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MODELING STUDIES OF MULTIPHASE FLUID AND HEAT FLOW PROCESSES IN NUCLEAR WASTE ISOLATION

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ABSTRACT

Multiphase fluid and heat flow plays an important role in many problems relating to the disposal of nuclear wastes in geologic media. Examples include boiling and condensation processes near heat-generating wastes, flow of water and formation gas in partially saturated formations, evolution of a free gas phase from waste package corrosion in initially water-saturated environments, and redistribution (dissolution, transport, and precipitation) of rock minerals in non-isothermal flow fields. Such processes may strongly impact upon waste package and repository design considerations and performance.

This paper summarizes important physical phenomena occurring in multiphase and nonisothermal flows, as well as techniques for their mathematical modeling and numerical simulation. Illustrative applications are given for a number of specific fluid and heat flow problems, including: thermohydrologic conditions near heat-generating waste packages in the unsaturated zone; repository-wide convection effects in the unsaturated zone; effects of quartz dissolution and precipitation for disposal in the saturated zone; and gas pressurization and flow effects from corrosion of low-level waste packages.

INTRODUCTION

Research efforts are currently underway in many countries to find methods for the safe disposal of radioactive wastes generated from nuclear power development. The preferred disposal method is emplacement in stable geologic formations, where the wastes would remain isolated from the biosphere for the long time periods required for their radioactivity to decay to innocuous levels. Most research in the disposal of nuclear wastes is directed at finding suitable host formations for a geologic repository below the water table, in rock formations of low intrinsic permeability with a low density of fracturing. In contrast, the U.S. program for disposal of high-level nuclear wastes from civilian power reactors is exploring the feasibility of developing a repository in thick unsaturated zones in desert environments.

From the viewpoint of fluid flow and heat transfer, the saturated zone represents a single-phase flow system at rather large (essentially hydrostatic) pressures, while in the unsaturated zone two-phase (liquid-gas) conditions and ambient pressures near 1 bar are present. Multiphase flow effects take on a rather different nature and significance in these different environments. We will first summarize the major multiphase fluid and heat flow phenomena that can arise in the context of geologic disposal of nuclear wastes. Then we discuss methods for simulating these processes by means of digital computers, and present applications of numerical simulators to several illustrative problems. The paper concludes with an examination of some challenging open problems and future research directions.

MULTIPHASE FLOW PROCESSES

There are several mechanisms by which multiphase processes can be induced in the saturated zone. The heat released from high-level nuclear waste packages will cause formation temperatures to rise, while simultaneously pore fluid pressures will be reduced near a repository, reaching ambient pressures of 1 bar at the walls of the excavations during the open (operational) phase. When host rock temperatures reach the saturation temperature of water vapor at prevailing fluid pressures, boiling will commence and two-phase flow of liquid and vapor will be induced. Another multiphase flow effect occurs under nonisothermal conditions in flow systems in which only a liquid phase is

present. Namely, the solubility of mineral phases such as quartz depends on temperature [1] so that nonisothermal flow will in general be accompanied by dissolution, transport, and precipitation effects. This can cause significant changes in formation porosity and permeability. Further multiphase effects in the saturated zone can develop from corrosive gas release as metallic waste packages interact chemically with formation waters.

Multiphase flow effects play a more significant and obvious role in the unsaturated zone, where two fluid phases (liquid water and formation gas) are present under natural conditions. The emplacement of heat generating high-level nuclear wastes in a partially saturated permeable medium will give rise to a complex interplay of two-phase flow processes with phase transformation and heat transfer effects. A vapor-liquid counterflow process known as "heat pipe" may develop which provides a very efficient heat transfer mechanism [2,3,4]. Especially favorable conditions for the development of heat pipe conditions exist in fractured-porous media with large fracture permeability and strong capillary effects in the rock matrix.

NUMERICAL SIMULATION TECHNIQUES

Recently developed modeling techniques for multiphase processes in nuclear waste isolation borrow heavily from techniques used in the simulation of geothermal and petroleum reservoirs [5,6]. Table I summarizes the various processes that have been considered in recent modeling developments [7]. Processes marked with an asterisk (*) have been modeled with the MULKOM and TOUGH simulators developed at Lawrence Berkeley Laboratory, which were used in the simulation studies summarized below. Due to space limitations we can only highlight the main concepts used in the simulation of multiphase processes; further details can be found in the literature [8,6,9].

Table I. Physical Processes in Multiphase Fluid and Heat Flow

1. Fluid Flow	2. Heat Flow
* pressure forces	* conduction
* viscous forces	* flow of latent and sensible heat
inertial forces	radiation
* gravity	3. Vaporization and Condensation
* interference between liquid and gas	* temperature and pressure effects
* dissolution of air in liquid	* capillarity and adsorption
* capillarity and adsorption	4. Changes in Rock Mass
differential heat of wetting	(*) thermal expansion
chemical potential gradients	(*) compression under stress
* mixing of vapor and air	thermal stress cracking
* vapor pressure lowering	(*) change in porosity and
* binary diffusion	permeability
Knudsen diffusion	
thermodiffusion	

For a flow system with K mass components and one heat "pseudo-component", the governing equations consist of (K+1) mass- and energy-balance equations. These are written in integral form for an arbitrary subdomain ("grid block" in finite-difference parlance) V_n as follows.

$$\frac{d}{dt} \int_{V_n} M^{(k)} dV = \int_{\Gamma_n} \tilde{F}^{(k)} \cdot \underline{n} d\Gamma + \int_{V_n} q^{(k)} dV \quad (1)$$

Here M denotes the "accumulation" term, i.e., the amount of component k (k = water, air, heat, etc.) present per unit formation volume. F is the flux of component k on the closed surface Γ_n around V_n , and q represents sink and source terms. Thus, Eq. (1) expresses the simple fact that the

rate of change in the amount of k within V_n is equal to the total rate at which k flows across the surface Γ_n of V_n , plus the contribution of sinks and sources from within V_n . (We mention in passing that the heat "component" is not strictly conserved because of the possibility of conversion of heat into mechanical work and vice versa; this fine point is immaterial for the present discussion.)

Note that the conservative quantities for which Eqs. (1) are written are not the phases but the components (different chemical species, or mixtures of species, such as air, which can be treated as a single "pseudo-component" for the processes of interest). The accumulation term M is a sum over contributions from the various phases (liquid, gaseous, solid) in which component k is present. This formulation automatically includes the description of phase change processes subject to the constraint of "local thermodynamic equilibrium" between all phases. Description of non-equilibrium phase change effects would require separate conservation equations for different phases, with appropriate sink and source terms to represent phase transformations. The flux terms F are likewise sums of the separate contributions made by the different flowing phases, the main term being a multiphase version of Darcy's law, that includes relative permeability and capillary pressure effects. In addition, diffusive and dispersive mass fluxes can be present. Heat flux includes conductive and convective components; the latter includes latent heat effects represented by different specific enthalpies of different phases.

The transport Eqs. (1) need to be complemented with constitutive relationships, which express all parameters as functions of a set of primary thermodynamic variables. Phase transitions from single-phase liquid to two-phase liquid-gas to single-phase gas conditions are handled in MULKOM and TOUGH by appropriate "switching" of primary variables. An important feature of multiphase flow systems is that the governing Eqs. (1) have the same form, regardless of the nature and number of fluid and solid components and phases present; the peculiar properties of specific fluid mixtures and solid phases enter only through the constitutive relationships. This allows for a flexible "modular" architecture of a numerical simulator (see Fig. 1), in which different fluid systems can be described by interfacing a module for setting up the transport equations with different thermophysical property modules ("equation-of-state packages"). Presently used thermophysical property modules for MULKOM are listed in Table II.

Fig. 1. Modular architecture of MULKOM and TOUGH.

Table II. MULKOM fluid property modules

Components	Number of Components
water	1
water at near-critical conditions	1
two waters*	2
water, CO ₂ †	2
water, NaCl	2
water, air	2
water, SiO ₂ ‡	2
water, volatile hydrocarbon, non-volatile hydrocarbon	3
water, natural gas, foam	3

* water with tracer

† with mineral buffer

‡ includes dissolution and precipitation, as well as associated changes in porosity and permeability

In MULKOM and TOUGH, thermophysical properties of water substance are described by steam table equations [10,11]. Non-condensable gases such as air, hydrogen, carbon dioxide etc. are represented as ideal or real gases, and additivity of pressures is assumed for the gaseous components. Vapor pressure lowering due to capillary and phase adsorption effects is described by Kelvin's equation, and dissolution of noncondensable gases in the liquid phase is represented by Henry's law. Aqueous silica concentrations are described by the equilibrium quartz solubilities given by Fournier and Potter [12]. All thermophysical and hydrologic parameters (including porosity and permeability) which appear in the governing equations can be arbitrary (nonlinear and differentiable) functions of the primary thermodynamic variables.

For numerical solution, the mass and energy balance Eqs. (1) must be discretized in space and time. In MULKOM and TOUGH, space discretization is made directly from the integrals, without first converting Eqs. (1) into partial differential equations. This "integral" finite difference method [13] avoids any reference to a global system of coordinates, and thus offers the advantage of being applicable to regular or irregular discretizations in one, two, or three dimensions. It also facilitates applications to fractured media (see below). Time is discretized fully implicitly as a first-order backward finite difference. This together with 100% upstream weighting of flux terms at interfaces is necessary to achieve unconditional stability [5], and to avoid impractical time step limitations for multiphase flow problems in fractured media with their usually small but highly active fracture volume. Space and time discretization results in a set of nonlinear algebraic equations. These are usually strongly coupled and are solved completely simultaneously by means of Newton/Raphson iteration. If convergence is not achieved within a predetermined number of iterations (typically eight), the time step size is automatically reduced. The linear equations arising at each iteration step are solved with a sparse version of LU-decomposition and backsubstitution [14].

APPLICATIONS

High-level waste packages in the unsaturated zone

Simulation studies of fluid and heat flow near high-level waste packages emplaced in partially saturated fractured rock have been carried out to gain some insight into possible thermohydrological conditions [15,16]. Problem parameters were chosen representative of the conditions at Yucca Mountain, Nevada. A highly idealized flow geometry was used, in which an infinite linear string of waste packages is intersected at a right angle by a set of plane, parallel, equidistant fractures. Neglecting gravity effects, the resulting symmetry element is then small enough to permit a detailed resolution of fluid and heat flow processes at matrix-fracture interfaces on a sub-millimeter scale. The major thermohydrologic phenomena observed in the simulations are indicated in Figure 2.

Heat from the waste packages enters the host rock where it causes vaporization of formation water. Most of the vapor flows towards the fractures which, because of their large permeability, act as essentially constant-pressure sinks. In the fractures the vapor flows outward and condenses as it encounters cooler wall rock (see Figure 2). The fate of the condensate depends on the relative permeability characteristics of the fractures, which are unknown at the present time. At ambient suction

Fig. 2. Schematic of simulated thermohydrologic phenomena near high-level nuclear waste packages emplaced in an unsaturated fractured porous medium (after Pruess et al., 1985).

Fig. 3. Predicted host rock temperatures at a distance of 0.34 m from the waste package centerline (after Pruess et al., 1985).

conditions, estimated to be near - 1 MPa, the bulk of most fractures will be drained; however, liquid could still be present in surface roughness, or as a thin adsorbed film on the fracture walls. If such liquid is assumed to have appreciable mobility most of the condensate will flow in the fracture surfaces back towards the heat source; if liquid is not mobile in the fractures the condensate will be sucked into the rock matrix and will then migrate down the saturation profile towards the heat source. Either way the aforementioned "heat pipe" process with vapor-liquid counterflow will develop.

The numerical simulation studies suggest that the seemingly subtle issue of liquid mobility in drained fractures may have a major impact on the thermo-hydrologic conditions near the waste packages. When liquid is assumed immobile in the fractures the backflow of liquid towards the heat source is impeded by the low permeability of the rock matrix, so that the heat pipe is imbalanced: Outflow of vapor exceeds backflow of liquid, and the vicinity of the waste packages is predicted to dry up. Heat transfer away from the waste packages occurs then by conduction, with temperatures in the host rock reaching approximately 250 °C (see Figure 3). If liquid is assumed mobile in the fractures, however, the heat pipe approaches a balanced counterflow after an initial transient period, maintaining wet (two-phase) conditions all the way to the surface of the waste canister emplacement hole. Due to the high fracture permeability pressure remains near ambient 1 bar, so that the two-phase conditions then constrain maximum formation temperatures to near 100°C.

It is of interest to note that possible evidence for heat pipe processes was observed in field experiments with electric resistance heaters in G-tunnel, Nevada Test Site, under conditions believed to be similar to those at the target repository horizon at Yucca Mountain [17,18]. Indeed, several of the thermocouples emplaced in the host rock near the heaters quickly reached a temperature of 94°C, and then remained at that temperature for periods from a few days to almost one month, before registering higher temperatures. 94°C happens to be the boiling temperature at ambient barometric pressure at G-tunnel, suggesting the presence of persistent two-phase conditions.

The explicit representation of fractures in the simulations discussed above is useful for a study of fundamental processes, but it is impractical for modeling of fluid and heat flows over the space and time scales of interest in nuclear waste isolation. Based on the results of the "explicit fracture" simulations, we have developed an "effective continuum" approximation in which fracture effects are represented by means of appropriately modified hydrologic parameters. Test calculations have shown that this approximation can accurately reproduce the complexity of nonisothermal multiphase flow in a fractured-porous medium (see Figure 3, as well as more detailed evaluations presented by Pruess et al. [15,19]).

The effective continuum approximation reduces the computational effort in modeling flow in a fractured-porous medium to that of a straight porous medium model. It permits large-scale simulations of fluid and heat flow in fractured media. As an example, Figure 4 shows a diagram of a schematic two-dimensional axisymmetric model of a repository in the unsaturated zone at Yucca Mountain. From numerical simulations it was predicted that the repository heat load would induce significant thermal buoyancy flow in the gas phase, with typical pore velocities of order 10 - 100 m/year ([20]; see Figure 5). This raises concerns about the potential release of gaseous contaminants, such as C-14 in the form of carbon dioxide [21]. Significant gas phase flows in the unsaturated zone can also be induced under natural conditions from an interplay of barometric pressure effects and seasonal temperature variations [22].

Silica redistribution

Large effects of silica redistribution on rock permeability have been observed in laboratory experiments [23,24]. Forced convection of water through rock samples held in large temperature gradients of approximately 26°C/cm indicated that a mere 8% reduction in original porosity resulted in 96% reduction in permeability of a granitic rock core [24]. Such dramatic effects can not be understood when conceptualizing permeable media as systems of flow channels with uniform cross section, as has often been done in the literature. Verma and Pruess [25,26] proposed that an essential feature of natural permeable media is the converging-diverging nature of flow channels (see also

Fig. 4. Schematic diagram of a nuclear waste repository in a thick unsaturated zone (after Tsang and Pruess, 1987).

Fig. 5. Simulated gas convection velocities along the repository centerline at 100 years after waste emplacement (after Tsang and Pruess, 1987).

[27]). This conceptualization includes “bottlenecks” which can account for the observation of drastic changes in permeability from minor changes in average porosity (Figure 6).

Numerical simulation studies have been carried out to examine whether severe porosity-permeability relationships as depicted in Figure 6 (curves for the “series model”) could give rise to significant thermal and hydrologic effects in nuclear waste isolation. All fluid and solid phases were assumed to be in local thermodynamic equilibrium, and dissolved silica concentration was assumed to correspond to equilibrium quartz solubility, as given by Fournier and Potter [12]. These assumptions were made to provide a conservative (maximum) estimate of quartz dissolution and precipitation effects, which in turn will provide conservative estimates for associated porosity and permeability changes and their thermohydrologic impacts.

Fig. 6. Hypothetical porosity-permeability relationships for different pore channel models (after Verma and Pruess, 1988).

Both a room-scale and a repository-scale problem with parameters appropriate for the Basalt Waste Isolation Project (BWIP) were studied. In the room-scale problem, ambient fluid pressure is

130 bars, while pressure in the room is maintained at 1 bar for an open period assumed to be 50 years. Thus, fluid flows towards the storage room and in the direction of the temperature gradient, so that quartz dissolution will take place coupled with enhancement of porosity and permeability. For the most severe porosity-permeability relationship examined (the series model with $\phi_c = 0.95$ in Figure 6), fluid flow rate was predicted to be enhanced by at most 20% compared to a reference case without allowance for silica redistribution effects. Pore pressures near the storage room were lowered from the enhancement in porosity and permeability, resulting in an increased extent of the boiling zone around the room from a maximum radial extent of 0.13 m for the reference case to 0.67 m when silica redistribution effects were included. Due to enhanced fluid flow, formation temperatures were predicted to be typically 10 - 20°C lower.

Simulations of a repository-scale model in the saturated zone indicated that effects from silica redistribution were negligibly small, with maximum predicted temperature effects less than 10°C [26].

Corrosive gas release

The "Nationale Genossenschaft fuer die Lagerung radioaktiver Abfaelle" (NAGRA) of Switzerland is studying the feasibility of emplacing low and intermediate level nuclear wastes at a site in the Oberbauenstock mountain [28,29,30]. The potential repository horizon is located in dense marl, with an estimated permeability of the intact rock matrix of order 0.1 microdarcies. Large-scale formation permeability is dominated by fractures and is estimated as approximately 10 microdarcies. The repository horizon is below the water table, with fluid pore pressure near 10 bar. The formation was originally believed to be water-saturated; however, recent site investigations have indicated the presence of significant amounts of gas. Origin and distribution of the gas have not yet been determined.

The proposed nuclear waste repository at Oberbauenstock would contain concrete, metals, and organic materials in contact with groundwater. Detailed studies have indicated that corrosion of the metals and microbial degradation of the organic materials will evolve large amounts of gas, the chief constituent being hydrogen, with minor amounts of methane, carbon dioxide, and others [28,31,32,33].

The expected gas release raises several concerns. From the data given by Wiborgh et al. [33] it can be estimated that gas pressures in the repository could build up to levels of several hundred bars, endangering the integrity of engineered barriers, unless specific design provisions are made for gas venting. Gas escaping from the repository could alter existing groundwater flow patterns in the host rock, and thereby impact on the travel time of contaminants to the biosphere.

We have initiated a numerical simulation study of the gas release and its effects on pore pressures and groundwater flow in the host rock. For this study a modified version of our TOUGH simulator is being used, in which the air component was replaced with hydrogen. Preliminary results for a porous medium model as well as for a dual-permeability fractured reservoir model are given in Figure 7. In the porous medium model it takes approximately 2.0 years for the released gas to exceed the solubility limit, and to initiate formation of a separate gas phase. The subsequent increase in gas saturation is accompanied by an increase in fluid pressure. Fluid pressures decline after a mobile gas saturation (5%) is established; for the porous medium this occurs after 20 years. At this time also the rate of corrosive gas generation is reduced, so that pressure decline after 20 years is rapid. The depressurization is accompanied by a further increase in gas saturation from expansion effects.

Our dual-permeability model employs the method of "multiple interacting continua" (MINC; [34]). For a first exploratory calculation only one fracture and one matrix continuum were defined. Interporosity flow between matrix and fractures was calculated using idealized matrix blocks in the shape of vertical slabs with $10 \times 10 \text{ m}^2$ cross section. Global flow can occur in both fracture and matrix continua. A comparison with the porous medium case (Figure 7) shows that pressures and gas saturations begin to rise at an earlier time. This was expected because of the smaller average fracture porosity (1%) than the porous medium porosity (3%). Pressure increase again ceases soon

Fig. 7. Simulated temporal evolution of gas pressures and saturations at a low-level repository in water-saturated rock.

after a mobile gas saturation (5%) is reached. Additional strong pressure decline occurs in response to the reduction in gas generation rate after 20 years. Gas saturations in the fractured medium model are larger at all times. Overall the behavior of the dual permeability model is similar to that of the porous medium model.

The gas migration simulations presented here are preliminary. Some of the important parameters governing system response, such as relative permeabilities and capillary pressures in the fractures, are poorly known. Further work is underway to determine the features with the most significant impact on gas pressurization and flow predictions, and to reduce the uncertainty in expected system behavior to acceptable levels.

DISCUSSION AND CONCLUSIONS

Phase change and multiphase flow effects involving gaseous, liquid, and solid phases may occur in a variety of conditions in the geologic disposal of high- and low-level nuclear wastes. These processes can be described by means of highly non-linear integro-differential or partial differential equations. Numerical simulation techniques have been developed that permit to obtain approximate solutions to these equations in a robust and efficient manner.

Illustrative applications of numerical simulation have provided valuable insight into fluid and heat flow conditions in geologic repositories for nuclear waste in the unsaturated as well as in the saturated zone. Thermo-hydrologic conditions near heat-generating waste packages emplaced in the unsaturated zone have been studied. It was found that the expected temperature and moisture regime near the waste packages depends on subtle multiphase flow characteristics of fractures (relative permeabilities), which are unknown at the present time. Repository-wide modeling has suggested that high-level waste disposal in the unsaturated zone will induce strong thermal buoyancy flow of formation gas. Silica redistribution and associated porosity and permeability effects have been studied for high-level wastes emplaced in saturated formations. Although laboratory experiments had suggested a potential for strong effects it was found that because of the relatively weak temperature gradients encountered near nuclear waste packages silica redistribution effects should be insignificant.

Preliminary simulation results were presented for an unusual two-phase flow problem, in which waste package corrosion will evolve a free gas phase in a water-saturated medium.

An added complication in modeling arises from the fact that the host rocks under consideration for nuclear waste isolation usually have predominant fracture permeability. Porous medium models are often inadequate under these conditions, and special techniques such as effective continuum or multiple-porosity approaches must be employed. The most serious drawback of present efforts to simulate multiphase flow processes is the lack of basic data. For example, there seem to be no experimental data available in the open literature for relative permeability functions of "real" rough-walled fractures. Carefully controlled laboratory experiments as well as advances in our ability to characterize fractured media in the field will be needed to improve the reliability of numerical simulation predictions.

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