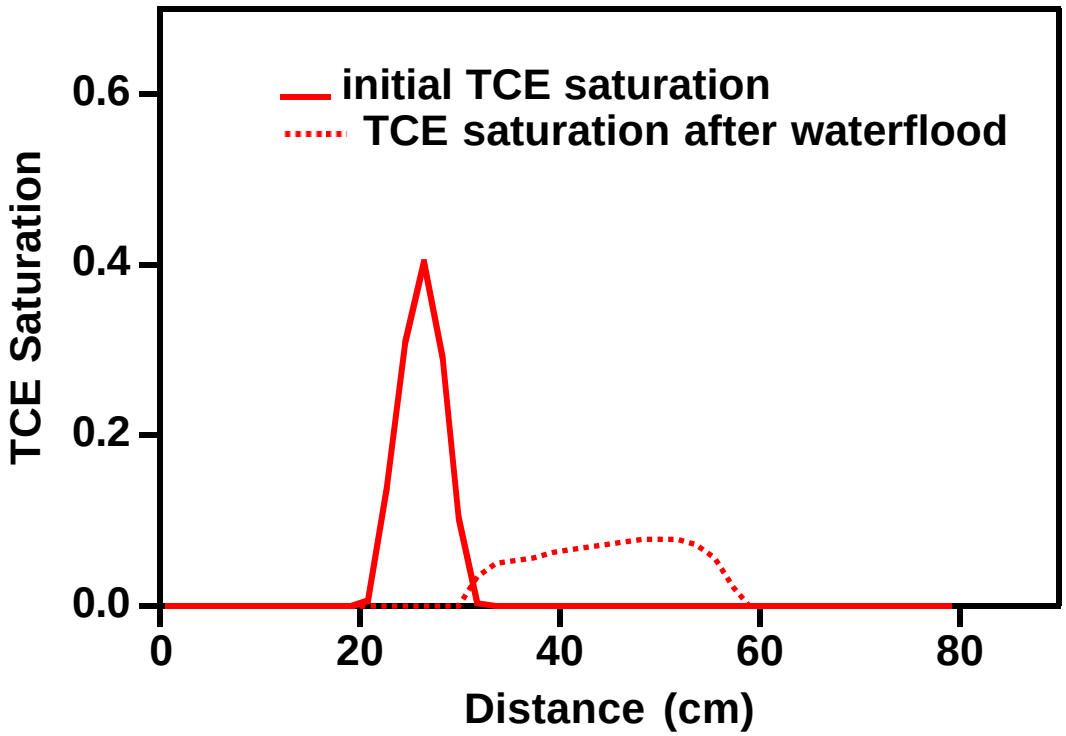

Figure 12. T2VOC input file for part 2 of problem 3.

```
*rtce2*  STMVOC problem 3 PART 2: INJECTION OF TCE-->WATERFLOODING
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.      .385   1.6E-11   1.6E-11   1.6E-11       3.1     1000.
     0.e-8        0.      2.85       0.0

CHEMP----1----*--TCE data----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    30.170     .2287-2.229E-04 8.244E-08
     1462.     293.0   8.0E-06     273.0      1.60
        0.        0.      0.59    293.15     256.0
1.50954E-4        0.        0.        0.
        0.        0.        0.
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1 100     100100000 00 0002 4 00 0 00   0.00E-5
            18000.00        2.     8000.              9.8060
     1.E-5     1.E00
            1.0133e5               0.00               .9950                22.0
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

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
AA  1INJ 1                        COM1 3.5395E-04 9.2332E+4
AA 50PRO 1                        DELV 3.5917E-12 1.0140E+5

INCON -- INITIAL CONDITIONS FOR   50 ELEMENTS AT TIME   .120000E+03
AA  1            .38500000E+00
  .1014265923124E+06  .5000000000000E+02  .4750407556490E-11  .2200000000000E+02
AA  2            .38500000E+00
  .1014797756339E+06  .5000000000000E+02  .2556161513894E-10  .2200000000000E+02
AA  3            .38500000E+00
  .1015329589538E+06  .5000000000000E+02  .1368924548834E-09  .2200000000000E+02
AA  4            .38500000E+00
  .1015861422718E+06  .5000000000000E+02  .7281884665449E-09  .2200000000000E+02
AA  5            .38500000E+00
  .1016393255880E+06  .5000000000000E+02  .3837076560212E-08  .2200000000000E+02
AA  6            .38500000E+00
  .1016925089021E+06  .5000000000000E+02  .1995411542515E-07  .2200000000000E+02
AA  7            .38500000E+00
  .1017456922143E+06  .5000000000000E+02  .1018836835343E-06  .2200000000000E+02
AA  8            .38500000E+00
  .1017988755242E+06  .5000000000000E+02  .5070340749548E-06  .2200000000000E+02
AA  9            .38500000E+00
  .1018520588320E+06  .5000000000000E+02  .2432264353017E-05  .2200000000000E+02
AA 10            .38500000E+00
  .1019052421374E+06  .5000000000000E+02  .1103520550423E-04  .2200000000000E+02
AA 11            .38500000E+00
  .1019584254403E+06  .5000000000000E+02  .4549223790574E-04  .2200000000000E+02
AA 12            .38500000E+00
  .1020931691282E+06  .9944561285886E+00  .5000000000000E+02  .2200000000000E+02
```

Figure 13. Printed output for part 2 of problem 3.

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [  10,  0] *****                                THE TIME IS   .12000E+03 SECONDS, OR   .13889E-02 DAYS

                        PHASES PRESENT                                                  COMPONENT MASS IN PLACE (KG)
*********************************************************        *********************************************************
 PHASES       *      GAS          AQUEOUS         NAPL           COMPONENTS    *     WATER           AIR            VOC
*********************************************************        *********************************************************
              *                                                   PHASES        *
 VOLUME (M^3) *  .00000000E+00  .69776551E-03  .17949492E-04      GAS PHASE     *  .00000000E+00  .00000000E+00  .00000000E+00
 MASS   (KG)  *  .00000000E+00  .69632411E+00  .26180765E-01      AQUEOUS       *  .69622488E+00  .00000000E+00  .99234541E-04
*********************************************************        NAPL          *  .00000000E+00  .00000000E+00  .26180765E-01
                                                                  ADSORBED      *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                  TOTAL         *  .69622488E+00  .00000000E+00  .26280000E-01
                                                                 *********************************************************

*****************************************************************************************************************************


...ITERATING...  AT [  11,  1] --- DELTEX =  .200000E+01   MAX. RES. =  .831084E-01  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  11,  2] --- DELTEX =  .200000E+01   MAX. RES. =  .787663E-01  AT ELEMENT AA 15  EQUATION   1
...ITERATING...  AT [  11,  3] --- DELTEX =  .200000E+01   MAX. RES. =  .926110E-02  AT ELEMENT AA 13  EQUATION   3
...ITERATING...  AT [  11,  4] --- DELTEX =  .200000E+01   MAX. RES. =  .195293E-04  AT ELEMENT AA 12  EQUATION   3
AA 13(  11,  5) ST =  .122000E+03 DT =  .200000E+01 DX1=  .792803E+04 DX2= -.103492E-02 T =  22.000 P =   110557. S =  .000000E+00
...ITERATING...  AT [  12,  1] --- DELTEX =  .200000E+01   MAX. RES. =  .151057E+00  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  12,  2] --- DELTEX =  .200000E+01   MAX. RES. =  .627735E-02  AT ELEMENT AA 18  EQUATION   3
AA 16(  12,  3) ST =  .124000E+03 DT =  .200000E+01 DX1=  .534368E+02 DX2= -.626798E-02 T =  22.000 P =   109388. S =  .000000E+00
...ITERATING...  AT [  13,  1] --- DELTEX =  .400000E+01   MAX. RES. =  .343309E+00  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  13,  2] --- DELTEX =  .400000E+01   MAX. RES. =  .465294E-01  AT ELEMENT AA 18  EQUATION   3
AA 18(  13,  3) ST =  .128000E+03 DT =  .400000E+01 DX1=  .203517E+02 DX2= -.182405E-02 T =  22.000 P =   107600. S =  .000000E+00
...ITERATING...  AT [  14,  1] --- DELTEX =  .800000E+01   MAX. RES. =  .743193E+00  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  14,  2] --- DELTEX =  .800000E+01   MAX. RES. =  .180943E+00  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  14,  3] --- DELTEX =  .800000E+01   MAX. RES. =  .175817E-03  AT ELEMENT AA 18  EQUATION   1
AA 18(  14,  4) ST =  .136000E+03 DT =  .800000E+01 DX1=  .578753E+02 DX2= -.740444E-02 T =  22.000 P =   107658. S =  .000000E+00
...ITERATING...  AT [  15,  1] --- DELTEX =  .160000E+02   MAX. RES. =  .120269E+01  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  15,  2] --- DELTEX =  .160000E+02   MAX. RES. =  .154044E+00  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  15,  3] --- DELTEX =  .160000E+02   MAX. RES. =  .715392E-03  AT ELEMENT AA 18  EQUATION   1
AA 18(  15,  4) ST =  .152000E+03 DT =  .160000E+02 DX1=  .135503E+03 DX2= -.262293E-01 T =  22.000 P =   107794. S =  .000000E+00
...ITERATING...  AT [  16,  1] --- DELTEX =  .320000E+02   MAX. RES. =  .136106E+01  AT ELEMENT AA 18  EQUATION   3
...ITERATING...  AT [  16,  2] --- DELTEX =  .320000E+02   MAX. RES. =  .208200E+01  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  16,  3] --- DELTEX =  .320000E+02   MAX. RES. =  .176501E+01  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  16,  4] --- DELTEX =  .320000E+02   MAX. RES. =  .419323E+00  AT ELEMENT AA 20  EQUATION   3
...ITERATING...  AT [  16,  5] --- DELTEX =  .320000E+02   MAX. RES. =  .128607E-02  AT ELEMENT AA 19  EQUATION   3
AA 19(  16,  6) ST =  .184000E+03 DT =  .320000E+02 DX1=  .578554E+02 DX2= -.490029E+02 T =  22.000 P =   107398. S =  .000000E+00
...ITERATING...  AT [  17,  1] --- DELTEX =  .320000E+02   MAX. RES. =  .879924E+00  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  17,  2] --- DELTEX =  .320000E+02   MAX. RES. =  .928130E+00  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  17,  3] --- DELTEX =  .320000E+02   MAX. RES. =  .691553E-02  AT ELEMENT AA 19  EQUATION   1
AA 19(  17,  4) ST =  .216000E+03 DT =  .320000E+02 DX1=  .883214E+02 DX2= -.113594E-01 T =  22.000 P =   107487. S =  .000000E+00
...ITERATING...  AT [  18,  1] --- DELTEX =  .640000E+02   MAX. RES. =  .151375E+01  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  18,  2] --- DELTEX =  .640000E+02   MAX. RES. =  .638700E+00  AT ELEMENT AA 19  EQUATION   1
...ITERATING...  AT [  18,  3] --- DELTEX =  .640000E+02   MAX. RES. =  .573412E+00  AT ELEMENT AA 20  EQUATION   3
...ITERATING...  AT [  18,  4] --- DELTEX =  .640000E+02   MAX. RES. =  .470332E+00  AT ELEMENT AA 20  EQUATION   1
...ITERATING...  AT [  18,  5] --- DELTEX =  .640000E+02   MAX. RES. =  .282278E-03  AT ELEMENT AA 20  EQUATION   1
AA 20(  18,  6) ST =  .280000E+03 DT =  .640000E+02 DX1=  .304821E+02 DX2= -.490010E+02 T =  22.000 P =   107182. S =  .000000E+00
...ITERATING...  AT [  19,  1] --- DELTEX =  .640000E+02   MAX. RES. =  .744618E+00  AT ELEMENT AA 19  EQUATION   3
...ITERATING...  AT [  19,  2] --- DELTEX =  .640000E+02   MAX. RES. =  .191294E+01  AT ELEMENT AA 20  EQUATION   3
...ITERATING...  AT [  19,  3] --- DELTEX =  .640000E+02   MAX. RES. =  .411155E-01  AT ELEMENT AA 20  EQUATION   1
...ITERATING...  AT [  19,  4] --- DELTEX =  .640000E+02   MAX. RES. =  .137638E-04  AT ELEMENT AA 20  EQUATION   3
AA 20(  19,  5) ST =  .344000E+03 DT =  .640000E+02 DX1=  .752357E+02 DX2= -.721879E-02 T =  22.000 P =   107257. S =  .000000E+00
```

Figure 13. (continued)

```
*rtce2*  STMVOC problem 3 PART 2: INJECTION OF TCE-->WATERFLOODING

         OUTPUT DATA AFTER (  43,  4)-2-TIME STEPS                                                    THE TIME IS   .20833E+00 DAYS

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Figure 13. (continued)

rtce2 STMVOC problem 3 PART 2: INJECTION OF TCE-->WATERFLOODING

KCYC = 43 - ITER = 4 - TIME = .18000E+05

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
AA 1	1	.0000E+00	.6395E-37	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 2	2	.0000E+00	.1911E-35	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 3	3	.0000E+00	.3015E-34	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 4	4	.0000E+00	.3358E-33	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 5	5	.0000E+00	.2978E-32	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 6	6	.0000E+00	.2252E-31	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 7	7	.0000E+00	.1518E-30	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 8	8	.0000E+00	.9399E-30	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 9	9	.0000E+00	.5470E-29	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 10	10	.0000E+00	.3038E-28	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 11	11	.0000E+00	.1625E-27	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 12	12	.0000E+00	.4566E-21	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 13	13	.0000E+00	.3869E-16	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 14	14	.0000E+00	.6288E-12	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 15	15	.0000E+00	.3902E-07	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 16	16	.0000E+00	.8111E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 17	17	.0000E+00	.7434E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 18	18	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.8791E+00	.0000E+00
AA 19	19	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.8313E+00	.1703E-04
AA 20	20	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.8261E+00	.5875E-04
AA 21	21	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.8158E+00	.1446E-03
AA 22	22	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7972E+00	.1974E-03
AA 23	23	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7839E+00	.2425E-03
AA 24	24	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7734E+00	.2832E-03
AA 25	25	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7647E+00	.3207E-03
AA 26	26	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7574E+00	.3543E-03
AA 27	27	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7519E+00	.3815E-03
AA 28	28	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7492E+00	.3955E-03
AA 29	29	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7521E+00	.3806E-03
AA 30	30	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.7675E+00	.3080E-03
AA 31	31	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.8113E+00	.1563E-03
AA 32	32	.0000E+00	.1098E+01	.0000E+00	.1459E+04	.1000E+01	.5737E-03	.0000E+00	.0000E+00	.0000E+00	.9216E+00	.0000E+00
AA 33	33	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 34	34	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 35	35	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 36	36	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 37	37	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 38	38	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 39	39	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 40	40	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 41	41	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 42	42	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 43	43	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 44	44	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 45	45	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 46	46	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 47	47	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 48	48	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 49	49	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 50	50	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00

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Figure 13. (continued)

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        *rtce2*  STMVOC problem 3 PART 2: INJECTION OF TCE-->WATERFLOODING

                                                                                                KCYC =   43  -  ITER =    4  -  TIME =  .18000E+05

ELEMENT SOURCE INDEX  GENERATION RATE    ENTHALPY      FF(GAS)      FF(AQ. )     FF(NAPL)     FF(VOCG)    FF(VOCAQ)      P(WB)
                       (KG/S) OR (W)      (J/KG)                                                                                (PA)

 AA  1   INJ 1    1        .35400E-03    .92330E+05
 AA 50   PRO 1    2       -.35412E-03    .92317E+05   .00000E+00   .10000E+01   .00000E+00   .00000E+00   .10998E-02   .10140E+06

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Figure 14. T2VOC input file for part 3 of problem 3.

```
*rtce3*  STMVOC problem 3 PART 3: Steamflooding
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.      .385   1.6E-11   1.6E-11   1.6E-11       3.1     1000.
     0.e-8        0.      2.85       0.0

CHEMP----1----*--TCE data----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    30.170     .2287-2.229E-04 8.244E-08
     1462.     293.0   8.0E-06     273.0      1.60
        0.        0.      0.59    293.15     256.0
1.50954E-4        0.        0.        0.
        0.        0.        0.
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    4    3    6
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 800     8001000 0 0010002 4 00 2 00   0.00E-5
            27000.00       -1.     2000.              9.8060
       20.
     1.E-5     1.E00
           1.0133e5                50.0                 0.0                22.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6           .150       .05      .005        3.
    8          0.000      1.84       10.       11.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
     23.e3
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                        COM1 3.5341E-05   1.562e6
AA 50PRO 1                        DELV 3.5917E-12 1.0140E+5

INCON -- INITIAL CONDITIONS FOR   50 ELEMENTS AT TIME   .180000E+05
AA  1            .38500000E+00
  .1114577077819E+06  .5000000000000E+02  .8787539166409E-41  .2200000000000E+02
AA  2            .38500000E+00
  .1112691265526E+06  .5000000000000E+02  .2626276372803E-39  .2200000000000E+02
AA  3            .38500000E+00
  .1110805453035E+06  .5000000000000E+02  .4143523440258E-38  .2200000000000E+02
AA  4            .38500000E+00
  .1108919640346E+06  .5000000000000E+02  .4613876163171E-37  .2200000000000E+02
AA  5            .38500000E+00
  .1107033827459E+06  .5000000000000E+02  .4092264281965E-36  .2200000000000E+02
AA  6            .38500000E+00
  .1105148014373E+06  .5000000000000E+02  .3094542901588E-35  .2200000000000E+02
AA  7            .38500000E+00
  .1103262201089E+06  .5000000000000E+02  .2085268205004E-34  .2200000000000E+02
AA  8            .38500000E+00
  .1101376387606E+06  .5000000000000E+02  .1291502871036E-33  .2200000000000E+02
AA  9            .38500000E+00
  .1099490573926E+06  .5000000000000E+02  .7516279330179E-33  .2200000000000E+02
AA 10            .38500000E+00
  .1097604760047E+06  .5000000000000E+02  .4173876872718E-32  .2200000000000E+02
```

Figure 15. Printed output for part 3 of problem 3.

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [  43,  0] *****                                THE TIME IS   .18000E+05 SECONDS, OR   .20833E+00 DAYS

                          PHASES PRESENT                                                  COMPONENT MASS IN PLACE (KG)
*********************************************************        *********************************************************
 PHASES        *      GAS          AQUEOUS         NAPL          COMPONENTS    *     WATER           AIR            VOC
*********************************************************        *********************************************************
               *                                                   PHASES        *
 VOLUME (M^3) *  .00000000E+00  .70248274E-03  .13232261E-04       GAS PHASE     *  .00000000E+00  .00000000E+00  .00000000E+00
 MASS   (KG)  *  .00000000E+00  .70116108E+00  .19300308E-01       AQUEOUS       *  .70065591E+00  .00000000E+00  .50516978E-03
*********************************************************        NAPL          *  .00000000E+00  .00000000E+00  .19300308E-01
                                                                  ADSORBED      *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                  TOTAL         *  .70065591E+00  .00000000E+00  .19805478E-01
                                                                 *********************************************************

*****************************************************************************************************************************


...ITERATING...  AT [  44,  1] --- DELTEX =  .200000E+02   MAX. RES. =  .446173E+00  AT ELEMENT AA  1  EQUATION   1
...ITERATING...  AT [  44,  2] --- DELTEX =  .200000E+02   MAX. RES. =  .115205E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  44,  3] --- DELTEX =  .200000E+02   MAX. RES. =  .126983E-01  AT ELEMENT AA  2  EQUATION   4
...ITERATING...  AT [  44,  4] --- DELTEX =  .200000E+02   MAX. RES. =  .366867E-04  AT ELEMENT AA  1  EQUATION   4
AA  2(  44,  5) ST =  .180200E+05 DT =  .200000E+02 DX1= -.883723E+04 DX2=  .000000E+00 T =  22.588 P =   102432. S =  .000000E+00
...ITERATING...  AT [  45,  1] --- DELTEX =  .200000E+02   MAX. RES. =  .265826E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  45,  2] --- DELTEX =  .200000E+02   MAX. RES. =  .129743E-02  AT ELEMENT AA  1  EQUATION   1
AA  2(  45,  3) ST =  .180400E+05 DT =  .200000E+02 DX1=  .819997E+01 DX2=  .000000E+00 T =  23.657 P =   102440. S =  .000000E+00
...ITERATING...  AT [  46,  1] --- DELTEX =  .400000E+02   MAX. RES. =  .396017E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  46,  2] --- DELTEX =  .400000E+02   MAX. RES. =  .655080E-02  AT ELEMENT AA  1  EQUATION   1
AA  2(  46,  3) ST =  .180800E+05 DT =  .400000E+02 DX1=  .772011E+01 DX2=  .000000E+00 T =  27.104 P =   102448. S =  .000000E+00
...ITERATING...  AT [  47,  1] --- DELTEX =  .800000E+02   MAX. RES. =  .515743E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  47,  2] --- DELTEX =  .800000E+02   MAX. RES. =  .263426E-01  AT ELEMENT AA  2  EQUATION   4
...ITERATING...  AT [  47,  3] --- DELTEX =  .800000E+02   MAX. RES. =  .658459E-04  AT ELEMENT AA  2  EQUATION   4
AA  3(  47,  4) ST =  .181600E+05 DT =  .800000E+02 DX1=  .908118E+01 DX2=  .000000E+00 T =  25.772 P =   102439. S =  .000000E+00
...ITERATING...  AT [  48,  1] --- DELTEX =  .160000E+03   MAX. RES. =  .587601E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  48,  2] --- DELTEX =  .160000E+03   MAX. RES. =  .138834E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  48,  3] --- DELTEX =  .160000E+03   MAX. RES. =  .133708E+01  AT ELEMENT AA  1  EQUATION   1
...ITERATING...  AT [  48,  4] --- DELTEX =  .160000E+03   MAX. RES. =  .594658E+03  AT ELEMENT AA 50  EQUATION   1
...ITERATING...  AT [  48,  5] --- DELTEX =  .160000E+03   MAX. RES. =  .858671E+00  AT ELEMENT AA  1  EQUATION   1
...ITERATING...  AT [  48,  6] --- DELTEX =  .160000E+03   MAX. RES. =  .413390E+03  AT ELEMENT AA 50  EQUATION   1
...ITERATING...  AT [  48,  7] --- DELTEX =  .160000E+03   MAX. RES. =  .671993E+00  AT ELEMENT AA  1  EQUATION   1
...ITERATING...  AT [  48,  8] --- DELTEX =  .160000E+03   MAX. RES. =  .377626E+03  AT ELEMENT AA 50  EQUATION   1
...ITERATING...  AT [  48,  9] --- DELTEX =  .160000E+03   MAX. RES. =  .634239E+00  AT ELEMENT AA  1  EQUATION   1
+++++++++ REDUCE TIME STEP AT (  48,  9) ++++++++++++++++   NEW DELT =  .400000E+02
...ITERATING...  AT [  48,  1] --- DELTEX =  .400000E+02   MAX. RES. =  .146900E+00  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  48,  2] --- DELTEX =  .400000E+02   MAX. RES. =  .182704E-02  AT ELEMENT AA  1  EQUATION   1
AA  2(  48,  3) ST =  .182000E+05 DT =  .400000E+02 DX1=  .712956E+01 DX2=  .000000E+00 T =  41.685 P =   102461. S =  .000000E+00
...ITERATING...  AT [  49,  1] --- DELTEX =  .800000E+02   MAX. RES. =  .244574E+00  AT ELEMENT AA  2  EQUATION   4
...ITERATING...  AT [  49,  2] --- DELTEX =  .800000E+02   MAX. RES. =  .871706E-02  AT ELEMENT AA  1  EQUATION   1
AA  3(  49,  3) ST =  .182800E+05 DT =  .800000E+02 DX1=  .131871E+01 DX2=  .000000E+00 T =  32.680 P =   102449. S =  .000000E+00
...ITERATING...  AT [  50,  1] --- DELTEX =  .160000E+03   MAX. RES. =  .409042E+00  AT ELEMENT AA  2  EQUATION   4
...ITERATING...  AT [  50,  2] --- DELTEX =  .160000E+03   MAX. RES. =  .450662E+00  AT ELEMENT AA  1  EQUATION   4
TEMPERATURE =  -.28915E+02  OUT OF RANGE IN SAT
+++++++++   CANNOT FIND PARAMETERS AT ELEMENT *AA  2*         XX(M) =  .759502E+05  .500000E+02  .891790E-39 -.289148E+02
+++++++++ REDUCE TIME STEP AT (  50,  2) ++++++++++++++++   NEW DELT =  .400000E+02
...ITERATING...  AT [  50,  1] --- DELTEX =  .400000E+02   MAX. RES. =  .102261E+00  AT ELEMENT AA  2  EQUATION   4
...ITERATING...  AT [  50,  2] --- DELTEX =  .400000E+02   MAX. RES. =  .701747E-01  AT ELEMENT AA  1  EQUATION   4
...ITERATING...  AT [  50,  3] --- DELTEX =  .400000E+02   MAX. RES. =  .128559E+04  AT ELEMENT AA  2  EQUATION   4
```

Figure 15. (continued)

```
*rtce3*  STMVOC problem 3 PART 3: Steamflooding

         OUTPUT DATA AFTER ( 373,  3)-2-TIME STEPS                                                    THE TIME IS   .26620E+00 DAYS

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Figure 15. (continued)

rtce3 STMVOC problem 3 PART 3: Steamflooding

KCYC = 373 - ITER = 3 - TIME = .23000E+05

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
AA 1	1	.0000E+00	.0000E+00	.7004E+00	.0000E+00	.1222E-04	.1000E+01	.0000E+00	.0000E+00	.5006E+00	.8011E-02	.0000E+00
AA 2	2	.1466-319	.0000E+00	.6985E+00	.0000E+00	.1222E-04	.1000E+01	.0000E+00	.0000E+00	.5005E+00	.8016E-02	.0000E+00
AA 3	3	.6734-320	.0000E+00	.6966E+00	.0000E+00	.1221E-04	.1000E+01	.0000E+00	.0000E+00	.5005E+00	.8021E-02	.0000E+00
AA 4	4	.5352-319	.0000E+00	.6947E+00	.0000E+00	.1221E-04	.1000E+01	.0000E+00	.0000E+00	.5004E+00	.8028E-02	.0000E+00
AA 5	5	.5649-319	.0000E+00	.6928E+00	.0000E+00	.1221E-04	.1000E+01	.0000E+00	.0000E+00	.5002E+00	.8035E-02	.0000E+00
AA 6	6	.2353-319	.0000E+00	.6909E+00	.0000E+00	.1220E-04	.1000E+01	.0000E+00	.0000E+00	.5001E+00	.8044E-02	.0000E+00
AA 7	7	.0000E+00	.0000E+00	.6890E+00	.0000E+00	.1220E-04	.1000E+01	.0000E+00	.0000E+00	.4999E+00	.8054E-02	.0000E+00
AA 8	8	.0000E+00	.0000E+00	.6871E+00	.0000E+00	.1220E-04	.1000E+01	.0000E+00	.0000E+00	.4997E+00	.8067E-02	.0000E+00
AA 9	9	.4962-319	.0000E+00	.6852E+00	.0000E+00	.1219E-04	.1000E+01	.0000E+00	.0000E+00	.4995E+00	.8082E-02	.0000E+00
AA 10	10	.8376-311	.1272-311	.6833E+00	.0000E+00	.1219E-04	.1000E+01	.0000E+00	.0000E+00	.4992E+00	.8101E-02	.0000E+00
AA 11	11	.9186-295	.1398-295	.6813E+00	.0000E+00	.1219E-04	.1000E+01	.0000E+00	.0000E+00	.4989E+00	.8123E-02	.0000E+00
AA 12	12	.8601-281	.1312-281	.6794E+00	.0000E+00	.1218E-04	.1000E+01	.0000E+00	.0000E+00	.4984E+00	.8152E-02	.0000E+00
AA 13	13	.2946-263	.4503-264	.6774E+00	.0000E+00	.1218E-04	.1000E+01	.0000E+00	.0000E+00	.4979E+00	.8186E-02	.0000E+00
AA 14	14	.3424-251	.5246-252	.6754E+00	.0000E+00	.1218E-04	.1000E+01	.0000E+00	.0000E+00	.4972E+00	.8228E-02	.0000E+00
AA 15	15	.5436-205	.8348-206	.6735E+00	.0000E+00	.1217E-04	.1000E+01	.0000E+00	.0000E+00	.4964E+00	.8280E-02	.0000E+00
AA 16	16	.4517-186	.6952-187	.6715E+00	.0000E+00	.1217E-04	.1000E+01	.0000E+00	.0000E+00	.4955E+00	.8343E-02	.0000E+00
AA 17	17	.3933-173	.6067-174	.6695E+00	.0000E+00	.1217E-04	.1000E+01	.0000E+00	.0000E+00	.4943E+00	.8420E-02	.0000E+00
AA 18	18	.1581-168	.2445-169	.6674E+00	.0000E+00	.1216E-04	.1000E+01	.0000E+00	.0000E+00	.4929E+00	.8515E-02	.0000E+00
AA 19	19	.1224-137	.1897-138	.6654E+00	.0000E+00	.1216E-04	.1000E+01	.0000E+00	.0000E+00	.4912E+00	.8631E-02	.0000E+00
AA 20	20	.1562-132	.2428-133	.6633E+00	.0000E+00	.1216E-04	.1000E+01	.0000E+00	.0000E+00	.4891E+00	.8773E-02	.0000E+00
AA 21	21	.5837-129	.9093-130	.6612E+00	.0000E+00	.1215E-04	.1000E+01	.0000E+00	.0000E+00	.4865E+00	.8949E-02	.0000E+00
AA 22	22	.6341-126	.9902-127	.6591E+00	.0000E+00	.1215E-04	.1000E+01	.0000E+00	.0000E+00	.4834E+00	.9166E-02	.0000E+00
AA 23	23	.2767-123	.4331-124	.6570E+00	.0000E+00	.1214E-04	.1000E+01	.0000E+00	.0000E+00	.4797E+00	.9434E-02	.0000E+00
AA 24	24	.5473-121	.8591-122	.6548E+00	.0000E+00	.1214E-04	.1000E+01	.0000E+00	.0000E+00	.4752E+00	.9766E-02	.0000E+00
AA 25	25	.5417-119	.8526-120	.6526E+00	.0000E+00	.1214E-04	.1000E+01	.0000E+00	.0000E+00	.4698E+00	.1018E-01	.0000E+00
AA 26	26	.2561-117	.4040-118	.6504E+00	.0000E+00	.1213E-04	.1000E+01	.0000E+00	.0000E+00	.4634E+00	.1069E-01	.0000E+00
AA 27	27	.1207-115	.1910-116	.6481E+00	.0000E+00	.1213E-04	.1000E+01	.0000E+00	.0000E+00	.4557E+00	.1133E-01	.0000E+00
AA 28	28	.3189E-60	.5060E-61	.6458E+00	.0000E+00	.1212E-04	.1000E+01	.0000E+00	.0000E+00	.4466E+00	.1212E-01	.0000E+00
AA 29	29	.3424E-45	.5448E-46	.6433E+00	.0000E+00	.1212E-04	.1000E+01	.0000E+00	.0000E+00	.4360E+00	.1312E-01	.0000E+00
AA 30	30	.8865E-32	.1415E-32	.6409E+00	.0000E+00	.1211E-04	.1000E+01	.0000E+00	.0000E+00	.4234E+00	.1439E-01	.0000E+00
AA 31	31	.8421E-27	.1348E-27	.6383E+00	.0000E+00	.1211E-04	.1000E+01	.0000E+00	.0000E+00	.4085E+00	.1603E-01	.0000E+00
AA 32	32	.4388E-23	.7050E-24	.6356E+00	.0000E+00	.1211E-04	.1000E+01	.0000E+00	.0000E+00	.3903E+00	.1826E-01	.0000E+00
AA 33	33	.6920E-20	.1116E-20	.6327E+00	.0000E+00	.1210E-04	.1000E+01	.0000E+00	.0000E+00	.3674E+00	.2146E-01	.0000E+00
AA 34	34	.4317E-17	.6986E-18	.6297E+00	.0000E+00	.1209E-04	.1000E+01	.0000E+00	.0000E+00	.3375E+00	.2644E-01	.0000E+00
AA 35	35	.1196E-14	.1944E-15	.6263E+00	.0000E+00	.1209E-04	.1000E+01	.0000E+00	.0000E+00	.2967E+00	.3502E-01	.0000E+00
AA 36	36	.2450E-12	.4001E-13	.6225E+00	.0000E+00	.1208E-04	.1000E+01	.0000E+00	.0000E+00	.2391E+00	.5207E-01	.0000E+00
AA 37	37	.2705E-08	.4444E-09	.6178E+00	.0000E+00	.1207E-04	.1000E+01	.0000E+00	.0000E+00	.1555E+00	.9505E-01	.0000E+00
AA 38	38	.1223E+01	.2556E+00	.1676E+01	.0000E+00	.1275E-04	.1000E+01	.0000E+00	.0000E+00	.4277E-01	.2676E+00	.0000E+00
AA 39	39	.0000E+00	.1075E+01	.0000E+00	.1377E+04	.1000E+01	.3067E-03	.0000E+00	.0000E+00	.0000E+00	.2460E+00	.2666E-01
AA 40	40	.0000E+00	.1089E+01	.0000E+00	.1419E+04	.1000E+01	.4162E-03	.0000E+00	.0000E+00	.0000E+00	.2778E+00	.2148E-01
AA 41	41	.0000E+00	.1094E+01	.0000E+00	.1439E+04	.1000E+01	.4878E-03	.0000E+00	.0000E+00	.0000E+00	.3822E+00	.1057E-01
AA 42	42	.0000E+00	.1096E+01	.0000E+00	.1449E+04	.1000E+01	.5270E-03	.0000E+00	.0000E+00	.0000E+00	.7056E+00	.6765E-03
AA 43	43	.0000E+00	.1097E+01	.0000E+00	.1453E+04	.1000E+01	.5479E-03	.0000E+00	.0000E+00	.0000E+00	.9937E+00	.0000E+00
AA 44	44	.0000E+00	.1097E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 45	45	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 46	46	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 47	47	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 48	48	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 49	49	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
AA 50	50	.0000E+00	.1098E+01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00

@@@

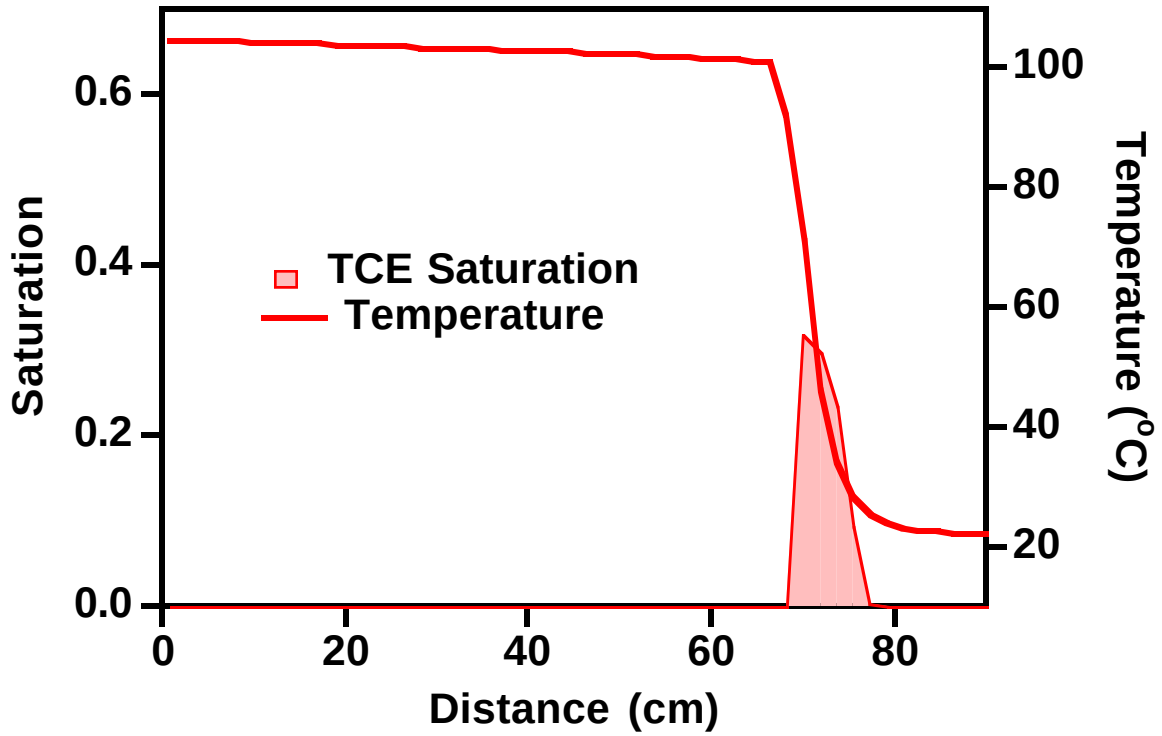
Figure 15. (continued)

```
*rtce3*  STMVOC problem 3 PART 3: Steamflooding

         OUTPUT DATA AFTER ( 520,  3)-2-TIME STEPS                                                    THE TIME IS   .31250E+00 DAYS

@@@
```

Figure 15. (continued)

```
        *rtce3*  STMVOC problem 3 PART 3: Steamflooding

                                                                                                  KCYC =  520  -  ITER =    3  -  TIME =  .27000E+05

ELEMENT SOURCE INDEX  GENERATION RATE    ENTHALPY      FF(GAS)      FF(AQ. )     FF(NAPL)     FF(VOCG)    FF(VOCAQ)      P(WB)
                       (KG/S) OR (W)      (J/KG)                                                                            (PA)

 AA  1   INJ 1    1        .35340E-04    .15620E+07
 AA 50   PRO 1    2       -.35562E-04    .15556E+07   .50281E+00   .49719E+00   .00000E+00   .12645E-22   .13210E-26   .10140E+06

@@@
```

Figure 16. Calculated separate phase trichloroethylene distribution and temperature profile after 5000 s of steam injection.



12.4 Problem No. 4 - Steam Displacement of NAPL in a 2-D 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.

The first part of the simulation involves generation of a computational grid and development of a gravity-capillary equilibrium in a saturated-unsaturated flow system. The input file used for this part of the simulation is shown in Figure 17. A rather coarse two dimensional vertical section (X-Z mesh) is used. Printout from the mesh generation portion of the T2VOC run is shown in Figure 18, and Figure 19 shows a scale diagram of the mesh.

Generation of gravity-capillary equilibrium proceeds from initial conditions of partial saturation and no VOC present, using the options NK = NEQ = 2 in **MULTI** for convenience. After 20 time steps the simulation has reached a rather accurate static equilibrium and a time of 6.068×10^5 days. Some printed output from this run is shown in Figure 20. The capillary pressure and relative permeability functions used throughout this simulation are similar to those in the previous example, except that the capillary pressure between the gas phase and the NAPL is neglected. Even though no VOC is present in the system during this first part of the simulation, data block **CHEMP** must be included for any T2VOC simulation. In the input file shown in Figure 17 (and in the other input files used for this 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 (`A11 9`) at a rate of 1.4667×10^{-4} kg/s for a period of 4.8×10^6 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. The input file used for this part of the problem is shown in Figure 21. The previously generated mesh could have been used, but in this as well as in the following segments of the simulation we have again included the MESHMaker data in the input file, so that each segment may be executed independently by the user. Note that we now specify NK = NEQ = 3 in **MULTI**, to be able to represent VOC. The file SAVE generated from the gravity-capillary equilibration run has been merged into the input file as block **INCON**, and MOP(19) = 1 is used to convert NK = 2 input data to NK = 3 formats needed in the present simulation. A deliverability boundary condition, which will be maintained for the remainder

of the simulation, is used in the production elements `A1117` through `A5117`. Part of the T2VOC output after xylene injection for 4.8×10^6 s is given in Figure 22.

In the next part of the simulation, the previously injected xylene is simply allowed to redistribute itself. No additional fluids are injected or produced, except that the deliverability boundary condition is still maintained at the production end of the mesh. The input file is shown in Figure 23 and is similar to the previous input file (Figure 21), except that the o-xylene injection specified in block **GENER** has been removed, and the SAVE file from the previous part of the simulation was imported as block **lNCON**. This part of the simulation is run for a period of 3.156×10^8 s (10 years), and part of the T2VOC output at this time is shown in Figure 24. A contour plot of the separate phase xylene (NAPL) saturation distribution is shown in Figure 25.

In the final part of this simulation, steam with a specific enthalpy of 2.676×10^6 J/kg is injected at the left boundary (elements `A11 1` through `A51 1`) for a period of 1.48×10^7 s (171.3 days). The total steam injection rate of 7.4×10^{-4} kg/s is evenly divided between the five injection elements. Again, at the production boundary, the deliverability boundary condition is used. The input file for this part of the simulation is shown in Figure 26, and is similar to the previous input file (Figure 23). NEQ = 4 is now used in **MULTI**, for a nonisothermal run. Again, the SAVE file from the previous part of the simulation was imported as data block **INCON**. Data block **GENER** has been changed to include steam injection in the boundary elements `A11 1` through `A51 1`. A printout after 9.2×10^6 s (106.5 days) of steam injection is specified in data block TIMES (a total time of 9.608×10^8 s), and part of this output is shown in Figure 27. A contour plot of the xylene saturation distribution along with the steam front location at this time, shown in Figure 28, indicates that the steam is achieving an effective sweep of the xylene plume. By the end of the simulation, after 1.48×10^7 s (171.3 days) of steam injection, all of the xylene has been removed, and the entire system is at the steam temperature, see Figure 29.

Figure 17. T2VOC input file for part 1 of problem 4.

```
*rfs1*...2-D X-Z field scale problem: generate gravity-capillary equilibrium.
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX       1       0.3
NX      15       1.2
NX       1       0.3
NY       1       1.0
NZ       5       1.2


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.       .40   2.5E-13   2.5E-13   2.5E-13       3.1    1000.0
        0.        0.      2.85       0.0

CHEMP----1----o-Xylene data--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    -15.85     .5962 -3.443E-4  7.528E-8
     880.0     293.0    8.0E-6     273.0      1.60
    -3.332   1.039E3 -1.768E-3  1.076E-6      369.
  2.975E-5        0.        0.        0.
        0.        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  20      201000000001000104 0001000   0.00E-5
                          -1.                        9.8060
      1.e5
     1.E-5     1.E00                                  1.E-8
               1.12e5                50.0                22.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6           .100       .05       .01        3.
    8          0.000      1.84      5.E4      5.24
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1   16    1            .40
              1.01e5                0.10                22.0
A21 1   16    1            .40
              1.01e5                0.10                22.0
A31 1   16    1            .40
              1.01e5                0.95                22.0

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 18. Meshmaker output for problem 4.

```
*****************************************************************************************************************
*                    CARTESIAN MESH WITH NX*NY*NZ =   17 *   1 *   5  GRID BLOCKS                                 *
*****************************************************************************************************************
*                                                                                                                 *
*                    THE MESH WILL BE PRINTED AS SLICES FOR J = 1 TO J = NY =   1                                 *
*                                                                                                                 *
*                    IN EACH MESH SLICE, ROWS WILL GO FROM  K = 1 TO K = NZ =   5                                 *
*                                                                                                                 *
*                    IN EACH ROW, COLUMNS WILL GO FROM      I = 1 TO I = NX =  17                                 *
*                                                                                                                 *
*****************************************************************************************************************

SLICE WITH J =   1

  COLUMN I =  1     2     3     4     5     6     7     8     9    10    11    12    13    14    15    16    17    18    19    20
ROWS
 K =    1   A11 1 A11 2 A11 3 A11 4 A11 5 A11 6 A11 7 A11 8 A11 9 A1110 A1111 A1112 A1113 A1114 A1115 A1116 A1117
 K =    2   A21 1 A21 2 A21 3 A21 4 A21 5 A21 6 A21 7 A21 8 A21 9 A2110 A2111 A2112 A2113 A2114 A2115 A2116 A2117
 K =    3   A31 1 A31 2 A31 3 A31 4 A31 5 A31 6 A31 7 A31 8 A31 9 A3110 A3111 A3112 A3113 A3114 A3115 A3116 A3117
 K =    4   A41 1 A41 2 A41 3 A41 4 A41 5 A41 6 A41 7 A41 8 A41 9 A4110 A4111 A4112 A4113 A4114 A4115 A4116 A4117
 K =    5   A51 1 A51 2 A51 3 A51 4 A51 5 A51 6 A51 7 A51 8 A51 9 A5110 A5111 A5112 A5113 A5114 A5115 A5116 A5117

*****************************************************************************************************************

MESH GENERATION COMPLETE --- EXIT FROM MODULE *MESHMAKER*


DOMAIN NO.  1     MATERIAL NAME -- DIRT1
HAVE READ UNKNOWN BLOCK LABEL "----*" --- IGNORE THIS, AND CONTINUE READING INPUT DATA

WRITE FILE *INCON* FROM INPUT DATA

WRITE FILE *GENER* FROM INPUT DATA

                        ***********************************************************************************
                        *                        EVALUATE FLOATING POINT ARITHMETIC                         *
                        ***********************************************************************************
                        *                                                                                 *
                        * FLOATING POINT PROCESSOR HAS APPROXIMATELY 15 SIGNIFICANT DIGITS                *
                        *                                                                                 *
                        * DEFAULT VALUE OF INCREMENT FACTOR FOR NUMERICAL DERIVATIVES IS DFAC =  .1051E-07 *
                        * USER-SPECIFIED VALUE DFAC =  .1000E-07 WILL BE USED                             *
                        *                                                                                 *
                        ***********************************************************************************



MESH HAS   85 ELEMENTS (   85 ACTIVE) AND  148 CONNECTIONS (INTERFACES) BETWEEN THEM
GENER HAS   0 SINKS/SOURCES


END OF TOUGH2 INPUT JOB --- ELAPSED TIME =    .0000 SECONDS
```

Figure 19. Mesh diagram for problem 4.

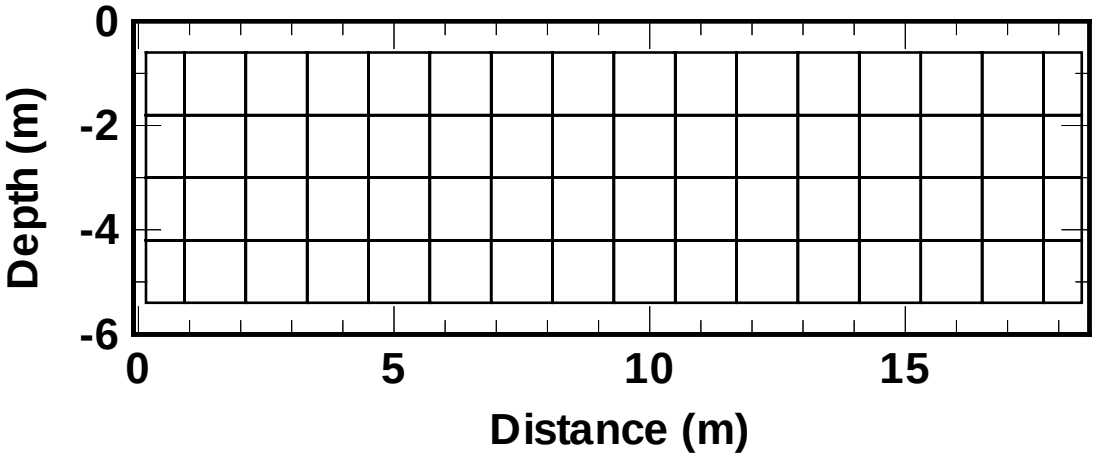


Figure 20. Printed output for part 1 of problem 4.

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [   0,  0] *****                                THE TIME IS   .00000E+00 SECONDS, OR   .00000E+00 DAYS


                        PHASES PRESENT                                                  COMPONENT MASS IN PLACE (KG)
*********************************************************        *********************************************************
 PHASES       *      GAS          AQUEOUS         NAPL           COMPONENTS    *     WATER           AIR            VOC
*********************************************************        *********************************************************
              *                                                   PHASES        *
 VOLUME (M^3) *  .16516800E+02  .28123200E+02  .00000000E+00      GAS PHASE     *  .32076273E+00  .19171294E+02  .00000000E+00
 MASS   (KG)  *  .19492057E+02  .28063919E+05  .00000000E+00      AQUEOUS       *  .28063757E+05  .16198725E+00  .00000000E+00
*********************************************************        NAPL          *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                  ADSORBED      *  .00000000E+00  .00000000E+00  .00000000E+00
                                                                  TOTAL         *  .28064078E+05  .19333281E+02  .00000000E+00
                                                                 *********************************************************

*****************************************************************************************************************************


...ITERATING...  AT [   1,  1] --- DELTEX =  .100000E+06   MAX. RES. =  .631493E+01  AT ELEMENT A21 1  EQUATION   1
...ITERATING...  AT [   1,  2] --- DELTEX =  .100000E+06   MAX. RES. =  .197393E+01  AT ELEMENT A2117  EQUATION   1
...ITERATING...  AT [   1,  3] --- DELTEX =  .100000E+06   MAX. RES. =  .363121E+00  AT ELEMENT A2117  EQUATION   1
...ITERATING...  AT [   1,  4] --- DELTEX =  .100000E+06   MAX. RES. =  .182445E-01  AT ELEMENT A2115  EQUATION   1
...ITERATING...  AT [   1,  5] --- DELTEX =  .100000E+06   MAX. RES. =  .513958E-04  AT ELEMENT A2111  EQUATION   1
A21 7(   1,  6) ST =  .100000E+06 DT =  .100000E+06 DX1=  .821535E+01 DX2=  .704254E-01 T =  22.000 P =   101008. S =  .829575E+00
...ITERATING...  AT [   2,  1] --- DELTEX =  .100000E+06   MAX. RES. =  .413186E+00  AT ELEMENT A21 7  EQUATION   1
...ITERATING...  AT [   2,  2] --- DELTEX =  .100000E+06   MAX. RES. =  .419837E-01  AT ELEMENT A2117  EQUATION   1
...ITERATING...  AT [   2,  3] --- DELTEX =  .100000E+06   MAX. RES. =  .533051E-03  AT ELEMENT A21 1  EQUATION   1
A2113(   2,  4) ST =  .200000E+06 DT =  .100000E+06 DX1= -.208931E+01 DX2=  .173031E-01 T =  22.000 P =   101006. S =  .812272E+00
...ITERATING...  AT [   3,  1] --- DELTEX =  .200000E+06   MAX. RES. =  .184323E+00  AT ELEMENT A2113  EQUATION   1
...ITERATING...  AT [   3,  2] --- DELTEX =  .200000E+06   MAX. RES. =  .779317E-02  AT ELEMENT A2116  EQUATION   1
...ITERATING...  AT [   3,  3] --- DELTEX =  .200000E+06   MAX. RES. =  .151057E-04  AT ELEMENT A21 2  EQUATION   1
A21 1(   3,  4) ST =  .400000E+06 DT =  .200000E+06 DX1= -.728606E+00 DX2=  .579437E-02 T =  22.000 P =   101005. S =  .806477E+00
...ITERATING...  AT [   4,  1] --- DELTEX =  .400000E+06   MAX. RES. =  .598771E-01  AT ELEMENT A2113  EQUATION   1
...ITERATING...  AT [   4,  2] --- DELTEX =  .400000E+06   MAX. RES. =  .693335E-03  AT ELEMENT A21 8  EQUATION   1
A21 7(   4,  3) ST =  .800000E+06 DT =  .400000E+06 DX1= -.150817E+00 DX2=  .108689E-02 T =  22.000 P =   101005. S =  .805390E+00
...ITERATING...  AT [   5,  1] --- DELTEX =  .800000E+06   MAX. RES. =  .155191E-01  AT ELEMENT A11 6  EQUATION   1
...ITERATING...  AT [   5,  2] --- DELTEX =  .800000E+06   MAX. RES. =  .558415E-04  AT ELEMENT A2112  EQUATION   1
A3117(   5,  3) ST =  .160000E+07 DT =  .800000E+06 DX1=  .146775E+00 DX2= -.142285E-02 T =  22.000 P =   101019. S =  .147413E+00
...ITERATING...  AT [   6,  1] --- DELTEX =  .160000E+07   MAX. RES. =  .269266E-01  AT ELEMENT A1112  EQUATION   1
...ITERATING...  AT [   6,  2] --- DELTEX =  .160000E+07   MAX. RES. =  .150181E-03  AT ELEMENT A1113  EQUATION   1
A3117(   6,  3) ST =  .320000E+07 DT =  .160000E+07 DX1=  .502030E-02 DX2= -.205215E-02 T =  22.000 P =   101019. S =  .149465E+00
...ITERATING...  AT [   7,  1] --- DELTEX =  .320000E+07   MAX. RES. =  .413256E-01  AT ELEMENT A1113  EQUATION   1
...ITERATING...  AT [   7,  2] --- DELTEX =  .320000E+07   MAX. RES. =  .470530E-03  AT ELEMENT A1116  EQUATION   1
A1117(   7,  3) ST =  .640000E+07 DT =  .320000E+07 DX1= -.526019E-01 DX2=  .285057E-02 T =  22.000 P =   100991. S =  .892221E+00
...ITERATING...  AT [   8,  1] --- DELTEX =  .640000E+07   MAX. RES. =  .528873E-01  AT ELEMENT A1113  EQUATION   1
...ITERATING...  AT [   8,  2] --- DELTEX =  .640000E+07   MAX. RES. =  .853817E-03  AT ELEMENT A11 8  EQUATION   1
A11 1(   8,  3) ST =  .128000E+08 DT =  .640000E+07 DX1= -.527035E-01 DX2=  .288574E-02 T =  22.000 P =   100991. S =  .889336E+00
...ITERATING...  AT [   9,  1] --- DELTEX =  .128000E+08   MAX. RES. =  .521444E-01  AT ELEMENT A1113  EQUATION   1
...ITERATING...  AT [   9,  2] --- DELTEX =  .128000E+08   MAX. RES. =  .764499E-03  AT ELEMENT A1116  EQUATION   1
A1117(   9,  3) ST =  .256000E+08 DT =  .128000E+08 DX1= -.367649E-01 DX2=  .202915E-02 T =  22.000 P =   100991. S =  .887306E+00
...ITERATING...  AT [  10,  1] --- DELTEX =  .256000E+08   MAX. RES. =  .360059E-01  AT ELEMENT A11 1  EQUATION   1
...ITERATING...  AT [  10,  2] --- DELTEX =  .256000E+08   MAX. RES. =  .278389E-03  AT ELEMENT A1116  EQUATION   1
A11 1(  10,  3) ST =  .512000E+08 DT =  .256000E+08 DX1= -.160226E-01 DX2=  .888314E-03 T =  22.000 P =   100991. S =  .886418E+00
...ITERATING...  AT [  11,  1] --- DELTEX =  .512000E+08   MAX. RES. =  .156392E-01  AT ELEMENT A1117  EQUATION   1
...ITERATING...  AT [  11,  2] --- DELTEX =  .512000E+08   MAX. RES. =  .338520E-04  AT ELEMENT A11 2  EQUATION   1
A3117(  11,  3) ST =  .102400E+09 DT =  .512000E+08 DX1= -.856914E-03 DX2= -.208116E-03 T =  22.000 P =   101019. S =  .157835E+00
...ITERATING...  AT [  12,  1] --- DELTEX =  .102400E+09   MAX. RES. =  .387867E-02  AT ELEMENT A1117  EQUATION   1
```

Figure 20. (continued)

rfs1...2-D X-Z field scale problem: generate gravity-capillary equilibrium.

OUTPUT DATA AFTER (20, 1)-2-TIME STEPS THE TIME IS .60681E+06 DAYS

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Figure 21. T2VOC input file for part 2 of problem 4.

```
*rfs2*...2-D X-Z field scale problem: inject o-Xylene.
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX       1       0.3
NX      15       1.2
NX       1       0.3
NY       1       1.0
NZ       5       1.2


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.       .40   2.5E-13   2.5E-13   2.5E-13       3.1    1000.0
        0.        0.      2.85       0.0

CHEMP----1----o-Xylene data--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    -15.85     .5962 -3.443E-4  7.528E-8
     880.0     293.0    8.0E-6     273.0      1.60
    -3.332   1.039E3 -1.768E-3  1.076E-6      369.
  2.975E-5        0.        0.        0.
        0.        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  20      201000000001000104 0101000   0.00E-5
               4.8e6       -1.                       9.8060
      1.e5
     1.E-5     1.E00                                 1.E-8
              1.12e5               50.0               22.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6           .100       .05       .01        3.
    8          0.000      1.84      5.E4      5.24
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 9INO 1                        COM3  1.4667E-4    3.80E4
A5117PRO 5                   5    DELV    2.0e-12   1.232e5       1.2
A4117PRO 4                        DELV    2.0e-12   1.232e5       1.2
A3117PRO 3                        DELV    2.0e-12   1.232e5       1.2
A2117PRO 2                        DELV    2.0e-12   1.232e5       1.2
A1117PRO 1                        DELV    2.0e-12   1.232e5       1.2

INCON -- INITIAL CONDITIONS FOR   85 ELEMENTS AT TIME   .524288E+11
A11 1            .40000000E+00
  .1009912017795E+06  .1138339596073E+00  .2200000000000E+02
A21 1            .40000000E+00
  .1010050884085E+06  .1940257313915E+00  .2200000000000E+02
A31 1            .40000000E+00
  .1010189769660E+06  .8421354014011E+00  .2200000000000E+02
A41 1            .40000000E+00
  .1115416826634E+06  .5000000000008E+02  .2200000000000E+02
A51 1            .40000000E+00
  .1232841286996E+06  .5000000000000E+02  .2200000000000E+02
A11 2            .40000000E+00
  .1009912017795E+06  .1138339596073E+00  .2200000000000E+02
A21 2            .40000000E+00
  .1010050884085E+06  .1940257313915E+00  .2200000000000E+02
A31 2            .40000000E+00
  .1010189769660E+06  .8421354014011E+00  .2200000000000E+02
```

Figure 22. Printed output for part 2 of problem 4.

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*rfs2*...2-D X-Z field scale problem: inject o-Xylene.

         OUTPUT DATA AFTER (  10,  4)-2-TIME STEPS                                                    THE TIME IS   .55556E+02 DAYS

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Figure 22. (continued)

ELEM	INDEX	P (PA)	T (DEG.C)	SO	SW	SG	PVOC (PA)	PAIR (PA)	PSATO (PA)	PSATW (PA)	PCO (PA)	PCW (PA)
A51 9	45	128844.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	281.	741.	2642.	0.	0.
A1110	46	106054.	22.000	.7111E-03	.1143E+00	.8850E+00	741.	102671.	741.	2642.	-3.	-24554.
A2110	47	106070.	22.000	.7257E-03	.2011E+00	.7982E+00	741.	102687.	741.	2642.	-1.	-12396.
A3110	48	106751.	22.000	.6917E-01	.8237E+00	.1071E+00	741.	103368.	741.	2642.	0.	-1321.
A4110	49	117100.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	3373.	741.	2642.	0.	0.
A5110	50	128820.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	43.	741.	2642.	0.	0.
A1111	51	106054.	22.000	.0000E+00	.1142E+00	.8858E+00	70.	103342.	741.	2642.	-3.	-24591.
A2111	52	106069.	22.000	.0000E+00	.1993E+00	.8007E+00	44.	103383.	741.	2642.	-1.	-12531.
A3111	53	106371.	22.000	.0000E+00	.8672E+00	.1328E+00	331.	103398.	741.	2642.	0.	-1081.
A4111	54	117035.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	139.	741.	2642.	0.	0.
A5111	55	128774.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	1.	741.	2642.	0.	0.
A1112	56	106053.	22.000	.0000E+00	.1141E+00	.8859E+00	4.	103407.	741.	2642.	-3.	-24609.
A2112	57	106068.	22.000	.0000E+00	.1984E+00	.8016E+00	1.	103425.	741.	2642.	-1.	-12602.
A3112	58	106296.	22.000	.0000E+00	.8676E+00	.1324E+00	6.	103648.	741.	2642.	0.	-1079.
A4112	59	116977.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	9.	741.	2642.	0.	0.
A5112	60	128726.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A1113	61	106052.	22.000	.0000E+00	.1141E+00	.8859E+00	0.	103410.	741.	2642.	-3.	-24620.
A2113	62	106067.	22.000	.0000E+00	.1978E+00	.8022E+00	0.	103425.	741.	2642.	-1.	-12650.
A3113	63	106256.	22.000	.0000E+00	.8658E+00	.1342E+00	0.	103614.	741.	2642.	0.	-1089.
A4113	64	116931.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	1.	741.	2642.	0.	0.
A5113	65	128683.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A1114	66	106052.	22.000	.0000E+00	.1140E+00	.8860E+00	0.	103410.	741.	2642.	-3.	-24628.
A2114	67	106067.	22.000	.0000E+00	.1973E+00	.8027E+00	0.	103425.	741.	2642.	-1.	-12683.
A3114	68	106232.	22.000	.0000E+00	.8639E+00	.1361E+00	0.	103590.	741.	2642.	0.	-1100.
A4114	69	116897.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A5114	70	128649.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A1115	71	106051.	22.000	.0000E+00	.1140E+00	.8860E+00	0.	103409.	741.	2642.	-3.	-24632.
A2115	72	106066.	22.000	.0000E+00	.1971E+00	.8029E+00	0.	103424.	741.	2642.	-1.	-12705.
A3115	73	106217.	22.000	.0000E+00	.8625E+00	.1375E+00	0.	103575.	741.	2642.	0.	-1107.
A4115	74	116873.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A5115	75	128626.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A1116	76	106051.	22.000	.0000E+00	.1140E+00	.8860E+00	0.	103409.	741.	2642.	-3.	-24635.
A2116	77	106066.	22.000	.0000E+00	.1969E+00	.8031E+00	0.	103424.	741.	2642.	-1.	-12717.
A3116	78	106209.	22.000	.0000E+00	.8617E+00	.1383E+00	0.	103567.	741.	2642.	0.	-1112.
A4116	79	116861.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A5116	80	128613.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A1117	81	106051.	22.000	.0000E+00	.1140E+00	.8860E+00	0.	103409.	741.	2642.	-3.	-24635.
A2117	82	106066.	22.000	.0000E+00	.1969E+00	.8031E+00	0.	103424.	741.	2642.	-1.	-12718.
A3117	83	106209.	22.000	.0000E+00	.8616E+00	.1384E+00	0.	103566.	741.	2642.	0.	-1112.
A4117	84	116859.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.
A5117	85	128612.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	0.	741.	2642.	0.	0.

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Figure 23. T2VOC input file for part 3 of problem 4.

```
*rfs3*...2-D X-Z field scale problem: spreading of o-Xylene.
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX       1       0.3
NX      15       1.2
NX       1       0.3
NY       1       1.0
NZ       5       1.2


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.       .40   2.5E-13   2.5E-13   2.5E-13       3.1    1000.0
        0.        0.      2.85       0.0

CHEMP----1----o-Xylene data--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    -15.85     .5962 -3.443E-4  7.528E-8
     880.0     293.0    8.0E-6     273.0      1.60
    -3.332   1.039E3 -1.768E-3  1.076E-6      369.
  2.975E-5        0.        0.        0.
        0.        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  40      40100000000100010470 01000   0.00E-5
             3.156e8       -1.      2.e7              9.8060
      2.e5
     1.E-5     1.E00                                   1.E-8
             1.12e5                50.0                 22.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6          .100       .05       .01        3.
    8         0.000      1.84      5.E4      5.24
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A5117PRO 5                  5     DELV    2.0e-12   1.232e5       1.2
A4117PRO 4                        DELV    2.0e-12   1.232e5       1.2
A3117PRO 3                        DELV    2.0e-12   1.232e5       1.2
A2117PRO 2                        DELV    2.0e-12   1.232e5       1.2
A1117PRO 1                        DELV    2.0e-12   1.232e5       1.2

INCON -- INITIAL CONDITIONS FOR   85 ELEMENTS AT TIME   .480000E+07
A11 1            .40000000E+00
  .1060511419408E+06  .1139940384325E+00  .6076167610022E-13  .2200000000000E+02
A21 1            .40000000E+00
  .1060660493631E+06  .1968846696062E+00  .1007832857023E-14  .2200000000000E+02
A31 1            .40000000E+00
  .1062085137667E+06  .8616285109018E+00  .1398886127020E-15  .2200000000000E+02
A41 1            .40000000E+00
  .1168589870921E+06  .5000000000008E+02  .5617176457889E-19  .2200000000000E+02
A51 1            .40000000E+00
  .1286117006033E+06  .5000000000000E+02  .2943810248792E-20  .2200000000000E+02
A11 2            .40000000E+00
  .1060511696326E+06  .1139952434164E+00  .8401506922224E-11  .2200000000000E+02
A21 2            .40000000E+00
  .1060660790209E+06  .1969032776091E+00  .1750375136797E-12  .2200000000000E+02
A31 2            .40000000E+00
  .1062094760462E+06  .8617310272224E+00  .6531878177701E-13  .2200000000000E+02
```

Figure 24. Printed output for part 3 of problem 4.

```
*rfs3*...2-D X-Z field scale problem: spreading of o-Xylene.

         OUTPUT DATA AFTER (  26,  3)-2-TIME STEPS                                                    THE TIME IS   .36528E+04 DAYS

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Figure 24. (continued)

ELEM	INDEX	P (PA)	T (DEG.C)	SO	SW	SG	PVOC (PA)	PAIR (PA)	PSATO (PA)	PSATW (PA)	PCO (PA)	PCW (PA)
A51 9	45	128526.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	556.	741.	2642.	0.	0.
A1110	46	106085.	22.000	.7180E-03	.1154E+00	.8839E+00	741.	102701.	741.	2642.	-3.	-24286.
A2110	47	106100.	22.000	.7363E-03	.1959E+00	.8033E+00	741.	102716.	741.	2642.	-1.	-12794.
A3110	48	106426.	22.000	.1689E+00	.8123E+00	.1878E-01	741.	103042.	741.	2642.	0.	-1384.
A4110	49	117342.	22.000	.4600E-01	.9540E+00	.0000E+00	0.	6760.	741.	2642.	0.	-558.
A5110	50	128526.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	168.	741.	2642.	0.	0.
A1111	51	106085.	22.000	.0000E+00	.1151E+00	.8849E+00	69.	103374.	741.	2642.	-3.	-24342.
A2111	52	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	196.	103261.	741.	2642.	-1.	-12794.
A3111	53	106355.	22.000	.1544E+00	.8250E+00	.2060E-01	741.	102972.	741.	2642.	0.	-1314.
A4111	54	116784.	22.000	.1919E-04	.1000E+01	.0000E+00	0.	2731.	741.	2642.	0.	0.
A5111	55	128526.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	18.	741.	2642.	0.	0.
A1112	56	106085.	22.000	.0000E+00	.1150E+00	.8850E+00	6.	103437.	741.	2642.	-3.	-24375.
A2112	57	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	36.	103421.	741.	2642.	-1.	-12794.
A3112	58	106246.	22.000	.1274E+00	.8449E+00	.2777E-01	741.	102863.	741.	2642.	0.	-1205.
A4112	59	116784.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	2775.	741.	2642.	0.	0.
A5112	60	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	20.	741.	2642.	0.	0.
A1113	61	106085.	22.000	.0000E+00	.1149E+00	.8851E+00	0.	103442.	741.	2642.	-3.	-24396.
A2113	62	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	8.	103449.	741.	2642.	-1.	-12794.
A3113	63	106116.	22.000	.2450E-01	.8685E+00	.1070E+00	741.	102733.	741.	2642.	0.	-1074.
A4113	64	116784.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	2145.	741.	2642.	0.	0.
A5113	65	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	12.	741.	2642.	0.	0.
A1114	66	106085.	22.000	.0000E+00	.1149E+00	.8851E+00	0.	103443.	741.	2642.	-3.	-24407.
A2114	67	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	0.	103457.	741.	2642.	-1.	-12794.
A3114	68	106114.	22.000	.0000E+00	.8689E+00	.1311E+00	3.	103469.	741.	2642.	0.	-1072.
A4114	69	116785.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	2039.	741.	2642.	0.	0.
A5114	70	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	11.	741.	2642.	0.	0.
A1115	71	106085.	22.000	.0000E+00	.1149E+00	.8851E+00	0.	103443.	741.	2642.	-3.	-24413.
A2115	72	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	0.	103457.	741.	2642.	-1.	-12793.
A3115	73	106114.	22.000	.0000E+00	.8690E+00	.1310E+00	0.	103472.	741.	2642.	0.	-1072.
A4115	74	116785.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	1917.	741.	2642.	0.	0.
A5115	75	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	10.	741.	2642.	0.	0.
A1116	76	106085.	22.000	.0000E+00	.1148E+00	.8852E+00	0.	103443.	741.	2642.	-3.	-24416.
A2116	77	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	0.	103457.	741.	2642.	-1.	-12793.
A3116	78	106114.	22.000	.0000E+00	.8690E+00	.1310E+00	0.	103472.	741.	2642.	0.	-1072.
A4116	79	116785.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	1872.	741.	2642.	0.	0.
A5116	80	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	9.	741.	2642.	0.	0.
A1117	81	106085.	22.000	.0000E+00	.1148E+00	.8852E+00	0.	103443.	741.	2642.	-3.	-24416.
A2117	82	106099.	22.000	.0000E+00	.1959E+00	.8041E+00	0.	103457.	741.	2642.	-1.	-12793.
A3117	83	106114.	22.000	.0000E+00	.8690E+00	.1310E+00	0.	103472.	741.	2642.	0.	-1072.
A4117	84	116785.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	1867.	741.	2642.	0.	0.
A5117	85	128527.	22.000	.0000E+00	.1000E+01	.0000E+00	0.	9.	741.	2642.	0.	0.

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Figure 24. (continued)

rfs3...2-D X-Z field scale problem: spreading of o-Xylene.

KCYC = 26 - ITER = 3 - TIME = .31560E+09

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
A11 1	1	.7826E-12	.4270E-11	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4489E-05	.0000E+00
A21 1	2	.5990E-13	.3269E-12	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 1	3	.7767E-13	.4238E-12	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2431E-02	.6238E+00	.0000E+00
A41 1	4	.0000E+00	.2422E-13	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 1	5	.0000E+00	.3104E-15	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 2	6	.9083E-10	.4956E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4490E-05	.0000E+00
A21 2	7	.3190E-10	.1741E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 2	8	.2623E-10	.1431E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2431E-02	.6238E+00	.0000E+00
A41 2	9	.0000E+00	.6701E-11	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 2	10	.0000E+00	.7661E-13	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 3	11	.6965E-08	.3800E-07	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4500E-05	.0000E+00
A21 3	12	.1501E-07	.8188E-07	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 3	13	.3606E-07	.1967E-06	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2432E-02	.6237E+00	.0000E+00
A41 3	14	.0000E+00	.1898E-08	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 3	15	.0000E+00	.1612E-10	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 4	16	.2604E-06	.1421E-05	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9193E+00	.4522E-05	.0000E+00
A21 4	17	.3212E-05	.1753E-04	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 4	18	.1186E-03	.6469E-03	.1241E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2435E-02	.6236E+00	.0000E+00
A41 4	19	.0000E+00	.4417E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 4	20	.0000E+00	.1249E-07	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 5	21	.1178E-04	.6429E-04	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9192E+00	.4560E-05	.0000E+00
A21 5	22	.3408E-03	.1859E-02	.1241E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 5	23	.3206E-01	.1749E+00	.1264E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.1252E-02	.6226E+00	.0000E+00
A41 5	24	.0000E+00	.2177E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 5	25	.0000E+00	.8007E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 6	26	.2414E-03	.1317E-02	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9189E+00	.4635E-05	.0000E+00
A21 6	27	.1575E-02	.8592E-02	.1241E+01	.0000E+00	.1820E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 6	28	.3206E-01	.1749E+00	.1265E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.7691E-05	.5669E+00	.2165E-02
A41 6	29	.0000E+00	.4737E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A51 6	30	.0000E+00	.3525E-04	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 7	31	.2989E-02	.1631E-01	.1242E+01	.0000E+00	.1818E-04	.1000E+01	.0000E+00	.0000E+00	.9185E+00	.4759E-05	.0000E+00
A21 7	32	.8471E-02	.4622E-01	.1246E+01	.0000E+00	.1813E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A31 7	33	.3206E-01	.1749E+00	.1267E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.1633E-05	.5228E+00	.3588E-02
A41 7	34	.0000E+00	.1749E+00	.0000E+00	.8782E+03	.1000E+01	.7867E-03	.0000E+00	.0000E+00	.0000E+00	.9999E+00	.0000E+00
A51 7	35	.0000E+00	.1481E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 8	36	.3206E-01	.1749E+00	.1263E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.9156E+00	.4971E-05	.0000E+00
A21 8	37	.3206E-01	.1749E+00	.1264E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.6849E+00	.1211E-02	.0000E+00
A31 8	38	.3206E-01	.1749E+00	.1267E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.9293E-06	.4958E+00	.4599E-02
A41 8	39	.0000E+00	.1749E+00	.0000E+00	.8782E+03	.1000E+01	.7867E-03	.0000E+00	.0000E+00	.0000E+00	.8544E+00	.0000E+00
A51 8	40	.0000E+00	.3591E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A11 9	41	.3206E-01	.1749E+00	.1263E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.7437E+00	.5192E-05	.5249E-05
A21 9	42	.3206E-01	.1749E+00	.1264E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.5604E+00	.1211E-02	.6531E-05
A31 9	43	.3206E-01	.1749E+00	.1268E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.5722E-06	.4833E+00	.5162E-02
A41 9	44	.0000E+00	.1749E+00	.0000E+00	.8782E+03	.1000E+01	.7867E-03	.0000E+00	.0000E+00	.0000E+00	.8229E+00	.1530E-03
A51 9	45	.0000E+00	.1127E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1110	46	.3206E-01	.1749E+00	.1263E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.9156E+00	.4971E-05	.0000E+00
A2110	47	.3206E-01	.1749E+00	.1264E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.6849E+00	.1211E-02	.0000E+00
A3110	48	.3206E-01	.1749E+00	.1267E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.9293E-06	.4958E+00	.4599E-02
A4110	49	.0000E+00	.1749E+00	.0000E+00	.8782E+03	.1000E+01	.7867E-03	.0000E+00	.0000E+00	.0000E+00	.8544E+00	.0000E+00
A5110	50	.0000E+00	.3591E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1111	51	.2989E-02	.1631E-01	.1242E+01	.0000E+00	.1818E-04	.1000E+01	.0000E+00	.0000E+00	.9185E+00	.4759E-05	.0000E+00
A2111	52	.8471E-02	.4622E-01	.1246E+01	.0000E+00	.1813E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00

Figure 24. (continued)

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
A3111	53	.3206E-01	.1749E+00	.1267E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.1633E-05	.5228E+00	.3588E-02
A4111	54	.0000E+00	.1749E+00	.0000E+00	.8782E+03	.1000E+01	.7867E-03	.0000E+00	.0000E+00	.0000E+00	.9999E+00	.0000E+00
A5111	55	.0000E+00	.1481E-03	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1112	56	.2414E-03	.1317E-02	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9189E+00	.4635E-05	.0000E+00
A2112	57	.1575E-02	.8592E-02	.1241E+01	.0000E+00	.1820E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3112	58	.3206E-01	.1749E+00	.1265E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.7691E-05	.5669E+00	.2165E-02
A4112	59	.0000E+00	.4737E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5112	60	.0000E+00	.3525E-04	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1113	61	.1178E-04	.6429E-04	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9192E+00	.4560E-05	.0000E+00
A2113	62	.3408E-03	.1859E-02	.1241E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3113	63	.3206E-01	.1749E+00	.1264E+01	.8782E+03	.1790E-04	.7867E-03	.0000E+00	.0000E+00	.1252E-02	.6226E+00	.0000E+00
A4113	64	.0000E+00	.2177E-02	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5113	65	.0000E+00	.8007E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1114	66	.2604E-06	.1421E-05	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9193E+00	.4522E-05	.0000E+00
A2114	67	.3212E-05	.1753E-04	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3114	68	.1186E-03	.6469E-03	.1241E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2435E-02	.6236E+00	.0000E+00
A4114	69	.0000E+00	.4417E-05	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5114	70	.0000E+00	.1260E-07	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1115	71	.6965E-08	.3800E-07	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4500E-05	.0000E+00
A2115	72	.1501E-07	.8188E-07	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3115	73	.3606E-07	.1967E-06	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2432E-02	.6237E+00	.0000E+00
A4115	74	.0000E+00	.1957E-08	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5115	75	.0000E+00	.1687E-10	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1116	76	.9083E-10	.4956E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4490E-05	.0000E+00
A2116	77	.3189E-10	.1740E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3116	78	.2623E-10	.1431E-09	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2431E-02	.6238E+00	.0000E+00
A4116	79	.0000E+00	.6813E-11	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5116	80	.0000E+00	.7755E-13	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1117	81	.7896E-12	.4309E-11	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.9194E+00	.4489E-05	.0000E+00
A2117	82	.5854E-13	.3194E-12	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.6868E+00	.1211E-02	.0000E+00
A3117	83	.7787E-13	.4249E-12	.1240E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.2431E-02	.6238E+00	.0000E+00
A4117	84	.0000E+00	.4955E-13	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5117	85	.0000E+00	.1588E-14	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00

@@@

Figure 25. Separate phase xylene saturation distribution prior to steam injection.

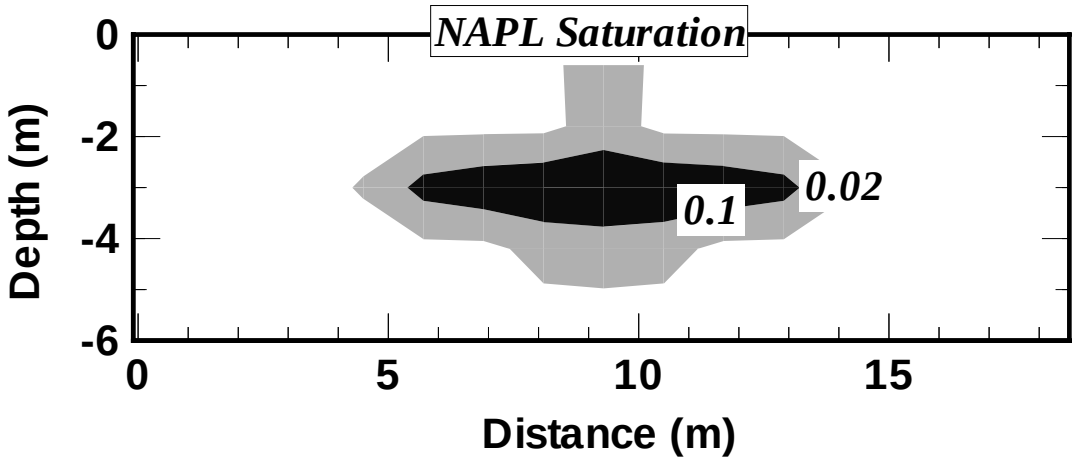

Figure 26. T2VOC input file for part 4 of problem 4.

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*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
      00.
NX       1       0.3
NX      15       1.2
NX       1       0.3
NY       1       1.0
NZ       5       1.2


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
DIRT1    1     2650.       .40   2.5E-13   2.5E-13   2.5E-13       3.1    1000.0
        0.        0.      2.85       0.0

CHEMP----1----o-Xylene data--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    -15.85     .5962 -3.443E-4  7.528E-8
     880.0     293.0    8.0E-6     273.0      1.60
    -3.332   1.039E3 -1.768E-3  1.076E-6      369.
  2.975E-5        0.        0.        0.
        0.        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    4    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3 300     30010000000100010400 01000   0.00E-5
             1.48e7       -1.      1.e5              9.8060
      1.e5
     1.E-5     1.E00                                  1.E-8
             1.12e5                50.0                22.0
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6          .100       .05       .01        3.
    8         0.000      1.84      5.E4      5.24
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
     9.2e6
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1INJ 1                        COM1    1.48e-4   2.676e6
A21 1INJ 2                        COM1    1.48e-4   2.676e6
A31 1INJ 3                        COM1    1.48e-4   2.676e6
A41 1INJ 4                        COM1    1.48e-4   2.676e6
A51 1INJ 5                        COM1    1.48e-4   2.676e6
A5117PRO 5                  5     DELV    2.0e-12   1.232e5       1.2
A4117PRO 4                        DELV    2.0e-12   1.232e5       1.2
A3117PRO 3                        DELV    2.0e-12   1.232e5       1.2
A2117PRO 2                        DELV    2.0e-12   1.232e5       1.2
A1117PRO 1                        DELV    2.0e-12   1.232e5       1.2

INCON -- INITIAL CONDITIONS FOR   85 ELEMENTS AT TIME   .315600E+09
A11 1            .40000000E+00
  .1060848028501E+06  .1148464608786E+00  .1705120693891E-12  .2200000000000E+02
A21 1            .40000000E+00
  .1060993959119E+06  .1959411157618E+00  .1305020322786E-13  .2200000000000E+02
A31 1            .40000000E+00
  .1061139893603E+06  .8689848999841E+00  .1691979745491E-13  .2200000000000E+02
A41 1            .40000000E+00
  .1167846788972E+06  .5000000030008E+02  .4119167811768E-17  .2200000000000E+02
```

Figure 27. Printed output for part 4 of problem 4 after 106.5 days of steam injection.

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*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.

        OUTPUT DATA AFTER ( 127,  6)-2-TIME STEPS                                                    THE TIME IS   .10648E+03 DAYS

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Figure 27. (continued)

ELEM	INDEX	P (PA)	T (DEG.C)	SO	SW	SG	PVOC (PA)	PAIR (PA)	PSATO (PA)	PSATW (PA)	PCO (PA)	PCW (PA)
A51 9	45	188081.	116.991	.0000E+00	.4554E+00	.5446E+00	7745.	0.	46076.	180336.	0.	-4054.
A1110	46	177481.	116.492	.0000E+00	.2006E+00	.7994E+00	25.	0.	45368.	177456.	-1.	-11780.
A2110	47	178323.	116.543	.0000E+00	.2386E+00	.7614E+00	578.	0.	45439.	177745.	-1.	-9507.
A3110	48	180357.	116.019	.0000E+00	.2945E+00	.7055E+00	5597.	0.	44703.	174760.	-1.	-7296.
A4110	49	183477.	110.545	.1320E+00	.3364E+00	.5316E+00	37568.	0.	37568.	145909.	0.	-6172.
A5110	50	181158.	107.037	.1319E+00	.8681E+00	.0000E+00	0.	709.	33501.	129572.	0.	-1028.
A1111	51	162094.	113.684	.0000E+00	.2310E+00	.7690E+00	166.	0.	41537.	161929.	-1.	-9920.
A2111	52	163092.	113.096	.0000E+00	.3025E+00	.6975E+00	4264.	4.	40769.	158825.	-1.	-7067.
A3111	53	171302.	108.487	.2441E+00	.3835E+00	.3724E+00	35137.	32.	35137.	136133.	0.	-5191.
A4111	54	170257.	92.643	.2538E+00	.7462E+00	.0000E+00	0.	18830.	20368.	77449.	0.	-1701.
A5111	55	179350.	83.433	.1685E-02	.9983E+00	.0000E+00	0.	1916.	14444.	54341.	0.	-84.
A1112	56	141296.	108.493	.0000E+00	.3181E+00	.6819E+00	4999.	135.	35144.	136162.	-1.	-6648.
A2112	57	148275.	102.947	.2075E+00	.5773E+00	.2152E+00	29218.	6598.	29218.	112459.	0.	-2833.
A3112	58	158109.	78.123	.3037E+00	.6841E+00	.1217E-01	11732.	102504.	11732.	43873.	0.	-2096.
A4112	59	166971.	67.271	.1239E-01	.9876E+00	.0000E+00	0.	22427.	7485.	27662.	0.	-260.
A5112	60	178286.	63.519	.0000E+00	.1000E+01	.0000E+00	0.	1240.	6356.	23398.	0.	0.
A1113	61	132070.	82.602	.1038E+00	.7116E+00	.1847E+00	13988.	65505.	13988.	52576.	0.	-1918.
A2113	62	142656.	66.674	.2731E-01	.9015E+00	.7119E-01	7295.	108418.	7295.	26942.	0.	-872.
A3113	63	154333.	54.313	.6978E-01	.9149E+00	.1535E-01	4175.	134928.	4175.	15230.	0.	-800.
A4113	64	165361.	50.251	.0000E+00	.1000E+01	.0000E+00	0.	16660.	3437.	12490.	0.	0.
A5113	65	177057.	48.101	.0000E+00	.1000E+01	.0000E+00	0.	1003.	3093.	11219.	0.	0.
A1114	66	129936.	49.148	.1172E-02	.8285E+00	.1703E+00	3257.	114856.	3257.	11823.	0.	-1282.
A2114	67	140772.	45.578	.0000E+00	.9667E+00	.3335E-01	2701.	128201.	2727.	9870.	0.	-460.
A3114	68	152341.	40.323	.7425E-04	.9807E+00	.1921E-01	2082.	142757.	2082.	7503.	0.	-337.
A4114	69	163829.	38.562	.0000E+00	.1000E+01	.0000E+00	0.	13384.	1897.	6828.	0.	0.
A5114	70	175553.	37.487	.0000E+00	.1000E+01	.0000E+00	0.	817.	1791.	6442.	0.	0.
A1115	71	128200.	34.612	.1759E-05	.8426E+00	.1574E+00	1533.	121166.	1533.	5502.	0.	-1213.
A2115	72	139086.	34.130	.0000E+00	.9695E+00	.3047E-01	1452.	132278.	1493.	5357.	0.	-438.
A3115	73	150686.	32.186	.0000E+00	.9785E+00	.2151E-01	1299.	144582.	1340.	4804.	0.	-360.
A4115	74	162049.	31.358	.0000E+00	.1000E+01	.0000E+00	0.	11062.	1280.	4583.	0.	0.
A5115	75	173764.	30.863	.0000E+00	.1000E+01	.0000E+00	0.	640.	1244.	4456.	0.	0.
A1116	76	126052.	28.373	.0000E+00	.8515E+00	.1485E+00	1013.	121178.	1080.	3861.	0.	-1166.
A2116	77	137030.	28.508	.0000E+00	.9697E+00	.3028E-01	1009.	132129.	1088.	3892.	0.	-437.
A3116	78	148657.	27.835	.0000E+00	.9777E+00	.2226E-01	960.	143955.	1047.	3742.	0.	-367.
A4116	79	160001.	27.460	.0000E+00	.1000E+01	.0000E+00	0.	9337.	1024.	3661.	0.	0.
A5116	80	171720.	27.228	.0000E+00	.1000E+01	.0000E+00	0.	487.	1011.	3612.	0.	0.
A1117	81	124360.	27.498	.0000E+00	.8963E+00	.1037E+00	941.	119750.	1027.	3669.	0.	-917.
A2117	82	135572.	27.666	.0000E+00	.9724E+00	.2761E-01	947.	130919.	1037.	3705.	0.	-415.
A3117	83	147245.	27.168	.0000E+00	.9780E+00	.2205E-01	909.	142737.	1007.	3599.	0.	-365.
A4117	84	158605.	26.856	.0000E+00	.1000E+01	.0000E+00	0.	8764.	989.	3534.	0.	0.
A5117	85	170333.	26.664	.0000E+00	.1000E+01	.0000E+00	0.	446.	978.	3494.	0.	0.

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Figure 27. (continued)

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*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.

                                                                                                KCYC =  127  -  ITER =    6  -  TIME =  .92000E+07
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ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
A11 1	1	.8123E-22	.6481E-23	.1426E+01	.0000E+00	.1310E-04	.1000E+01	.0000E+00	.0000E+00	.7693E+00	.3829E-03	.0000E+00
A21 1	2	.3464E-20	.2759E-21	.1428E+01	.0000E+00	.1311E-04	.1000E+01	.0000E+00	.0000E+00	.7506E+00	.5138E-03	.0000E+00
A31 1	3	.5567E-19	.4426E-20	.1431E+01	.0000E+00	.1311E-04	.1000E+01	.0000E+00	.0000E+00	.7420E+00	.5834E-03	.0000E+00
A41 1	4	.0000E+00	.0000E+00	.1434E+01	.0000E+00	.1311E-04	.1000E+01	.0000E+00	.0000E+00	.7333E+00	.6614E-03	.0000E+00
A51 1	5	.0000E+00	.0000E+00	.1439E+01	.0000E+00	.1312E-04	.1000E+01	.0000E+00	.0000E+00	.6887E+00	.1184E-02	.0000E+00
A11 2	6	.3706E-17	.3003E-18	.1403E+01	.0000E+00	.1308E-04	.1000E+01	.0000E+00	.0000E+00	.7841E+00	.2974E-03	.0000E+00
A21 2	7	.3436E-19	.2781E-20	.1405E+01	.0000E+00	.1308E-04	.1000E+01	.0000E+00	.0000E+00	.7517E+00	.5053E-03	.0000E+00
A31 2	8	.1975E-18	.1595E-19	.1408E+01	.0000E+00	.1309E-04	.1000E+01	.0000E+00	.0000E+00	.7333E+00	.6611E-03	.0000E+00
A41 2	9	.0000E+00	.0000E+00	.1411E+01	.0000E+00	.1309E-04	.1000E+01	.0000E+00	.0000E+00	.7132E+00	.8688E-03	.0000E+00
A51 2	10	.4226E-22	.3397E-23	.1415E+01	.0000E+00	.1309E-04	.1000E+01	.0000E+00	.0000E+00	.6253E+00	.2393E-02	.0000E+00
A11 3	11	.3309E-17	.2754E-18	.1365E+01	.0000E+00	.1305E-04	.1000E+01	.0000E+00	.0000E+00	.7863E+00	.2862E-03	.0000E+00
A21 3	12	.4424E-19	.3677E-20	.1367E+01	.0000E+00	.1305E-04	.1000E+01	.0000E+00	.0000E+00	.7478E+00	.5361E-03	.0000E+00
A31 3	13	.0000E+00	.0000E+00	.1369E+01	.0000E+00	.1305E-04	.1000E+01	.0000E+00	.0000E+00	.7227E+00	.7656E-03	.0000E+00
A41 3	14	.0000E+00	.0000E+00	.1372E+01	.0000E+00	.1305E-04	.1000E+01	.0000E+00	.0000E+00	.6929E+00	.1125E-02	.0000E+00
A51 3	15	.0000E+00	.0000E+00	.1375E+01	.0000E+00	.1306E-04	.1000E+01	.0000E+00	.0000E+00	.5720E+00	.4003E-02	.0000E+00
A11 4	16	.2433E-17	.2084E-18	.1325E+01	.0000E+00	.1301E-04	.1000E+01	.0000E+00	.0000E+00	.7821E+00	.3083E-03	.0000E+00
A21 4	17	.0000E+00	.0000E+00	.1327E+01	.0000E+00	.1301E-04	.1000E+01	.0000E+00	.0000E+00	.7405E+00	.5963E-03	.0000E+00
A31 4	18	.1327E-15	.1134E-16	.1329E+01	.0000E+00	.1301E-04	.1000E+01	.0000E+00	.0000E+00	.7113E+00	.8912E-03	.0000E+00
A41 4	19	.0000E+00	.0000E+00	.1331E+01	.0000E+00	.1301E-04	.1000E+01	.0000E+00	.0000E+00	.6741E+00	.1408E-02	.0000E+00
A51 4	20	.0000E+00	.0000E+00	.1334E+01	.0000E+00	.1302E-04	.1000E+01	.0000E+00	.0000E+00	.5274E+00	.5923E-02	.0000E+00
A11 5	21	.1820E-17	.1609E-18	.1283E+01	.0000E+00	.1297E-04	.1000E+01	.0000E+00	.0000E+00	.7752E+00	.3468E-03	.0000E+00
A21 5	22	.0000E+00	.0000E+00	.1284E+01	.0000E+00	.1297E-04	.1000E+01	.0000E+00	.0000E+00	.7312E+00	.6810E-03	.0000E+00
A31 5	23	.1083E-15	.9546E-17	.1286E+01	.0000E+00	.1297E-04	.1000E+01	.0000E+00	.0000E+00	.6987E+00	.1047E-02	.0000E+00
A41 5	24	.0000E+00	.0000E+00	.1289E+01	.0000E+00	.1297E-04	.1000E+01	.0000E+00	.0000E+00	.6554E+00	.1740E-02	.0000E+00
A51 5	25	.0000E+00	.0000E+00	.1292E+01	.0000E+00	.1298E-04	.1000E+01	.0000E+00	.0000E+00	.4872E+00	.8243E-02	.0000E+00
A11 6	26	.1514E-17	.1385E-18	.1238E+01	.0000E+00	.1292E-04	.1000E+01	.0000E+00	.0000E+00	.7662E+00	.4027E-03	.0000E+00
A21 6	27	.0000E+00	.0000E+00	.1239E+01	.0000E+00	.1292E-04	.1000E+01	.0000E+00	.0000E+00	.7194E+00	.8002E-03	.0000E+00
A31 6	28	.8853E-16	.8079E-17	.1241E+01	.0000E+00	.1292E-04	.1000E+01	.0000E+00	.0000E+00	.6836E+00	.1259E-02	.0000E+00
A41 6	29	.0000E+00	.0000E+00	.1244E+01	.0000E+00	.1293E-04	.1000E+01	.0000E+00	.0000E+00	.6345E+00	.2175E-02	.0000E+00
A51 6	30	.0000E+00	.0000E+00	.1247E+01	.0000E+00	.1293E-04	.1000E+01	.0000E+00	.0000E+00	.4481E+00	.1119E-01	.0000E+00
A11 7	31	.1354E-17	.1289E-18	.1189E+01	.0000E+00	.1287E-04	.1000E+01	.0000E+00	.0000E+00	.7542E+00	.4865E-03	.0000E+00
A21 7	32	.6699E-19	.6365E-20	.1191E+01	.0000E+00	.1287E-04	.1000E+01	.0000E+00	.0000E+00	.7038E+00	.9817E-03	.0000E+00
A31 7	33	.7245E-16	.6870E-17	.1193E+01	.0000E+00	.1287E-04	.1000E+01	.0000E+00	.0000E+00	.6635E+00	.1589E-02	.0000E+00
A41 7	34	.0000E+00	.0000E+00	.1196E+01	.0000E+00	.1288E-04	.1000E+01	.0000E+00	.0000E+00	.6076E+00	.2858E-02	.0000E+00
A51 7	35	.0000E+00	.0000E+00	.1198E+01	.0000E+00	.1288E-04	.1000E+01	.0000E+00	.0000E+00	.4057E+00	.1537E-01	.0000E+00
A11 8	36	.5553E-17	.5521E-18	.1136E+01	.0000E+00	.1281E-04	.1000E+01	.0000E+00	.0000E+00	.7376E+00	.6222E-03	.0000E+00
A21 8	37	.5552E-16	.5511E-17	.1138E+01	.0000E+00	.1281E-04	.1000E+01	.0000E+00	.0000E+00	.6813E+00	.1293E-02	.0000E+00
A31 8	38	.2284E-15	.2260E-16	.1142E+01	.0000E+00	.1282E-04	.1000E+01	.0000E+00	.0000E+00	.6328E+00	.2216E-02	.0000E+00
A41 8	39	.0000E+00	.0000E+00	.1144E+01	.0000E+00	.1282E-04	.1000E+01	.0000E+00	.0000E+00	.5642E+00	.4297E-02	.0000E+00
A51 8	40	.1362E-13	.1347E-14	.1143E+01	.0000E+00	.1282E-04	.1000E+01	.0000E+00	.0000E+00	.3481E+00	.2326E-01	.0000E+00
A11 9	41	.1209E-05	.1266E-06	.1078E+01	.0000E+00	.1274E-04	.1000E+01	.0000E+00	.0000E+00	.7134E+00	.8668E-03	.0000E+00
A21 9	42	.2164E-04	.2259E-05	.1081E+01	.0000E+00	.1275E-04	.1000E+01	.0000E+00	.0000E+00	.6458E+00	.1930E-02	.0000E+00
A31 9	43	.1715E-03	.1782E-04	.1086E+01	.0000E+00	.1275E-04	.1000E+01	.0000E+00	.0000E+00	.5761E+00	.3855E-02	.0000E+00
A41 9	44	.1240E-02	.1286E-03	.1088E+01	.0000E+00	.1275E-04	.1000E+01	.0000E+00	.0000E+00	.4759E+00	.9016E-02	.0000E+00
A51 9	45	.2535E+00	.2785E-01	.1279E+01	.0000E+00	.1235E-04	.1000E+01	.0000E+00	.0000E+00	.2096E+00	.6156E-01	.0000E+00
A1110	46	.8350E-03	.9311E-04	.1011E+01	.0000E+00	.1266E-04	.1000E+01	.0000E+00	.0000E+00	.6748E+00	.1396E-02	.0000E+00
A2110	47	.1895E-01	.2110E-02	.1030E+01	.0000E+00	.1264E-04	.1000E+01	.0000E+00	.0000E+00	.5819E+00	.3654E-02	.0000E+00
A3110	48	.1836E+00	.2077E-01	.1179E+01	.0000E+00	.1239E-04	.1000E+01	.0000E+00	.0000E+00	.4614E+00	.1010E-01	.0000E+00
A4110	49	.1250E+01	.1666E+00	.2091E+01	.7998E+03	.1099E-04	.3185E-03	.0000E+00	.0000E+00	.1947E+00	.1812E-01	.4618E-02
A5110	50	.0000E+00	.1670E+00	.0000E+00	.8031E+03	.1000E+01	.3277E-03	.0000E+00	.0000E+00	.0000E+00	.6216E+00	.1933E-02
A1111	51	.5464E-02	.6622E-03	.9323E+00	.0000E+00	.1255E-04	.1000E+01	.0000E+00	.0000E+00	.5997E+00	.3087E-02	.0000E+00
A2111	52	.1410E+00	.1739E-01	.1051E+01	.0000E+00	.1233E-04	.1000E+01	.0000E+00	.0000E+00	.4457E+00	.1139E-01	.0000E+00

Figure 27. (continued)

ELEM	INDEX	CVOCGAS (KG/M**3)	CVOCAQ. (KG/M**3)	DGAS (KG/M**3)	DNAPL (KG/M**3)	VISGAS (KG/M*S)	VISNAPL (KG/M*S)	DIFFO (M**2/S)	DIFFW (M**2/S)	KRGAS	KRAQ.	KRNAPL
A3111	53	.1176E+01	.1668E+00	.1964E+01	.8018E+03	.1093E-04	.3238E-03	.0000E+00	.0000E+00	.6528E-01	.3126E-01	.2135E-01
A4111	54	.0000E+00	.1689E+00	.0000E+00	.8165E+03	.1000E+01	.3700E-03	.0000E+00	.0000E+00	.0000E+00	.3701E+00	.1378E-01
A5111	55	.0000E+00	.1699E+00	.0000E+00	.8249E+03	.1000E+01	.4018E-03	.0000E+00	.0000E+00	.0000E+00	.9944E+00	.0000E+00
A1112	56	.1673E+00	.2374E-01	.9566E+00	.0000E+00	.1210E-04	.1000E+01	.0000E+00	.0000E+00	.4160E+00	.1424E-01	.0000E+00
A2112	57	.9920E+00	.1676E+00	.1712E+01	.8070E+03	.1116E-04	.3389E-03	.0000E+00	.0000E+00	.1184E-01	.1492E+00	.1500E-01
A3112	58	.4265E+00	.1705E+00	.1716E+01	.8297E+03	.1657E-04	.4221E-03	.0000E+00	.0000E+00	.1395E-07	.2734E+00	.2461E-01
A4112	59	.0000E+00	.1717E+00	.0000E+00	.8394E+03	.1000E+01	.4690E-03	.0000E+00	.0000E+00	.0000E+00	.9593E+00	.0000E+00
A5112	60	.0000E+00	.1238E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1113	61	.5021E+00	.1700E+00	.1467E+01	.8257E+03	.1505E-04	.4049E-03	.0000E+00	.0000E+00	.7311E-02	.3137E+00	.2793E-02
A2113	62	.2741E+00	.1717E+00	.1558E+01	.8399E+03	.1736E-04	.4719E-03	.0000E+00	.0000E+00	.3143E-03	.7063E+00	.0000E+00
A3113	63	.1628E+00	.1728E+00	.1699E+01	.8507E+03	.1815E-04	.5365E-03	.0000E+00	.0000E+00	.2100E-06	.7422E+00	.2822E-03
A4113	64	.0000E+00	.1642E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5113	65	.0000E+00	.7655E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1114	66	.1290E+00	.1733E+00	.1450E+01	.8552E+03	.1805E-04	.5676E-03	.0000E+00	.0000E+00	.5652E-02	.5304E+00	.0000E+00
A2114	67	.1082E+00	.1719E+00	.1576E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.1746E-04	.8929E+00	.0000E+00
A3114	68	.8480E-01	.1739E+00	.1723E+01	.8628E+03	.1829E-04	.6275E-03	.0000E+00	.0000E+00	.1072E-05	.9371E+00	.0000E+00
A4114	69	.0000E+00	.1568E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5114	70	.0000E+00	.4338E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1115	71	.6360E-01	.1743E+00	.1474E+01	.8676E+03	.1815E-04	.6715E-03	.0000E+00	.0000E+00	.4396E-02	.5617E+00	.0000E+00
A2115	72	.6032E-01	.1695E+00	.1598E+01	.0000E+00	.1821E-04	.1000E+01	.0000E+00	.0000E+00	.1177E-04	.9018E+00	.0000E+00
A3115	73	.5434E-01	.1691E+00	.1738E+01	.0000E+00	.1823E-04	.1000E+01	.0000E+00	.0000E+00	.2093E-05	.9300E+00	.0000E+00
A4115	74	.0000E+00	.1480E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5115	75	.0000E+00	.2390E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1116	76	.4292E-01	.1639E+00	.1470E+01	.0000E+00	.1810E-04	.1000E+01	.0000E+00	.0000E+00	.3647E-02	.5821E+00	.0000E+00
A2116	77	.4272E-01	.1620E+00	.1596E+01	.0000E+00	.1814E-04	.1000E+01	.0000E+00	.0000E+00	.1144E-04	.9024E+00	.0000E+00
A3116	78	.4073E-01	.1602E+00	.1734E+01	.0000E+00	.1816E-04	.1000E+01	.0000E+00	.0000E+00	.2525E-05	.9276E+00	.0000E+00
A4116	79	.0000E+00	.1343E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5116	80	.0000E+00	.1353E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A1117	81	.3996E-01	.1601E+00	.1454E+01	.0000E+00	.1809E-04	.1000E+01	.0000E+00	.0000E+00	.1130E-02	.6925E+00	.0000E+00
A2117	82	.4022E-01	.1596E+00	.1583E+01	.0000E+00	.1813E-04	.1000E+01	.0000E+00	.0000E+00	.7490E-05	.9108E+00	.0000E+00
A3117	83	.3863E-01	.1576E+00	.1720E+01	.0000E+00	.1815E-04	.1000E+01	.0000E+00	.0000E+00	.2399E-05	.9283E+00	.0000E+00
A4117	84	.0000E+00	.1305E+00	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00
A5117	85	.0000E+00	.1136E-01	.0000E+00	.0000E+00	.1000E+01	.1000E+01	.0000E+00	.0000E+00	.0000E+00	.1000E+01	.0000E+00

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Figure 27. (continued)

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*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.

                                                                                                  KCYC =  127  -  ITER =    6  -  TIME =  .92000E+07

ELEMENT SOURCE INDEX  GENERATION RATE    ENTHALPY      FF(GAS)      FF(AQ. )     FF(NAPL)     FF(VOCG)    FF(VOCAQ)      P(WB)
                       (KG/S) OR (W)      (J/KG)                                                                            (PA)

 A11 1   INJ 1    1        .14800E-03    .26760E+07
 A21 1   INJ 2    2        .14800E-03    .26760E+07
 A31 1   INJ 3    3        .14800E-03    .26760E+07
 A41 1   INJ 4    4        .14800E-03    .26760E+07
 A51 1   INJ 5    5        .14800E-03    .26760E+07
 A5117   PRO 5    6       -.65318E-03    .11188E+06   .00000E+00   .10000E+01   .00000E+00   .00000E+00   .11394E-04   .17005E+06
 A4117   PRO 4    7       -.66064E-03    .11267E+06   .00000E+00   .10000E+01   .00000E+00   .00000E+00   .13094E-03   .15832E+06
 A3117   PRO 3    8       -.62433E-03    .11396E+06   .47457E-06   .10000E+01   .00000E+00   .10659E-07   .15816E-03   .14659E+06
 A2117   PRO 2    9       -.62772E-03    .11603E+06   .14696E-05   .10000E+01   .00000E+00   .37338E-07   .16021E-03   .13487E+06
 A1117   PRO 1   10       -.39877E-03    .11534E+06   .52846E-03   .99947E+00   .00000E+00   .14526E-04   .16058E-03   .12320E+06

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```

Figure 28. Separate phase xylene saturation distribution after 106.5 days of steam injection.

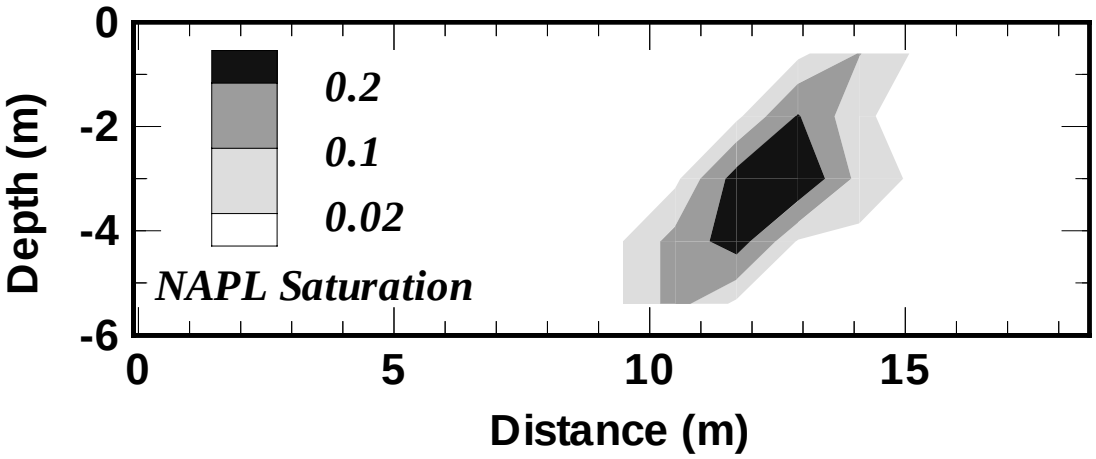

Figure 29. Printed output at the end of part 4 of problem 4.

```
*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.

         OUTPUT DATA AFTER ( 224,  2)-2-TIME STEPS                                                    THE TIME IS   .17130E+03 DAYS

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Figure 29. (continued)

ELEM	INDEX	P (PA)	T (DEG.C)	SO	SW	SG	PVOC (PA)	PAIR (PA)	PSATO (PA)	PSATW (PA)	PCO (PA)	PCW (PA)
A51 9	45	214797.	122.502	.0000E+00	.2792E+00	.7208E+00	0.	0.	54522.	214797.	-1.	-7767.
A1110	46	205072.	121.024	.0000E+00	.1499E+00	.8501E+00	0.	0.	52145.	205072.	-2.	-16723.
A2110	47	205159.	121.038	.0000E+00	.1637E+00	.8363E+00	0.	0.	52166.	205159.	-2.	-15032.
A3110	48	205299.	121.059	.0000E+00	.1752E+00	.8248E+00	0.	0.	52201.	205299.	-1.	-13842.
A4110	49	205476.	121.087	.0000E+00	.1942E+00	.8058E+00	0.	0.	52244.	205476.	-1.	-12210.
A5110	50	205711.	121.123	.0000E+00	.2861E+00	.7139E+00	0.	0.	52301.	205711.	-1.	-7539.
A1111	51	195494.	119.512	.0000E+00	.1519E+00	.8481E+00	0.	0.	49799.	195494.	-2.	-16485.
A2111	52	195586.	119.527	.0000E+00	.1661E+00	.8339E+00	0.	0.	49822.	195586.	-2.	-14786.
A3111	53	195733.	119.551	.0000E+00	.1780E+00	.8220E+00	0.	0.	49858.	195733.	-1.	-13595.
A4111	54	195913.	119.580	.0000E+00	.1975E+00	.8025E+00	0.	0.	49902.	195913.	-1.	-11973.
A5111	55	196147.	119.617	.0000E+00	.2926E+00	.7074E+00	0.	0.	49959.	196147.	-1.	-7335.
A1112	56	185336.	117.841	.0000E+00	.1542E+00	.8458E+00	0.	0.	47306.	185336.	-2.	-16206.
A2112	57	185441.	117.859	.0000E+00	.1690E+00	.8310E+00	0.	0.	47332.	185441.	-2.	-14500.
A3112	58	185606.	117.886	.0000E+00	.1814E+00	.8186E+00	0.	0.	47372.	185606.	-1.	-13308.
A4112	59	185800.	117.919	.0000E+00	.2014E+00	.7986E+00	0.	0.	47420.	185800.	-1.	-11708.
A5112	60	186039.	117.959	.0000E+00	.2990E+00	.7010E+00	0.	0.	47479.	186039.	-1.	-7146.
A1113	61	174496.	115.973	.0000E+00	.1571E+00	.8429E+00	0.	0.	44638.	174496.	-2.	-15875.
A2113	62	174623.	115.995	.0000E+00	.1725E+00	.8275E+00	0.	0.	44670.	174623.	-1.	-14165.
A3113	63	174822.	116.030	.0000E+00	.1855E+00	.8145E+00	0.	0.	44719.	174822.	-1.	-12971.
A4113	64	175048.	116.070	.0000E+00	.2061E+00	.7939E+00	0.	0.	44774.	175048.	-1.	-11402.
A5113	65	175305.	116.116	.0000E+00	.3053E+00	.6947E+00	0.	0.	44838.	175305.	-1.	-6967.
A1114	66	162826.	113.852	.0000E+00	.1606E+00	.8394E+00	0.	0.	41759.	162826.	-2.	-15481.
A2114	67	162994.	113.884	.0000E+00	.1768E+00	.8232E+00	0.	0.	41800.	162994.	-1.	-13771.
A3114	68	163254.	113.932	.0000E+00	.1905E+00	.8095E+00	0.	0.	41864.	163254.	-1.	-12574.
A4114	69	163541.	113.986	.0000E+00	.2119E+00	.7881E+00	0.	0.	41935.	163541.	-1.	-11036.
A5114	70	163843.	114.042	.0000E+00	.3123E+00	.6877E+00	0.	0.	42010.	163843.	-1.	-6779.
A1115	71	150118.	111.396	.0000E+00	.1652E+00	.8348E+00	0.	0.	38613.	150118.	-2.	-14984.
A2115	72	150358.	111.444	.0000E+00	.1826E+00	.8174E+00	0.	0.	38672.	150358.	-1.	-13267.
A3115	73	150722.	111.517	.0000E+00	.1974E+00	.8026E+00	0.	0.	38762.	150722.	-1.	-12061.
A4115	74	151120.	111.596	.0000E+00	.2202E+00	.7798E+00	0.	0.	38861.	151120.	-1.	-10545.
A5115	75	151507.	111.673	.0000E+00	.3218E+00	.6782E+00	0.	0.	38957.	151507.	-1.	-6533.
A1116	76	136043.	108.468	.0000E+00	.1760E+00	.8240E+00	0.	0.	35115.	136043.	-1.	-13907.
A2116	77	136413.	108.548	.0000E+00	.1977E+00	.8023E+00	0.	0.	35207.	136413.	-1.	-12070.
A3116	78	136936.	108.661	.0000E+00	.2162E+00	.7838E+00	0.	0.	35337.	136936.	-1.	-10811.
A4116	79	137515.	108.785	.0000E+00	.2429E+00	.7571E+00	0.	0.	35481.	137515.	-1.	-9358.
A5116	80	138008.	108.891	.0000E+00	.3466E+00	.6534E+00	0.	0.	35604.	138008.	-1.	-5941.
A1117	81	125895.	106.197	.0000E+00	.2255E+00	.7745E+00	0.	0.	32583.	125895.	-1.	-10286.
A2117	82	126333.	106.298	.0000E+00	.2804E+00	.7196E+00	0.	0.	32693.	126333.	-1.	-7829.
A3117	83	126899.	106.429	.0000E+00	.3313E+00	.6687E+00	0.	0.	32834.	126899.	-1.	-6318.
A4117	84	127605.	106.590	.0000E+00	.3888E+00	.6112E+00	0.	0.	33010.	127605.	-1.	-5103.
A5117	85	128017.	106.684	.0000E+00	.4758E+00	.5242E+00	0.	0.	33113.	128017.	0.	-3833.

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Figure 29. (continued)

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*rfs4*...2-D X-Z field scale problem: steam sweep of Xylene plume.

                                                                                                  KCYC =  224  -  ITER =    2  -  TIME =  .14800E+08

ELEMENT SOURCE INDEX  GENERATION RATE    ENTHALPY      FF(GAS)      FF(AQ. )     FF(NAPL)     FF(VOCG)    FF(VOCAQ)      P(WB)
                       (KG/S) OR (W)      (J/KG)                                                                            (PA)

 A11 1   INJ 1    1        .14800E-03    .26760E+07
 A21 1   INJ 2    2        .14800E-03    .26760E+07
 A31 1   INJ 3    3        .14800E-03    .26760E+07
 A41 1   INJ 4    4        .14800E-03    .26760E+07
 A51 1   INJ 5    5        .14800E-03    .26760E+07
 A5117   PRO 5    6       -.41377E-03    .98739E+06   .24122E+00   .75878E+00   .00000E+00   .18516E-07   .68236E-11   .12359E+06
 A4117   PRO 4    7       -.15037E-03    .26862E+07   .10000E+01   .00000E+00   .00000E+00   .36201E-08   .00000E+00   .12343E+06
 A3117   PRO 3    8       -.16849E-03    .26859E+07   .10000E+01   .00000E+00   .00000E+00   .22040E-09   .00000E+00   .12332E+06
 A2117   PRO 2    9       -.18076E-03    .26857E+07   .10000E+01   .00000E+00   .00000E+00   .10698E-10   .00000E+00   .12325E+06
 A1117   PRO 1   10       -.19718E-03    .26856E+07   .10000E+01   .00000E+00   .00000E+00   .10895E-11   .00000E+00   .12320E+06

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12.5 Problem No. 5 - TCE Spill in 3-D Heterogeneous Field Scale System

The purpose of this example is to demonstrate the ability of T2VOC to handle large three-dimensional problems, with a complexity approaching "real-life" field applications. The present problem involves contaminant migration and three-phase flow in a very heterogeneous soil. Both saturated and unsaturated zones are included, and there is regional groundwater flow in the saturated zone. Following a series of pre-processing steps to generate a heterogeneous permeability distribution, the simulation consists of four parts, namely, (i) development of gravity-capillary equilibrium, (ii) TCE injection, (iii) redistribution of contaminant, and (iv) remediation by vapor extraction.

Pre-processing involves generation of a three-dimensional X-Y-Z mesh with 15x15x20 = 4500 grid blocks using the MESHMAKER facility. A spatially correlated permeability field is then generated using simulated annealing techniques (Press et al., 1986; Datta Gupta, personal communication). A log-normal distribution is assumed with a (geometric) mean permeability of 10^{-10} m^2 and a standard deviation of one order of magnitude. The permeability field is annealed to a spherical variogram with a correlation length of 10 m in the horizontal direction. No vertical correlation is considered. The generated permeabilities are then ordered into 9 groups, covering values from 10^{-8} to 10^{-12} m^2. Each group has its own rock type. Porosities are in the range from 27 % to 43%, and are assumed to vary proportional to the logarithm of permeability. The strength of capillary pressures in the different domains was scaled according to Leverett (1941). The permeability distribution is shown in Figure 30.

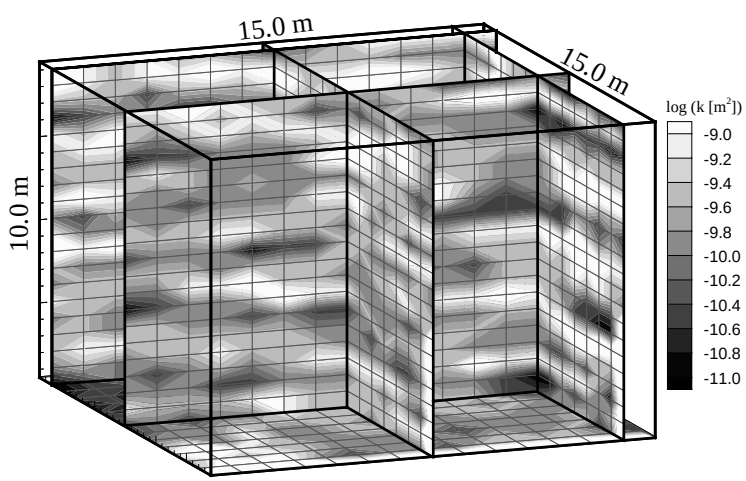


Figure 30. Permeability distribution for 3D sample problem

With up to 3 equations per grid block, a total of 13,500 coupled linear equations need to be solved, requiring the use of the preconditioned conjugate gradient package T2CG1 (Moridis and Pruess, 1995). The generalized minimum residual solver DSLUGM performed very well for this problem.

The first part of the simulation aims at developing a gravity-capillary equilibrium in a saturated-unsaturated flow system that exhibits a pressure gradient in the saturated zone. An atmospheric boundary condition is applied at the surface. A single-phase liquid Dirichlet boundary condition with hydrostatic pressure distribution is specified at the lower part of two opposite faces of the model. Depth to the water table is fixed at -6.0 m at the back face, and at -6.5 m at the front face. With a separation distance of 14 m between the two water table boundaries, the head gradient is 0.5/14 = .0357. The left and right vertical faces as well as the bottom are modeled as no flow boundaries.

Figure 31 shows the T2VOC input file used for generating a gravity-capillary equilibrium, prior to introducing the TCE contaminant. It does not include MESH or INCON data, which are provided separately on disk files MESH and INCON (not shown). The option NK = NEQ = 2 is used for a more efficient calculation in the absence of VOC. Nearly steady-state conditions are reached after 300 time steps.

Figure 31. T2VOC input file for part 1 of problem 5

```
Sample problem No. 5, part 1: Gravity-capillary equilibrium
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SOL 1    2  2600.e00       .27   1.0E-08   1.0E-08   1.0E-09      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84      300.      330.
SOL 2    2  2600.e00       .29   3.0e-09   3.0e-09   3.0e-09      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84      200.      220.
SOL 3    2  2600.e00       .31   1.0E-09   1.0E-09   1.0E-09      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84      100.      110.
SOL 4    2  2600.e00       .33   3.0E-10   3.0E-10   3.0E-10      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84       50.       55.
SOL 5    2  2600.e00       .35   1.0E-10   1.0E-10   1.0E-10      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84       30.       33.
SOL 6    2  2600.e00       .37   3.0E-11   3.0E-11   3.0E-11      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84       20.       22.
```

Figure 31 (continued)

```
SOL 7    2  2600.e00       .39   1.0E-11   1.0E-11   1.0E-11      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84       10.       11.
SOL 8    2  2600.e00       .41   3.0E-12   3.0E-12   3.0E-12      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84        5.       5.5
SOL 9    2  2600.e00       .43   1.0E-12   1.0E-12   1.0E-12      2.51      920.
     1.e-9
    6           .150       .05       .05        3.
    8          0.000      1.84        3.       3.3
 BACK    2  2600.e00       .35   1.0E-08   1.0E-08   1.0E-08      2.51   100000.
     1.e-9
    6           .150       .05       .05        3.
    9
FRONT    2  2600.e00       .35   1.0E-08   1.0E-08   1.0E-08      2.51   100000.
     1.e-9
    6           .150       .05       .05        3.
    9
ATMOS    2  2600.e00       .35   1.0e-08   1.6e-08   1.6e-08      2.51      920.

    6           .150       .05       .05        3.
    9

CHEMP----1----*--TCE data----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    30.170     .2287-2.229E-04 8.244E-08
     1462.     293.0   8.0E-06     273.0      1.60
        0.        0.      0.59    293.15     256.0
1.50954E-4        0.        0.        0.
        0.        0.
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2    3    6
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1-MOP: 123456789*123456789*1234----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2 350     99910000010002000040000 4000
                         -1.                          9.81
      1.e1
     1.e-5
                1.e5                0.25                 20.
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ATMOS
                1.e5                0.01                 20.

ENDCY
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       00.
NX      15       1.0
NY      15       1.0
NZ      20       0.5


ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

In the next part of the simulation, a total of 1000 kg of trichloroethylene (TCE) is injected at a rate of 2.5×10^{-3} kg/s. The file SAVE from the previous simulation is provided as the INCON file, and MOP(19) = 1 is specified to convert NK = 2 input data to NK = 3 formats. Contaminant distribution at the end of the 400,000 second injection period is shown in Figures 32a-c. TCE is present as a free NAPL phase, dissolved in the aqueous phase, and as VOC vapor in the gas phase.

Part 3 of the simulation allows for free redistribution of TCE over a 1 week period under the combined action of gravitational, capillary and pressure forces. No TCE is injected. However, there is a minor amount lost from the system by evaporation to the atmosphere, and by outflow of TCE dissolved in the aqueous phase through the front face of the model. The NAPL saturation as well as aqueous and gaseous TCE concentrations are shown in Figures 33a-c. Dissolved TCE is seen to migrate away from the spill point and downgradient by convection. TCE vapors sink by negative buoyancy and then spread on top of the water table.

In the final part of the simulation, soil gas is extracted from five wells at a constant rate of 5×10^{-2} kg/s. As shown in Figures 34a-c, the TCE vapor in the gaseous phase is quickly replaced by clean air from the surface. Higher TCE vapor concentrations, however, are still observed near the extraction wells, indicating that TCE in the NAPL phase is evaporating. The dissolved TCE content remains relatively high downstream from the spill, and will not be extracted even after long remediation times.

Figure 32. (a) NAPL saturation after injection

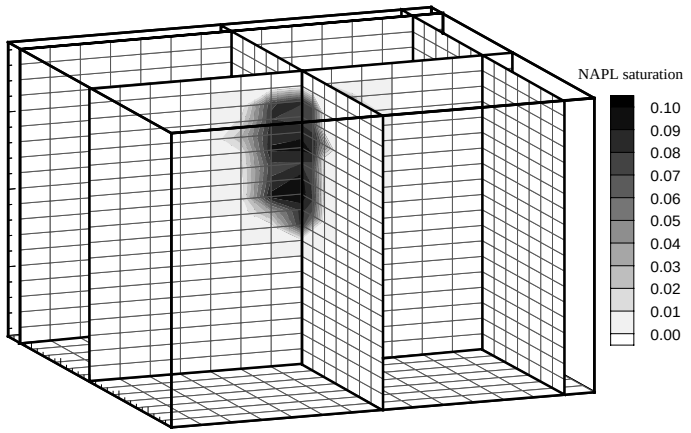


Figure 32. (b) Dissolved VOC content after injection

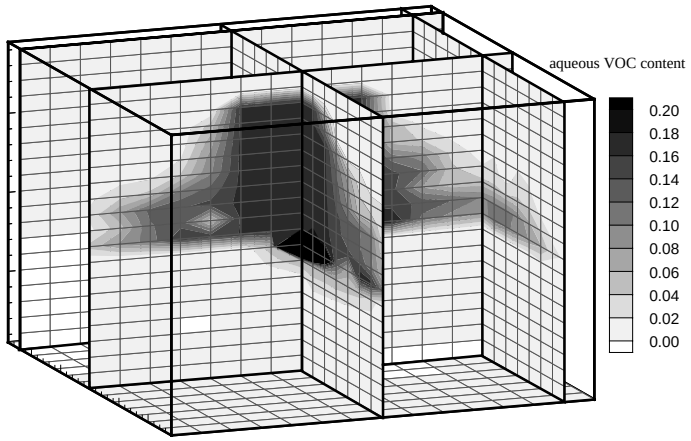


Figure 32. (c) Vaporized VOC content after injection

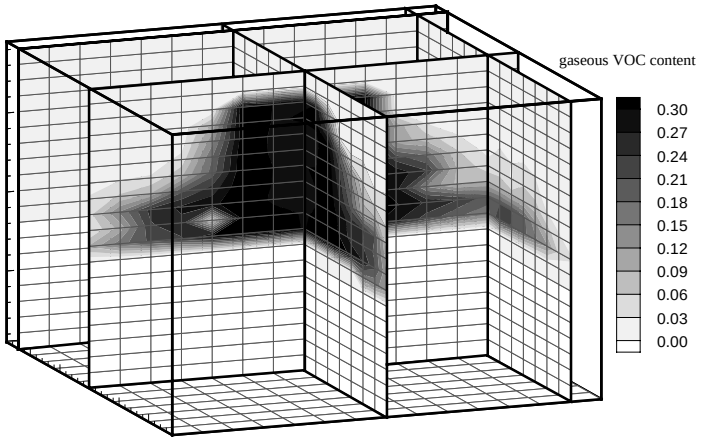


Figure 33. (a) NAPL saturation after redistribution

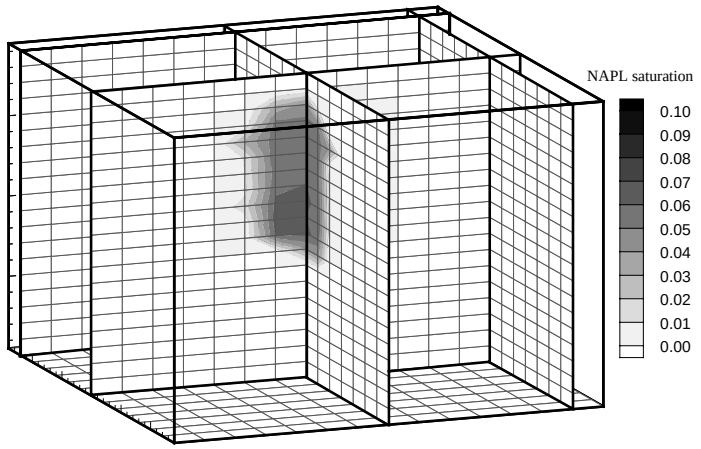


Figure 33. (b) Dissolved VOC content after redistribution

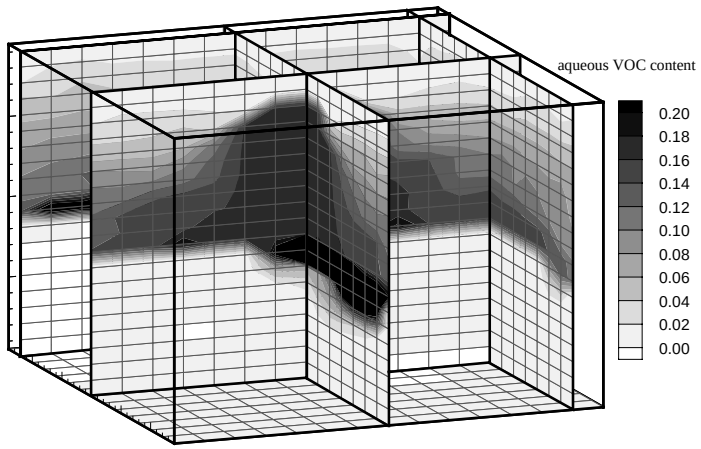


Figure 33. (c) Vaporized VOC content after redistribution

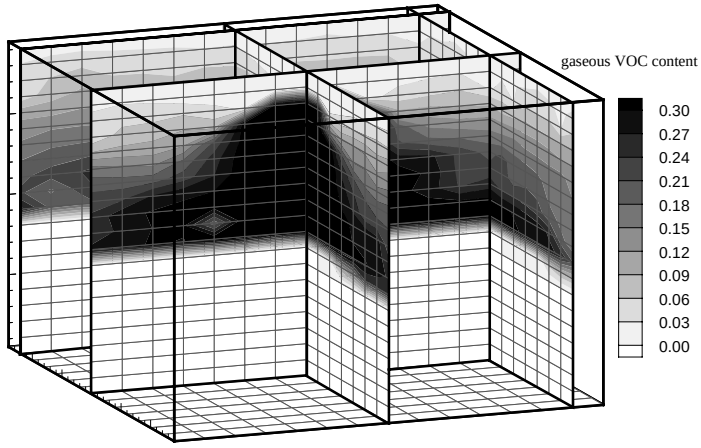


Figure 34. (a) NAPL saturation after 2 days of soil vapor extraction.

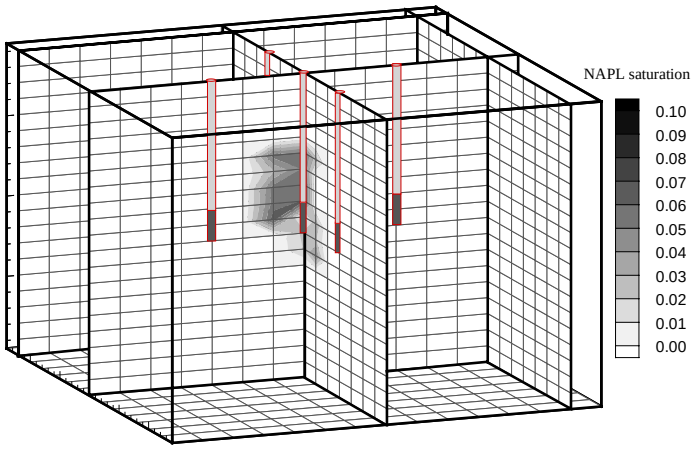


Figure 34. (b) Dissolved VOC content after 2 days of soil vapor extraction.

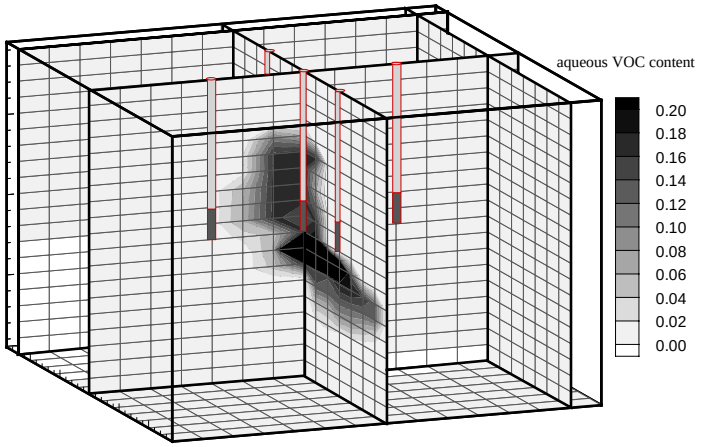
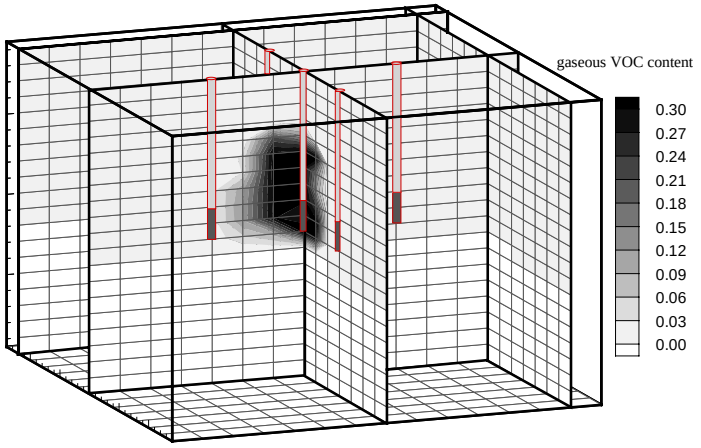


Figure 34. (c) Vaporized VOC content after 2 days of soil vapor extraction.



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NOTATION

A	area, m^2.
A_{nm}	area between grid blocks n and m, m^2.
b	Klinkenberg factor for gas permeability, Pa
C_{pn}	NAPL heat capacity, J/kg K .
C^0_{pn}	ideal gas molar heat capacity for chemical, J/mole K .
C_R	soil grain heat capacity, J/kg ˚C.
C^c_s	concentration of chemical in the solid phase, kg/m^3.
C_{va}	air heat capacity at constant volume, J/kg K .
C^κ_β	concentration of mass component κ in phase β, kg/m^3.
D^{ij}_g	binary i-j mixture molecular gas diffusivity, m^2/s.
D^{ijR}_g	reference binary i-j mixture molecular gas diffusivity, m^2/s.
D^κ_g	molecular diffusivity of mass component κ in a multicomponent gas, m^2/s.
F^0_p	polarity correction factor for pure vapor viscosity calculation.
$\mathbf{F}^\kappa$	total flux of component κ; for $\kappa \neq h$: kg/m^2s; for $\kappa = h$: J/m^2s.
$\mathbf{F}_\beta$	total mass flux in the β phase, kg/m^2s.
$\mathbf{F}^\kappa_\beta$	flux of component κ in the β phase; for $\kappa \neq h$: kg/m^2s; for $\kappa = h$: J/m^2s.
F_{nm}	flux from grid block m into n; for mass: kg/m^2s, for heat: 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^c_{vap}	chemical latent heat of vaporization, J/kg.
$h^c_{vap,b}$	chemical latent heat of vaporization at the normal boiling point, J/kg.
h_β	specific enthalpy of phase β, J/kg.

h_g^κ specific enthalpy of mass component κ in the gas phase, J/kg.

H_{gn}^κ Henry's constant for gas-NAPL partitioning of mass component κ, Pa.

H_{gw}^c Henry's constant for dissolution of VOC vapors in aqueous phase, Pa.

$\mathbf{J}_g^\kappa$ diffusive mass flux of component κ in the gas phase, kg/m^{2}s.

K overall porous medium thermal conductivity, W/m K.

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 β 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 grid block index; also used to denote exponent in the calculation of relative permeabilities and capillary pressures.

M^κ amount of component κ per unit porous medium volume (accumulation term); for $\kappa \neq h$ (mass components): kg/m^3; for $\kappa = h$ (heat component): J/m^3.

M_n^κ accumulation term for component κ in grid block n.

M_{wt}^{aw} mixture molecular weight of air and water vapor, g/mole.

M_{wt}^κ molecular weight of mass component κ, g/mole.

n grid block index; also used to denote exponent in the calculation of relative permeabilities and capillary pressures.

n inward unit normal vector.

P pressure, Pa.

PI well productivity index, m^3.

P_{cgn} gas-NAPL capillary pressure, Pa.

P_{cgw} gas-water capillary pressure, Pa.

P_{cnw} NAPL-water capillary pressure, Pa.

P_{crit} critical pressure, Pa

P_R reference pressure, Pa.

P_{sat}^c saturated NAPL vapor pressure, Pa.

P_{sat}^w saturated water vapor pressure, Pa.

P_{wb} wellbore pressure, Pa.

P_β pressure in the β phase, Pa.

PI productivity index, m^3.

q^{κ} rate of generation of component κ per unit volume; for $\kappa \neq h$: kg/m^3 s; for $\kappa = h$: J/m^3 s .

q_{β} mass rate of generation of phase β in a source element, kg/s.

$\hat{q}^{\kappa}$ rate of generation of component κ in a source element; for $\kappa \neq h$: kg/s; for $\kappa = h$: J/s.

r_w well radius, m.

r_e grid block radius, m.

R universal gas constant, mJ/moleK.

R_g^c chemical gas phase retardation coefficient.

$R_n^{\kappa, k+1}$ residual of conservation equation for component κ in grid block n at time step k+1.

s well skin factor, dimensionless.

S_{β} saturation of phase β.

$S_{\beta r}$ residual saturation of phase β.

S_m empirical constant used in the calculation of capillary pressures.

S_{β}^* scaled saturation of phase β, defined in Appendix C.

$\bar{S}_{\beta}$ scaled saturation of phase β, defined in Appendix C.

T temperature, $^{\circ}$C.

T_b chemical normal boiling temperature, K.

T_{br} chemical reduced boiling temperature.

T_b^w water normal boiling temperature, K.

T_{crit} critical temperature, K.

T_r reduced temperature.

T_{rR} reduced reference temperature.

T_R reference temperature, K

T_{ref} temperature at which enthalpy is zero, K.

u specific internal energy, J/kg.

u_{β} specific internal energy of phase β, J/kg.

u_g^{κ} specific internal energy of mass component κ in the gas phase, J/kg.

V_{crit}^{κ} critical molar volume for mass component κ, cm^3/mole.

V_n volume of region n of porous medium, m^3.

x generic notation for primary thermodynamic variable.

X_{β}^{κ} mass fraction of mass component κ in phase β.

Z_{crit} critical compressibility.

α_{gn} constant used in the calculation of the gas-NAPL capillary pressure, 1/m.

α_{gw} constant used in the calculation of the gas-water capillary pressure, 1/m.

α_{nw} constant used in the calculation of the NAPL-water capillary pressure, 1/m.

β phase index, β = g: gas phase; w: aqueous (water) phase; n: NAPL.

Δt time step, s.

ε convergence tolerance, dimensionless.

$\bar{\chi}_g^c$ saturated mole fraction of chemical vapor in the gas phase.

$\bar{\chi}_w^c$ chemical solubility in water (mole fraction).

χ_β^κ mole fraction of mass component κ in the β phase.

η_d dipole moment, debyes.

η_{dr} reduced dipole moment.

Γ_n surface area of region n, m^2.

κ component index, κ = w: water, a: air; c: chemical; h: heat.

λ overall porous media thermal conductivity, W/mK; also used to denote decay constant for biodegradation, s^{-1}.

λ_n NAPL thermal conductivity, W/mK.

λ_R rock grain thermal conductivity, W/mK.

λ_w liquid water thermal conductivity, W/mK.

μ_{nR} reference NAPL viscosity, kg/ms.

μ_g^{aw} air-water vapor viscosity, kg/ms.

μ_g^c chemical vapor viscosity, kg/ms.

μ_β β phase viscosity, kg/m s.

ρ density, kg/m^3.

ρ_{nsR} reference NAPL density, kg/m^3.

ρ_β density of the β phase, kg/m^3.

ρ_b soil dry bulk density, kg/m^3.

θ_{ij} exponent for variation of D_g^{ij} with temperature.

τ_g gas phase tortuosity.

ϕ porosity.

$\Phi_{aw,c}$ interaction parameter.

$\Phi_{c,aw}$ interaction parameter.

ω Pitzer's acentric factor.

Ω diffusion collision integral.

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APPENDIX A. SPACE AND TIME DISCRETIZATION†

The continuum equations (1) are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). Introducing appropriate volume averages, we have

$$\int_{V_n} M \, dV = V_n M_n \tag{A.1}$$

where M is a volume-normalized extensive quantity, and M_n is the average value of M over V_n. Surface integrals are approximated as a discrete sum of averages over surface segments A_{nm}:

$$\int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n} \, d\Gamma = \sum_m A_{nm} F_{nm} \tag{A.2}$$

Here F_{nm} is the average value of the (inward) normal component of **F** over the surface segment A_{nm} between volume elements V_n and V_m. The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Fig. 35.

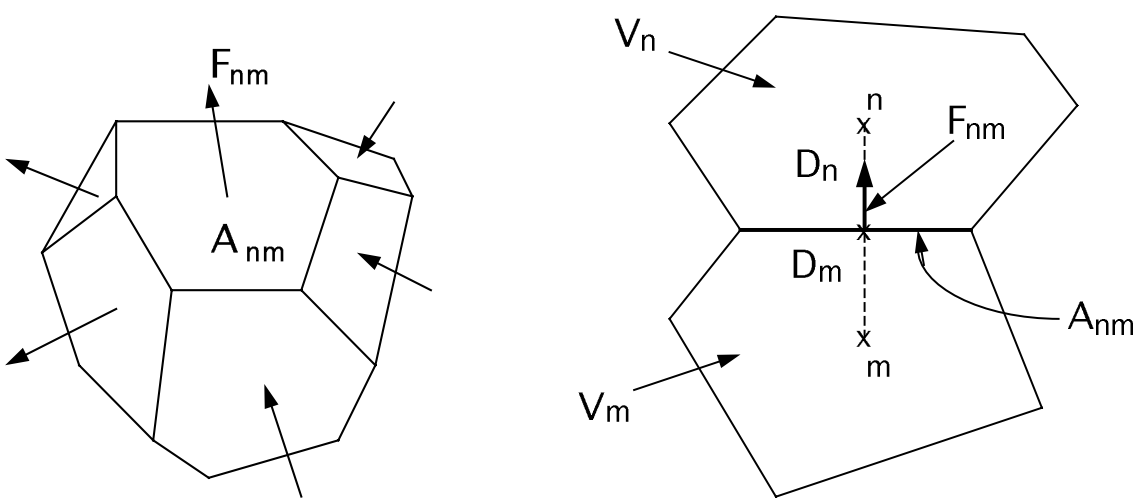

Figure 35. Space discretization and geometry data in the integral finite difference method.

† Adapted from TOUGH2 report, Pruess (1991).

The discretized flux is expressed in terms of averages over parameters for elements V_n and V_m. For the basic Darcy flux term, Eq. (11), we have

$$F_{\beta,nm} \quad = \quad - k_{nm} \left[\frac{k_{r\beta}\, \rho_\beta}{\mu_\beta} \right]_{nm} \left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}\, g_{nm} \right] \qquad (A.3)$$

where the subscripts (nm) denote a suitable averaging at the interface between grid blocks n and m (interpolation, harmonic weighting, upstream weighting). D_{nm} is the distance between the nodal points n and m, and g_{nm} is the component of gravitational acceleration in the direction from m to n.

The discretized form of the binary diffusive flux in the gas phase is

$$\mathbf{J}^{\kappa}_{g,nm} \quad = \quad - \left(\phi\, S_g\, \tau_g \right)_{nm} \left(D^{\kappa}_{g} \right)_{nm} \rho_{g,nm} \frac{X^{\kappa}_{g,n} - X^{\kappa}_{g,m}}{D_{nm}} \qquad (A.4).$$

For the group (ϕ S τ) harmonic weighting is used at the interface, while D and ρ are linearly interpolated between grid blocks n and m.

Substituting Eqs. (A.l) and (A.2) into the governing Eq. (1), a set of first-order ordinary differential equations in time is obtained.

$$\frac{d M^{\kappa}_{n}}{d t} \quad = \quad \frac{1}{V_n} \sum_{m} A_{nm}\, F^{\kappa}_{nm} + q^{\kappa}_{n} \qquad (A.5)$$

Time is discretized as a first order finite difference, and the flux and sink and source terms on the right hand side of Eq. (A.5) are evaluated at the new time level, $t^{k+l} = t^k + \Delta t$, to obtain the numerical stability needed for an efficient calculation of multiphase flow. This treatment of flux terms is known as "fully implicit," because the fluxes are expressed in terms of the unknown thermodynamic parameters at time level t^{k+l}, so that these unknowns are only implicitly defined in the resulting equations; see e.g. Peaceman (1977). However, our test calculations showed that fully implicit time differencing for the biodegradation term, Eq. (23), leads to rather severe time truncation errors. Accordingly, a centered-in-time differencing formulation was implemented for this term, as follows.

$$q^{c,k+1} = -\frac{\lambda}{2}\left(M_w^{c,k+1} + M_w^{c,k}\right) \tag{A.6}$$

The time discretization results in the following set of coupled non-linear, algebraic equations

$$\begin{aligned} R_n^{\kappa,k+1} &= M_n^{\kappa,k+1} - M_n^{\kappa,k} - \frac{\Delta t}{V_n}\left\{\sum_m A_{nm}\, F_{nm}^{\kappa,k+1} + V_n\, q_n^{\kappa,k+1}\right\} \\ &= 0 \end{aligned} \tag{A.7}$$

where we have introduced residuals $R_n^{\kappa,k+1}$. For each volume element (grid block) V_n there are NEQ equations (κ = 1, 2, ... NEQ; usually, NEQ = NK + 1), so that for a flow system with NEL grid blocks (A.7) represents a total of NEL • NEQ coupled non-linear equations. The unknowns are the NEL • NEQ independent primary variables $\{x_i;\ i = 1, ..., \text{NEL} \bullet \text{NEQ}\}$ which completely define the state of the flow system at time level t^{k+l}. These equations are solved by Newton/Raphson iteration, which is implemented as follows. We introduce an iteration index p and expand the residuals $R_n^{\kappa,k+1}$ in Eq. (A.7) at iteration step p + 1 in a Taylor series in terms of those at index p.

$$\begin{aligned} R_n^{\kappa,k+1}\left(x_{i,p+1}\right) &= R_n^{\kappa,k+1}\left(x_{i,p}\right) + \sum_i \left.\frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\right|_p \left(x_{i,p+1} - x_{i,p}\right) \\ &\quad + \ldots = 0 \end{aligned} \tag{A.8}$$

Retaining only terms up to first order, we obtain a set of NEL • NEQ linear equations for the increments $(x_{i,p+1} - x_{i,p})$:

$$-\sum_i \left.\frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\right|_p \left(x_{i,p+1} - x_{i,p}\right) = R_n^{\kappa,k+1}\left(x_{i,p}\right) \tag{A.9}$$

All terms $\partial R_n/\partial x_i$ in the Jacobian matrix are evaluated by numerical differentiation. Eq. (A.9) is solved by sparse direct matrix methods (Duff, 1977) or iteratively by means of preconditioned conjugate gradients (Moridis and Pruess, 1995). Iteration is continued until the residuals $R_n^{\kappa,k+1}$ are reduced below a preset convergence tolerance.

$$\left| \frac{R_{n,p+1}^{\kappa,k+1}}{M_{n,p+1}^{\kappa,k+1}} \right| \leq \varepsilon_1 \qquad \text{(A.10)}$$

The default (relative) convergence criterion is $\varepsilon_1 = 10^{-5}$ (T2VOC input parameter RE1). When the accumulation terms are smaller than ε_2 (T2VOC input parameter RE2, default $\varepsilon_2 = 1$), an absolute convergence criterion is imposed, $|R_n^{\kappa,k+1}| \leq \varepsilon_1 \cdot \varepsilon_2$. Convergence is usually attained in 3 - 4 iterations. If convergence cannot be achieved within a certain number of iterations (default 8), the time step size Δt is reduced and a new iteration process is started.

It is appropriate to add some comments about our space discretization technique. The entire geometric information of the space discretization in Eq. (A.7) is provided in the form of a list of grid block volumes V_n, interface areas A_{nm}, nodal distances D_{nm} and components g_{nm} of gravitational acceleration along nodal lines. There is no reference whatsoever to a global system of coordinates, or to the dimensionality of a particular flow problem. The discretized equations are in fact valid for arbitrary irregular discretizations in one, two or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution, however, because the accuracy of solutions depends upon the accuracy with which the various interface parameters in equations such as (A.3, A.4) can be expressed in terms of average conditions in grid blocks. A general requirement is that there exists approximate thermodynamic equilibrium in (almost) all grid blocks at (almost) all times (Pruess and Narasimhan, 1985). For systems of regular grid blocks referenced to global coordinates (such as r - z, x - y - z), Eq. (A.7) is identical to a conventional finite difference formulation (e.g. Peaceman, 1977).

APPENDIX B. DESCRIPTION OF FLOW IN FRACTURED MEDIA[#]

Figure 36 illustrates the classical double-porosity concept for modeling flow in fractured-porous media as developed by Warren and Root (1963). Matrix blocks of low permeability are embedded in a network of inter-connected fractures. Global flow in the reservoir occurs only through the fracture system, which is described as an effective porous continuum. Rock matrix and fractures may exchange fluid (or heat) locally by means of "interporosity flow," which is driven by the difference in pressures (or temperatures) between matrix and fractures. Warren and Root approximated the interporosity flow as being "quasi-steady," with rate of matrix-fracture interflow proportional to the difference in (local) average pressures.

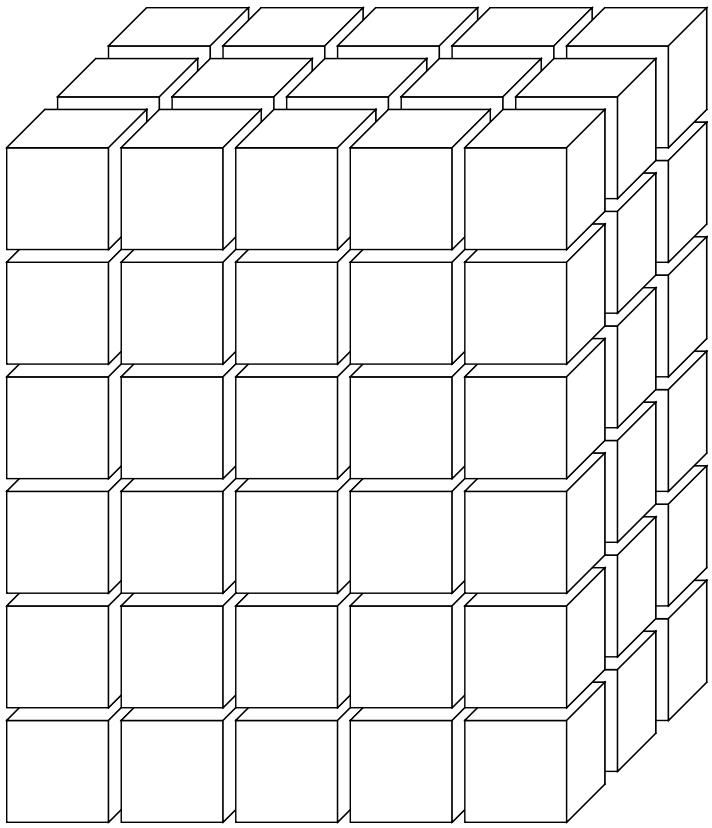

Figure 36. Idealized "double porosity" model of a fractured porous medium.

The quasisteady approximation is applicable to isothermal single phase flow of fluids with small compressibility, where pressure diffusivities are large, so that pressure

[#] Adapted from TOUGH2 report, Pruess (1991).

changes in the fractures penetrate quickly all the way into the matrix blocks. However, for multiphase flows, or coupled fluid and heat flows, the transient periods for interporosity flow can be very long (tens of years). In order to accurately describe such flows it is necessary to resolve the driving pressure, temperature and mass fraction gradients at the matrix/fracture interface. In the method of "multiple interacting continua" (MINC; Pruess and Narasimhan, 1982, 1985), resolution of these gradients is achieved by appropriate subgridding of the matrix blocks, as shown in Fig. 37. The MINC concept is based on the notion that changes in fluid pressures, temperatures, phase compositions, etc. due to the presence of sinks and sources (production and injection wells) will propagate rapidly through the fracture system, while invading the tight matrix blocks only slowly. Therefore, changes in matrix conditions will (locally) be controlled by the distance from the fractures. Fluid and heat flow from the fractures into the matrix blocks, or from the matrix blocks into the fractures, can then be modeled by means of one-dimensional strings of nested grid blocks, as shown in Fig. 37.

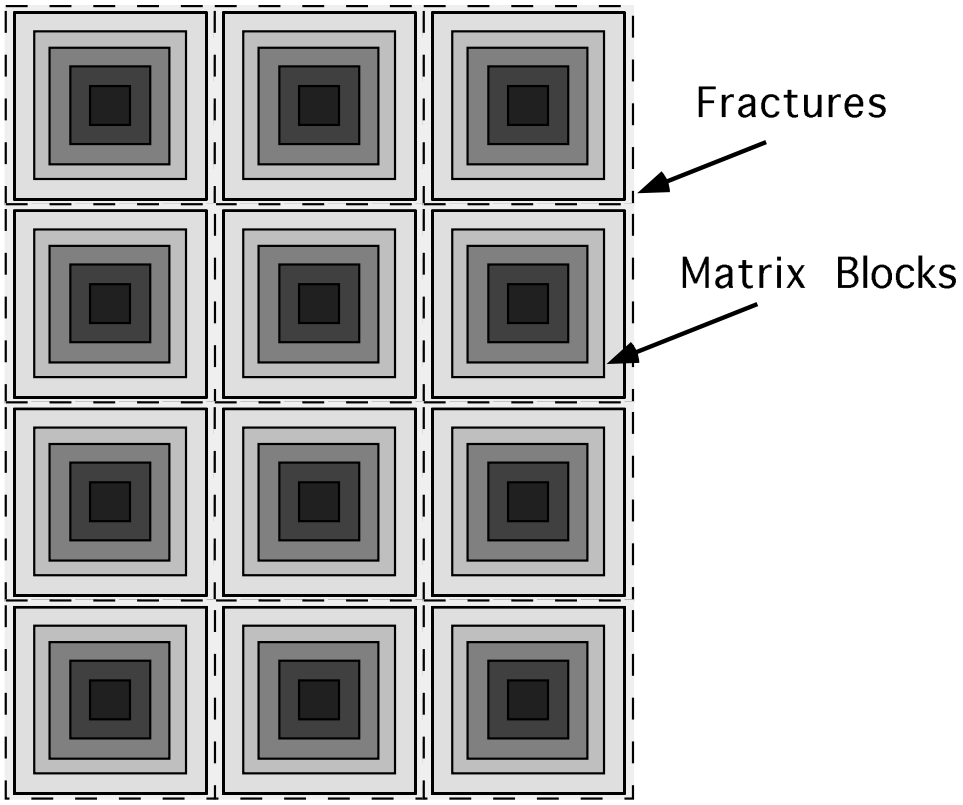

Figure 37. Subgridding in the method of "multiple interacting continua" (MINC).

In general it is not necessary to explicitly consider subgrids in all of the matrix blocks separately. Within a certain reservoir subdomain (corresponding to a finite difference grid block), all fractures will be lumped into continuum # 1, all matrix material within a certain distance from the fractures will be lumped into continuum # 2, matrix material at larger distance becomes continuum # 3, and so on. Quantitatively, the subgridding is specified by means of a set of volume fractions VOL(j), j = 1, ..., J, into which the "primary" porous medium grid blocks are partitioned. The MINC-process in the MESHMAKER module of T2VOC operates on the element and connection data of a porous medium mesh to calculate, for given data on volume fractions, the volumes, interface areas, and nodal distances for a "secondary" fractured medium mesh. The information on fracturing (spacing, number of sets, shape of matrix blocks) required for this is provided by a "proximity function" PROX(x) which expresses, for a given reservoir domain V_o, the total fraction of matrix material within a distance x from the fractures. If only two continua are specified (one for fractures, one for matrix), the MINC approach reduces to the conventional double-porosity method. Full details are given in a separate report (Pruess, 1983b).

The MINC-method as implemented in the MESHMAKER module can also describe global matrix-matrix flow. Figure 38 shows the most general approach, often referred to as "dual permeability," in which global flow occurs in both fracture and matrix continua. It is also possible to permit matrix-matrix flow only in the vertical direction. For any given fractured reservoir flow problem, selection of the most appropriate gridding scheme must be based on a careful consideration of the physical and geometric conditions of flow. The MINC approach is not applicable to systems in which fracturing is so sparse that the fractures cannot be approximated as a continuum.

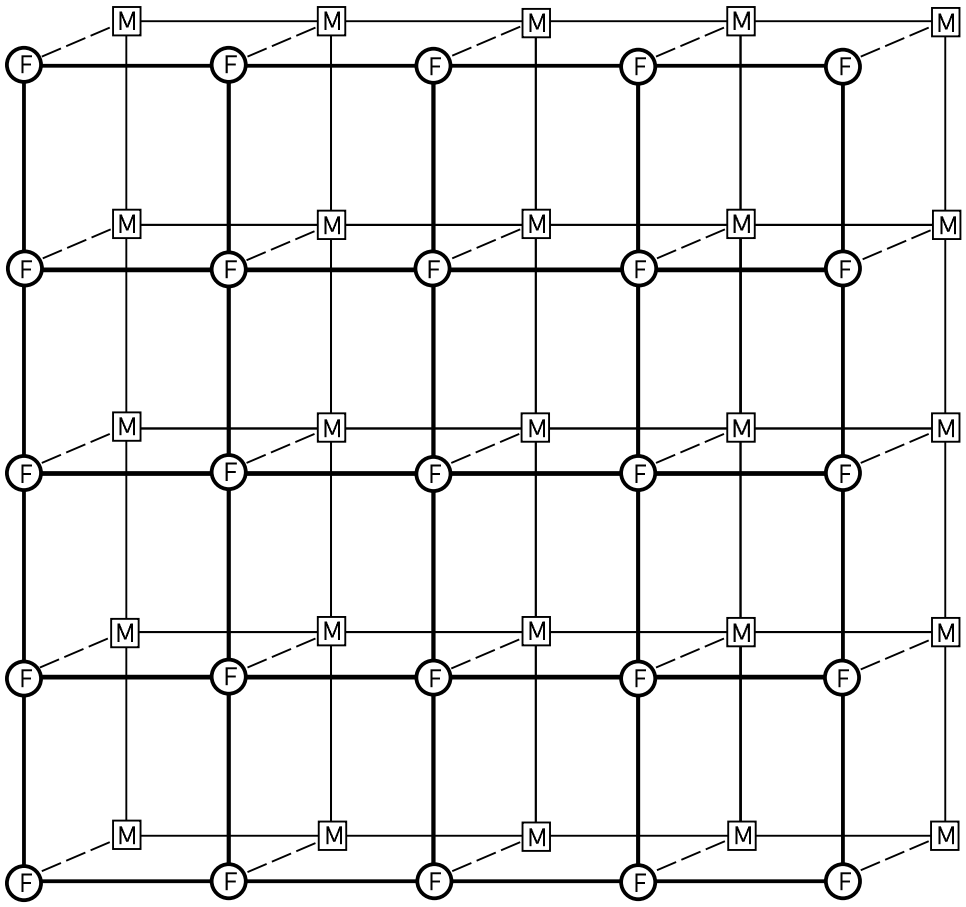

Figure 38. Flow connections in the “dual permeability” model. Global flow occurs between both fracture (F) and matrix (M) grid blocks. In addition there is F-M interporosity flow.

APPENDIX C: RELATIVE PERMEABILITY FUNCTIONS

Several relative permeability functions are provided in T2VOC for problems involving three-phase water-air-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. S_g, S_w, and $S_n = 1 - S_g - S_w$ are the saturations of gas, aqueous, and NAPL phases, respectively.

IRP = 5 "All perfectly mobile"

$k_{rw} = 1$
$k_{rg} = 1$
$k_{rn} = 1$
no parameters.

IRP = 6 Modified version of Stone's first three phase method (Stone, 1970).

$$k_{rg} = \left[\frac{S_g - S_{gr}}{1 - S_{wr}}\right]^n$$

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

$$k_{rn} = \left[\frac{1 - S_g - S_w - S_{nr}}{1 - S_g - S_{wr} - S_{nr}}\right]\left[\frac{1 - S_{wr} - S_{nr}}{1 - S_w - S_{nr}}\right]\left[\frac{\left(1 - S_g - S_{wr} - S_{nr}\right)\left(1 - S_w\right)}{\left(1 - S_{wr}\right)}\right]^n$$

When $S_n = 1 - S_g - S_w$ is near irreducible NAPL saturation, $S_{nr} \le S_n \le S_{nr} + .005$, NAPL relative permeability is taken to be

$$k'_{rn} = k_{rn} \cdot \frac{S_n - S_{nr}}{.005}$$

Parameters are S_{wr} = RP(1), S_{nr} = RP(2), S_{gr} = RP(3), n = RP(4).

IRP = 9 three phase functions of Parker et al. (1987).

$m = 1 - 1/n$

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

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

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

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

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

$$k_{rn} = \sqrt{\bar{S}_l - \bar{S}_w}\left\{\left[1 - (\bar{S}_w)^{1/m}\right]^m - \left[1 - (\bar{S}_l)^{1/m}\right]^m\right\}^2$$

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.

The relative permeability functions listed above should be considered preliminary. T2VOC users are encouraged to follow ongoing research into three-phase relative permeabilities and capillary pressures, and to add suitable formulations into subroutine RELP.

This routine has the following structure:

```
      SUBROUTINE RELP(SL,SG,REPL,REPG,REPO,NMAT)
C
      ...
      ...
      ...
C
      GOTO (10,11,12, ...),IRP(NMAT)
C
      ...
      ...
C
   10 CONTINUE                                  | (IRP = 1) |
      ...                                       |           |
      ...                                       |           |
      ...                                       |           |
      REPL= ...                                 |           |
      REPG= ...                                 |           |
      REPO= ...                                 |           |
      RETURN                                    |           |
C
   11 CONTINUE                                  | (IRP = 2) |
      ...                                       |           |
      ...                                       |           |
      ...                                       |           |
      REPL= ...                                 |           |
      REPG= ...                                 |           |
      REPO= ...                                 |           |
      RETURN                                    |           |
C
    12 CONTINUE
      ...
      ...
      ...
C
      END
```

Here, `SL` and `SG` are the aqueous and gas phase saturations (note that for NAPL saturation we have `SO = 1 - SL - SG`). `REPL`, `REPG`, and `REPO` are, respectively, the relative permeabilities of aqueous, gas, and NAPL phases. `NMAT` is the index of the domain to which the grid block belongs, and `IRP(NMAT)` is the index number of the relative permeability function in that domain.

To code an additional relative permeability function, the user needs to insert a code segment analogous to those shown above, beginning with a statement number that would also appear in the `GOTO` statement. The relative permeabilities `REPL`, `REPG`, and `REPO` need to be defined as functions of the phase saturations. The `RP( )` data read in the input file can be utilized as parameters in these functional relationships.

APPENDIX D: CAPILLARY PRESSURE FUNCTIONS

A three phase capillary pressure function has been included in T2VOC. 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 capillary pressure between the NAPL and the aqueous phases, P_{cnw} , is given by $P_{cnw} = P_{cgw} - P_{cgn}$.

ICP = 8 three phase capillary functions from Parker et al. (1987).

$m = 1 - 1/n$

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

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

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

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

where S_m = CP(1); n = CP(2); α_{gn} = CP(3); α_{nw} = CP(4).

These functions have been modified so that the capillary pressures remain finite at low aqueous saturations. This is done by calculating the slope of the capillary pressure functions at $\bar{S}_w$ and $\bar{S}_l$ = 0.1. If $\bar{S}_w$ or $\bar{S}_l$ 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.

ICP = 9 zero capillary pressures

$P_{cgn} = 0$

$P_{cgw} = 0$

no parameters.

Additional capillary pressure functions can be programmed into subroutine PCAP in a fashion completely analogous to that for relative permeabilities (see Appendix C).

APPENDIX E: VISCOSITY OF A PURE GAS

The chemical vapor viscosity μ_g^c is computed from the corresponding states method (Reid et al., 1987)

$$\mu_g^c = \frac{0.606\, T_r\, F_p^o}{0.176\left[\dfrac{T_{crit}}{\left(M_{wt}^c\right)^3\left(P_{crit}\right)^4}\right]^{1/6}} \qquad \text{(E.1)}$$

where $T_r = T/T_{crit}$ is the reduced temperature, and μ_g^c has units of centipoise. The value of the polarity correction factor, F_p^o, depends on the value of the reduced dipole moment of the chemical

$$\eta_{dr} = 52.46\,\frac{\left(\eta_d\right)^2 P_{crit}}{\left(T_{crit}\right)^2} \qquad \text{(E.2)}$$

in which η_d is the dipole moment of the chemical. The polarity correction factor is then

$$\left.\begin{aligned} F_p^o &= 1 && \} \quad 0 \le \eta_{dr} < 0.22 \\ F_p^o &= 1 + 30.55\left(0.292 - Z_{crit}\right)^{1.72} && \} \quad 0.22 \le \eta_{dr} < 0.75 \\ F_p^o &= 1 + 30.55\left(0.292 - Z_{crit}\right)^{1.72}\left[0.96 + 0.1\left(T_r - 0.7\right)\right] && \} \quad 0.75 \le \eta_{dr} \end{aligned}\right. \qquad \text{(E.3)}$$

where Z_{crit} is the critical compressibility factor.

APPENDIX F: CALCULATION OF BINARY GAS DIFFUSIVITIES

If direct experimental data for the binary gas diffusivity of two chemicals are not available, the diffusivity may be estimated by using the Wilke and Lee empirical correlation (Reid et al., 1987). Considering a binary system containing water and chemical vapor

$$D_g^{cw} = \frac{100\left(3.03-\left[0.98/\sqrt{M_{wt}^{cw}}\right]\right)T^{3/2}}{P\,\sigma_{cw}^2\,\Omega_d\,\sqrt{M_{wt}^{cw}}} \qquad \text{(F.1)}$$

where

$$M_{wt}^{cw} = \frac{2}{1/M_{wt}^{c} + 1/M_{wt}^{w}} \qquad \text{(F.2)}$$

The scale parameter, σ_{cw}, may be computed as

$$\sigma_{cw} = 0.388\left(\left[V_{crit}^{c}\right]^{0.3493} + \left[V_{crit}^{w}\right]^{0.3493}\right) \qquad \text{(F.3)}$$

while the diffusion collision integral, may be accurately calculated from

$$\Omega_d = \frac{A}{\left(T^*\right)^B} + \frac{C}{\exp\left(D\,T^*\right)} + \frac{E}{\exp\left(F\,T^*\right)} + \frac{G}{\exp\left(H\,T^*\right)} \qquad \text{(F.4)}$$

where

$$T^* = \frac{T}{\left[\left(1.15\,T_b\right)\left(1.15\,T_{bw}\right)\right]^{1/2}} \qquad \text{(F.5)}$$

In (F.3), V_{crit}^{c} is the critical molar volume of the chemical and V_{crit}^{w} is the critical molar volume of water. In (F.5), T_b is the boiling temperature of the chemical, T_{bw} is the boiling point of water, A=1.06036, B=0.15610, C=0.19300, D=0.47635, E=1.03587, F=1.52996, G=1.76474, and H=3.89411. The diffusivity calculated by this method is usually within ten percent of the experimental value (Reid et al., 1987).