CONF-831174--77

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

Presented at the Materials Research Society 1983
Annual Meeting, Boston, MA, November 14-17, 1983

LBL--16946

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UNSATURATED FLOW TO STUDY WASTE CANISTER
HEATING EFFECTS

DE84 006491

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December 1983

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TOUGH - A Numerical Model for Nonisothermal Unsaturated Flow
to Study Waste Canister Heating Effects

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ABSTRACT

The physical processes modeled and the mathematical and numerical methods employed in a simulator for non-isothermal flow of water, vapor, and air in permeable media are briefly summarized. The simulator has been applied to study thermohydrological conditions in the near vicinity of high-level nuclear waste packages emplaced in unsaturated rocks. The studies reported here specifically address the question whether or not the waste canister environment will dry up in the thermal phase.

INTRODUCTION

The unsaturated tuffs at the Nevada Test Site are currently being investigated as a host medium for disposal of high-level nuclear waste. Emplacement of heat-generating waste packages is expected to give rise to considerable forced convection of the gaseous phase, due to thermal expansion and accompanying pressurization. The conventional methods for modeling saturated-unsaturated flow treat the gaseous phase as a spectator [1] or consider diffusive-type vapor transport only [2] and are therefore not applicable to a strongly heat-driven problem.

We have developed a numerical model called "TOUGH" (transport of unsaturated groundwater and heat), which treats the two-phase flow of air and water in gaseous and liquid phases together with heat flow in a fully coupled way. The formulation used in TOUGH is analogous to the multiphase, multicomponent treatment customarily employed in simulators for geothermal reservoirs [3] or for steam-flooding of hydrocarbon reservoirs [4]. The governing equations account for gaseous diffusion and Darcy flow with relative permeability and capillary pressure effects. Vaporization and condensation with latent heat effects along with conductive and convective heat flow are included in the energy balance. Water, air, and rock are assumed to be in local thermodynamic equilibrium at all times. The flow domain can include liquid, gaseous, and two-phase regions. A logic for "switching" thermodynamic state variables provides for accurate and efficient calculation of phase transitions and component appearances/disappearances. The thermophysical properties of water substance are accurately represented by the steam table equations as given by the International Formulation Committee [5]. Air is approximated as an ideal gas, and additivity of partial pressures is assumed for air-vapor mixtures.

TOUGH employs an integral finite-difference method which is applicable for one-, two-, or three-dimensional flow problems in porous or fractured porous media [6]. The governing mass- and energy-balance equations are strongly nonlinear and are solved completely simultaneously, using Newton-Raphson iteration.

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CODE VERIFICATION

To our knowledge, no analytical or numerical solutions for strongly heat driven flow of water, steam, and air in porous or fractured media are presently available. We have verified the TOUGH simulator by comparison with existing solutions for isothermal saturated/unsaturated flow, and with non-isothermal single-component (no air) solutions available for geothermal reservoir problems. As an example, Figure 1 shows a comparison of a TOUGH-calculation for a one-dimensional infiltration problem with the semi-analytical similarity solution of Philip [7]. The agreement is excellent. Equally good agreement has been obtained with available solutions for geothermal problems with propagating boiling fronts [8].

CANISTER PROBLEM

We have applied the TOUGH simulator to an initial exploration of thermohydrological conditions in the near vicinity of high-level waste packages, which are emplaced in partially saturated rock. In keeping with the exploratory nature of the study, we have kept unessential detail to a minimum. We model a symmetry element of height $H = 3.353$ m (corresponding to one waste package) of an infinite linear string of canisters, embedded in an infinite uniform and homogeneous porous medium without gravity. Heat driven and capillary driven flows are assumed to be much stronger than gravity driven flow components. Sensitivity studies have been performed to obtain insight into the heat-driven multi-component, multiphase processes near buried canisters. A special focus of our studies is the question whether "dry" or "wet" conditions will prevail at the canister surface in the thermal phase. This together with the presence or absence of air (oxygen) is a crucial parameter determining the rate of corrosive processes, which may affect canister integrity.

A one-dimensional radial mesh is used in the calculations. The first grid block represents the canister and has a radius of $R_1 = 0.343$ m. Subsequent radial spacings for the rock formation are incremented according to $\Delta R_{n+1} = \alpha \Delta R_n$, with $\alpha = 1.1622682$, so that $R_{33} = R_1 (\alpha^{33}-1)/(\alpha-1) = 300$ m. The first node is on the canister-rock interface and subsequent nodes are placed at rock block centers. The canister thermal power at emplacement is 2.21 kW for 10-year-old high-level waste [8]. The simulation is carried out over 50 years, with an initial time step of $\Delta t_1 = 10^3$ sec, and with subsequent time steps increasing logarithmically if convergence is obtained within 4 or less iterations. Test calculations using a finer mesh and smaller time steps showed that spatial and temporal discretization errors were negligible.

The material properties used in the "reference case" calculations are tabulated in Table I; the parameter choices are discussed in ref. [8]. Initial conditions are $T = 20^\circ\text{C}$, $p = 1$ bar, $S_2 = 0.35$. Test calculations showed that the moisture status near the waste canister is determined primarily by (1) capillary pressure (moisture retention characteristics), (2) absolute permeability, and (3) relative permeability for liquid and gaseous phases, respectively. The capillary pressure functions and the permeability-saturation relationship are not well known, especially in the region close to residual saturation at elevated temperature, which is crucial in determining the behavior of the system. A simple algebraic function, as shown in Table I, is used to represent capillary pressure-saturation relationship. This functional relationship, in its inverse form expressing saturation as a function of pressure head, is frequently used in the soil science literature for fitting the characteristic curves

describing soil-water retention data [9,10]. The air entry pressure $P_{a.e.}$ - a cutoff to be exceeded before the pores can be desaturated - is usually neglected and set to zero in fitting the data of partially saturated soils. This algebraic function formula with $P_{a.e.}$ as a parameter is used in the saturated/unsaturated flow program TRUST [11] and is also programmed in TOUGH. TOUGH can also use five other functional forms in its current version and can be easily programmed for other empirical formulae for the capillary functions.

The capillary function with the parameters in Table I is illustrated in Figure 2. The region of particular interest to our study is in the vicinity of the residual liquid saturation S_{gr} . If the system dries up, the liquid saturation will decrease and cross over S_{gr} toward zero. The algebraic functional form is not defined for $S_L < S_{gr}$. A large negative value of the capillary pressure, e.g. at the permanent wilting point of -15 bar [10], is used as a cutoff to define the capillary function in the region $S_L < S_{gr} + \epsilon$. The concepts of inter-phase surface tension and capillary driven fluid movement are probably ill-defined for $S_L < S_{gr}$. Desorption of water in the final drying-up stage may be accomplished by stationary phase changes on the soil surfaces and does not contribute significantly to the multi-phase fluid fluxes driven by pressure gradients. Therefore a constant cutoff with $P_C = P_{wilt}$, with zero capillary pressure gradient for $S_L < S_{gr}$, is probably a good approximation in describing the drying-up process.

RESULTS

For our simulations, the system is assumed initially partially saturated at $S_L = 0.35$. After emplacement of the waste canisters, temperatures near the canisters rise quickly above 100°C, and vigorous boiling of liquid water in the rock matrix adjacent to the canister is initiated. As the liquid water saturation decreases, the capillary pressure decreases rapidly (to large negative values), and a strong suction gradient is established which drives liquid flow towards the canister, while gas phase flow (vapor and air) occurs away from the canister. The two competing processes - thermally driven desaturation versus capillary driven resaturation - determine if the system will cross over the residual saturation and dry up or will remain wet. For the reference case parameters (Table I), the canister will dry up, as shown in Figure 3, because the thermally driven desaturation mechanism is stronger than the capillary driven resaturation mechanism. Parameters used in the sensitivity studies are given in Table II. If we double the capillary strength P_{cap} - defined as the value of capillary pressure at the mid-saturation point $S_L = 0.5 (1 + S_{gr})$ - the canister will remain wet, with the liquid saturation recovering slowly after a decline at early time (Figure 3). The capillary driven mechanism can also be enhanced with stronger saturation dependence by setting the exponent n to a smaller value. With stronger saturation dependence, the capillary gradient is larger and the resaturation flux is stronger. The dry-or-wet condition is especially sensitive to the capillary function near the residual saturation. If a higher cutoff is used in the calculations, the canister also remains wet, and the liquid saturation remains near S_{gr} for a long period of time, before it again increases and recovers to its initial value. The fifth case in Table II uses a higher air entry pressure, together with a higher capillary strength, but the difference $P_{cap} - P_{a.e.}$ is the same as in the reference case. The canister behavior is indistinguishable from the reference case.

The capillary driven liquid flow is enhanced for higher absolute permeability (case 6), and the canister will stay wet as shown in Figure 3 and Table II. On the other hand, with the same higher absolute permeability

but with relative liquid permeability near the residual saturation decreased by using Corey's relative permeability curves [12], the canister will dry up. The relative permeabilities for the liquid and gaseous phases are presently not well-understood for the materials of interest in high-level nuclear waste isolation. A more systematic study on the combined effect of capillarity and relative permeability is underway and will be discussed in a future paper [8].

DISCUSSION

If the canister dries up, the more obvious consequence is that the canister temperature will be higher, as illustrated in Figure 4. This occurs because the steam-water counterflow mechanism is not operative for dry conditions, so that heat is removed less effectively from the near vicinity of the canisters.

Gas phase pressures near the canisters are controlled by the saturation pressure (partial pressure) of vapor at prevailing temperatures. When the canister remains wet, the controlling temperature for the gas phase pressure is the canister temperature. When the vicinity of the canister dries up, liquid phase is encountered at some distance from the canisters, and the temperature determining the two-phase saturation pressure is lower. Therefore, the controlling vapor pressure is lower if drying occurs (see Figure 5).

The capillary driven liquid flow from high liquid saturation to low liquid saturation (i.e. toward the canister) is almost equal in magnitude to the gas phase flow driven by vaporization and thermal expansion. This is shown in Figure 6 for a case where the canister stays wet (higher capillary strength). A liquid-gas counterflow with little net mass transport is a very efficient heat transport mechanism. It occurs naturally in vapor-dominated geothermal reservoirs, and has engineering applications in devices known as "heat pipes" [13].

The phase velocities, defined as the Darcy velocities divided by the effective porosities ϕS_L and ϕS_g for liquid and gaseous phases, respectively, are shown in Figure 7 for a case where the canisters stay wet (higher capillary strength). Due to the large density differences between liquid and vapor, the gas velocities are two orders of magnitude larger than the liquid velocities. The hot gas phase near the canister moves outward fast and the vapor will condense at some distance from the canister. The liquid flow will move slowly toward the canister to complete the vaporization-condensation cycle. The outward gas flow is of concern if volatile waste components are released from the canister. The inward liquid flow provides an additional containment mechanism for liquid soluble waste components. However, the cyclic gas-out, liquid-in process may result in the accumulation of dissolved mineral concentrations near the canister, and the liquid near the canister may be more corrosive than the ambient formation fluids away from the heat source.

Figure 8 shows the mass fraction of air present in the gas phase in case 2 as a function of time and radial distance. The continuous vaporization process is accompanied by gas phase flow away from the canisters, which effectively purges air from the vicinity of the canisters. Even in cases where the canister vicinity dries up, sufficient vaporization takes place to sweep the air component away from the canisters. Therefore, the environment of the waste packages will become air-free rapidly after emplacement, and the gas phase will consist solely of water vapor. The expected absence of gaseous oxygen at the waste packages will considerably slow corrosive processes.

SUMMARY

The thermohydrological processes expected near high-level waste packages emplaced in unsaturated rocks are of considerable complexity. Depending upon properties of the host medium such as capillary pressure and relative permeability relationships, and absolute permeability, the near vicinity of waste packages will or will not dry up during the thermal phase. Of critical importance for the drying behavior are capillary pressures and relative permeabilities in the vicinity of the residual liquid saturation, which are poorly known at present. Laboratory and field experimentation is needed to quantify these parameters. The vaporization process taking place near the canisters will purge air from the canister vicinity, creating a canister environment free of gaseous oxygen.

ACKNOWLEDGEMENT

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Contract Number DE-AC03-76SF00098.

REFERENCES

1. T.N. Narasimhan, Physics of Saturated-Unsaturated Subsurface Flow, In T.N. Narasimhan, ed., Recent Trends in Hydrogeology, Geological Society of America, Special Paper 189 (1982).
2. P.C.D. Milly, Moisture and Heat Transport in Hysteretic, Inhomogeneous Porous Media: A Matrix-Head Based Formulation and a Numerical Model, Water Resources Research 18 (3), pp. 489-498 (1982).
3. K. Pruess, Heat Transfer in Fractured Geothermal Reservoirs with Boiling, Water Resources Research 19 (1), pp. 201-208 (1983).
4. K.H. Coats, A Highly Implicit Steam Flood Model, Soc. Petr. Eng. J., October 1978, pp. 369-393.
5. International Formulation Committee, A Formulation of the Thermodynamic Properties of Ordinary Water Substance, IFC Secretariat, Dusseldorf, Germany (1967).
6. K. Pruess and T.N. Narasimhan, A Practical Method for Modeling Fluid and Heat Flow in Fractured Porous Media, Proc. Sixth SPE Symposium on Reservoir Simulation (paper SPE-10509), New Orleans, Louisiana, February 1982.
7. J.R. Philip, Numerical Solution of Equations of the Diffusion Type with Diffusivity Concentration Dependent, Trans. Faraday Soc., 51, pp. 885-892 (1955).
8. K. Pruess and J.S.Y. Wang, Mechanics and Parameters Controlling the Moisture Conditions near High-Level Nuclear Waste Packages Embedded in Unsaturated Rock, in preparation.
9. R. Haverkamp, M. Vauclin, J. Touma, P.J. Wierenga, and G. Vachaud, A Comparison of Numerical Simulation Models for One-Dimensional Infiltration, Soil Sci. Soc. Am. J., 41, pp. 285-294 (1977).
10. M.Th. van Genuchten, A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, Soil Sci. Soc. Am. J., 44, pp. 892-898 (1980).
11. T.N. Narasimhan and P.A. Witherspoon, Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media, 3. Applications, Water Resources Research, 14 (6), pp. 1017-1034 (1977).
12. C.R. Faust and J.W. Mercer, Geothermal Reservoir Simulation - 2. Numerical Solution Techniques for Liquid- and Vapor-Dominated Hydrothermal Systems, Water Resources Research, 15, (1), pp. 31-46, February 1979.
13. G.Y. Eastman, The Heat Pipe, Scientific American, 218, pp. 38-46 (1968).

TABLE I. Material Parameters for Reference Case.

Constitutive Relationship	Parameter	Value
Capillary Pressure:	Strength P_{cap}	0.5 bar
$P_C(S_L) = \begin{cases} -P_{a.e.} - (P_{cap} - P_{a.e.}) \left(\frac{1-S_L}{S_L - S_{Lr}} \right)^{1/\eta} & \text{if } P_C > -P_{wilt} \\ -P_{wilt}, & \text{otherwise} \end{cases}$	Exponent η	2
	Wilting Pressure P_{wilt}	15 bar
	Air Entry Pressure $P_{a.e.}$	0.1 bar
	Residual Liquid Saturation S_{Lr}	0.25
	Residual Liquid Saturation S_{Lr}	0.25
Relative Permeability:	Residual Liquid Saturation S_{Lr}	0.25
Liquid: $K_{rx}(S_L) = \frac{S_L - S_{Lr}}{1 - S_{Lr}}$		
Gas: $K_{rg}(S_g) = S_g = 1 - S_L$		
Rock Hydrological Properties	Permeability k	10^{-15} m^2
	Porosity ϕ	0.1
Rock Thermal Properties	Thermal conductivity	$2.1 \text{ W/m}^\circ\text{C}$
	Specific heat	$1000 \text{ J/kg}^\circ\text{C}$
	Density	2650 kg/m^3
Canister Thermal Properties	Thermal conductivity	$5.3 \text{ W/m}^\circ\text{C}$
	Specific heat	$1030 \text{ J/kg}^\circ\text{C}$
	Density	2780 kg/m^3

TABLE II. Parameters in Sensitivity Studies.

Case	Parameter	Canister Condition
1 reference case	Table I	dry
2 higher strength	$P_{cap} = 1$ bar	wet
3 stronger S-dependence	$\eta = 1$	wet
4 stronger wilting cutoff	$P_{wilt} = 150$ bar	wet
5 higher air entry pressure	$P_{a.e.} = 0.6$ bar $P_{cap} = 1$ bar	dry
6 higher permeability	$k = 2 \times 10^{-15} \text{ m}^2$	wet
7 smaller relative permeability for liquid near S_{gr}	Corey's curves $k = 2 \times 10^{-15} \text{ m}^2$	dry

FIG. 1. Liquid saturation for one-dimensional infiltration problem (points: analytic solutions, lines: numerical results).

FIG. 2. Capillary pressure function.

FIG. 3. Liquid saturation at the canister surface.

FIG. 4. Temperature at the canister surface.

FIG. 5. Gas phase pressure at the canister surface.

FIG. 6. Rates of liquid and gas flow.

FIG. 7. Liquid and gas pore velocities.

FIG. 8. Mass fraction of air in gas phase.

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