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MOUNTAIN SCALE MODELING OF TRANSIENT, COUPLED GAS FLOW, HEAT TRANSFER AND CARBON-14 MIGRATION

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ABSTRACT

We simulate mountain-scale coupled heat transfer and gas flow at Yucca Mountain. A coupled rock-gas flow and heat transfer model, TGIF2, is used to simulate mountain-scale two-dimensional transient heat transfer and gas flow.

The model is first verified against an analytical solution for the problem of an infinite horizontal layer of fluid heated from below. Our numerical results match very well with the analytical solution.

Then, we obtain transient temperature and gas flow distributions inside the mountain. These distributions are used by a transient semianalytical particle tracker to obtain carbon-14 travel times for particles starting at different locations within the repository.

Assuming that the repository is filled with 30-year-old waste at an initial areal power density of 57 kw/acre, we find that repository temperatures remain above 60 °C for more than 10,000 years. Carbon-14 travel times to the surface are mostly less than 1000 years, for particles starting at any time within the first 10,000 years.

INTRODUCTION

Subsurface gas flow at the potential repository site at Yucca Mountain, Nevada, is an important element in repository performance. Gas flow is significant for several reasons:

- Carbon-14 released from waste packages will migrate to the surface in the gas phase.[1]
- Vapor movement can redistribute water above the repository.[2]
- If gas flows are sufficiently large, convection will affect repository temperatures.[3]

Because gas flows are driven by heat and in turn affect temperatures, accurate calculations require a transient coupled model of heat transfer and gas flow. Until recently, the only models available for such calculations were various versions of TOUGH[4], which solves fully coupled equations for multi-phase flow of air, water, and heat both above and below the boiling point. By including so much physics, this model requires intensive use of computer resources and limits the size of feasible grids.

To model the migration of carbon-14, a relatively fine grid is needed to represent migration paths with reasonable accuracy. We have developed a model which, by simplifying the physics, allows finer grids to be used. The principal simplification in this model, called TGIF2, is the assumption that relative humidity is always near 100 %. This allows the numerically challenging problem of unsaturated water movement to be omitted entirely from the model. The assumption is well satisfied in the deep subsurface as long as temperatures remain below the boiling point.[5]

Using this model and a newly developed transient particle tracker, we have simulated the migration of carbon-14 from the potential repository to the surface. The simulations use three parallel, east-west cross-sections which are taken from the Sandia National Laboratories Interactive Graphics Information System (IGIS).[6] The latest information about mountain topography and stratigraphy has been incorporated in our simulations. The system is simulated with fixed temperature at a lower boundary far below the repository level and with the repository heated by a full load of waste packages with the heat input varying as a function of time.

For each simulation, travel paths are determined for a large number of particles traveling from points evenly distributed throughout the potential repository area to the surface. The travel times are calculated along each path line for a particle of carbon-14 that is

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retarded by isotopic exchange with bicarbonate dissolved in the aqueous phase[1]. The concentration of dissolved bicarbonate is determined by assuming thermodynamic equilibrium with solid calcite and the measured rock-gas composition.

The results of these calculations are presented as histograms of travel times. Each histogram represents the distribution of travel times throughout the repository (combining all three cross-sections).

THE MODELS

We analyze carbon-14 travel times at Yucca Mountain in two steps. First, we solve the transient, coupled gas flow and heat transfer by an explicit finite difference method using the TGIF2 model. Then we perform the transient particle tracking analysis (with the TRACK model) using velocity and temperature fields calculated by TGIF2 to obtain ^{14}C particle travel times.

The TGIF2 model analyzes a gas whose humidity is maintained at 100% by evaporation or condensation of the water when the gas flows through pressure and temperature gradients. Flow of liquid water is not modeled explicitly, but water is assumed to flow toward areas of evaporation readily enough to keep the medium partially saturated. This humidity constraint is physically realistic; unsaturated soils and rocks almost always contain some liquid water except very near the ground surface, and this water keeps the humidity close to 100%.[5]

With these assumptions, the governing equations consist of four equations[7]: a constitutive relation, Darcy's Law, a volume balance, and an energy balance. They are given by

$$\rho = \frac{1}{RT}\left[P_v\Omega_v + P_a\Omega_a\right] \tag{1}$$

$$q = -\frac{k}{\mu}(\nabla P - g\rho z) \tag{2}$$

$$\nabla \cdot q - q \cdot \left[\left(\frac{1}{T} + \frac{1}{P_a}\frac{dP_v}{dT}\right)\nabla T - \frac{1}{P_a}\nabla P\right] = 0 \tag{3}$$

$$K_t\nabla^2 T - c_p^{gas}\rho q\cdot\nabla T + \frac{1}{c}\left(1+\frac{P_v}{P_a}\right)q\cdot\nabla P_a - \frac{H_v\Omega_v}{RT}q\cdot\left[\left(1+\frac{P_v}{P_a}\right)\frac{dP_v}{dT}\nabla T - \frac{P_v}{P_a}\nabla P\right] = c_p^{rock}\rho_{rock}(1-n)\frac{\partial T}{\partial t} \tag{4}$$

where ρ is the gas density, R is the gas constant, T is temperature, Ω_v and Ω_a are the molar weights of water and dry air, g is the acceleration of gravity, k is the intrinsic permeability of the porous medium, μ is the gas viscosity, and z is a downward-pointing unit vector. The variable P_v is the vapor pressure of water, which depends only on temperature because of the assumption of 100% humidity. By definition, we have $P_a = P - P_v$. In the energy equation, K_t is the thermal conductivity of the porous medium, c is a conversion factor equal to 4.18×10^{-7} erg cal^{-1}, c_p^{gas} is the specific heat of gas at constant pressure, c_p^{rock} and ρ_{rock} are the specific heat and density of rock (including liquid water in the pores), H_v is the heat of vaporization of water, and n is the drained porosity.

For given initial and boundary conditions at Yucca Mountain, Equations (1), (2), (3), and (4) can be solved for fields of density ρ, pressure P, temperature T, and gas flux q. The solution is obtained by an explicit transient finite difference technique.

Carbon-14 will move more slowly than the uncondensible components of the gas, because it spends most of its time in the relatively immobile liquid phase as dissolved bicarbonate. This phenomenon has been incorporated in the model by using the reaction path model PHREEQE to model the geochemical system. The conceptual model of the geochemical system adopted here has three principal features[1,9]:

- Sufficient calcium carbonate is present in the unsaturated zone to determine the aqueous chemistry, and to buffer the pH of the water.

- A relatively minor amount of calcium is derived from silicate weathering reactions; calcium concentrations are the result of equilibration with calcium carbonate.

- Fractionation plays a negligible role in removing ^{14}C from the gas phase, and concentrations of ^{14}C are proportional to those of ^{12}C.

The relative concentrations of carbonate species in liquid and gas phases at equilibrium are used to calculate retardation factors for ^{14}C transport in the gas phase.

The transient particle tracking employs a newly developed transient semianalytical theory.[8]

NUMERICAL MODEL VERIFICATION

To verify the TGIF2 model, we use an analytical solution of the stability problem for an infinite horizontal layer of gas heated from below. This problem was solved recently[7] and is extremely useful for model verification because no other available analytical solution involves coupling among gas flow, water evaporation, and heat transfer, and experimental model validation is not possible on the full spatial and temporal scale of Yucca Mountain.

The convective instability occurs only because of interactions between heat transfer and fluid flow. The value of the critical Rayleigh number is a direct quantitative measure of the coupling between these two processes.[7] When the fluid is moist gas, the result is strongly affected by evaporation and condensation, reflecting also the coupling between gas and liquid. Consequently, the performance of a numerical model in computing the critical Rayleigh number for flow of moist gas is a very sensitive test of its accuracy in computing coupled heat transfer and two-phase fluid flow.

Table 1
Parameter Values Used in Model Verification (the subscript *s* stands for values at the top surface)

c_p^{gas}	2.4×10^{-1} cal g^{-1} K^{-1}
c_p^{rock}	2.5×10^{-1} cal g^{-1} K^{-1}
H	6.0×10^4 cm
K_t	4.0×10^{-3} cal cm^{-1} K^{-1} s^{-1}
n	0.1 dimensionless
P_s	8.88×10^5 g cm^{-1} s^{-2}
T_s	3.0×10^2 K
μ	1.86×10^{-4} g cm^{-1} s^{-1}
ρ_s	1.00×10^{-3} g cm^{-3}
ρ_{rock}	3.00 g cm^{-3}

The code is run with an upper no-flow boundary at 30°C and a lower boundary temperature of 74°C. Parameter values used in model verification are listed in Table 1. For these boundary conditions and system parameters, the analytical solution predicts a critical Rayleigh number of 0.512. The code is run with a range of permeabilities, corresponding to different Rayleigh numbers. Figure 1 shows gas fluxes for a typical solution above the critical Rayleigh number, with clearly defined convection cells. The maximum calculated gas velocity

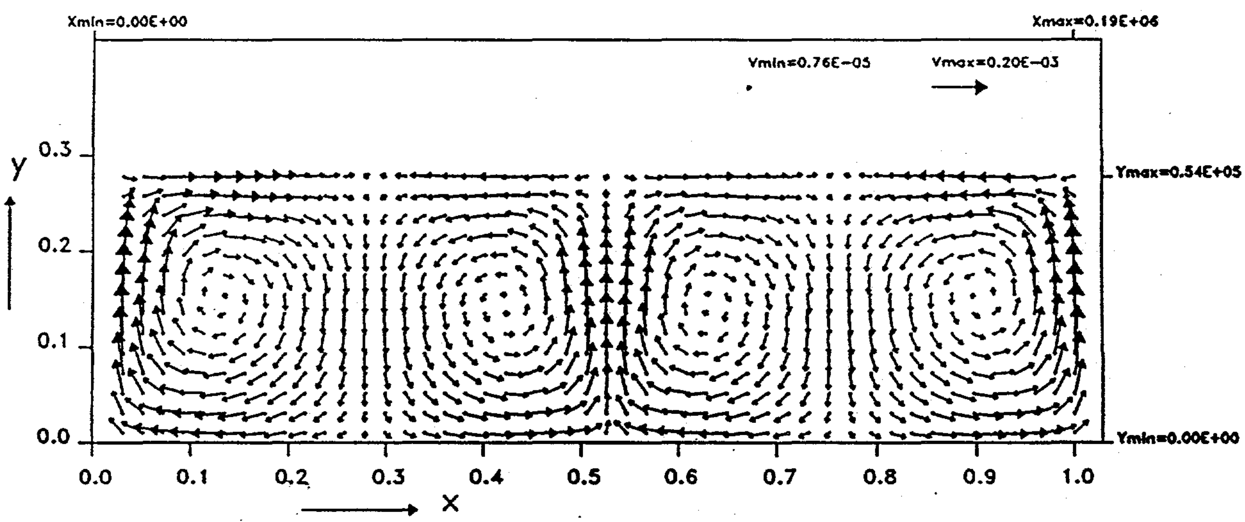

Figure 1 - Numerically calculated gas flux (Darcy velocity) at Rayleigh number 2.32. The unit for velocity is cm/s and the unit for coordinates showing on the right and upper boundaries is cm.

is plotted as a function of Rayleigh number in Figure 2. The numerically calculated onset of convection occurs at a Rayleigh number of approximately 1.2. Considering the extreme sensitivity of the simulation, the difference between an infinite layer and a finite numerical grid, and the approximations in the analytical solution, this represents good agreement.

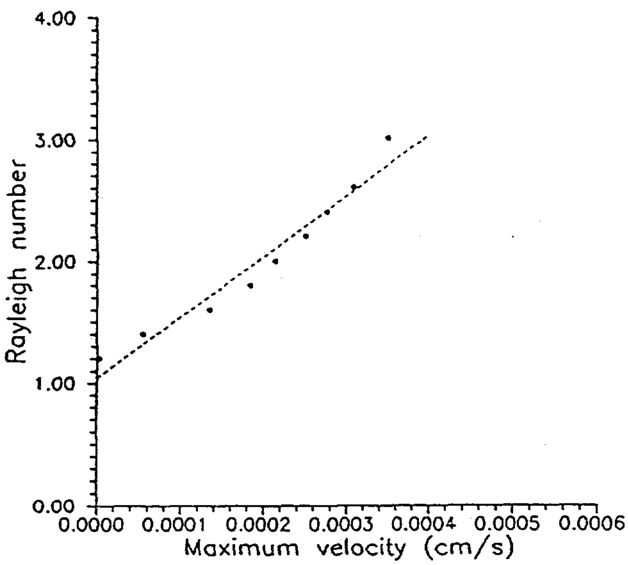

Figure 2 - Maximum gas flux calculated numerically, as a function of Rayleigh number.

SIMULATIONS AND RESULTS

We simulate gas flow, heat transfer, and carbon-14 travel times in three equally spaced east-west cross sections through Yucca Mountain. These cross sections are generated from Sandia's IGIS.[6] The cross-sections contain three hydrostratigraphic subdivisions of the Paintbrush Tuff Formation. They dip approximately six degrees to the east and differ in permeability. The upper and lower layers represent the Tiva Canyon welded unit and the Topopah Spring welded unit. These are thick, welded, densely fractured, and relatively permeable. A permeability of 10^{-7} cm^2 is used for these layers. This is within the range of measured values, near the upper end of the range.[10] The middle layer is the Paintbrush nonwelded unit, a thin (40~60 m) nonwelded tuff which includes all or part of several stratigraphic subdivisions of the Paintbrush Tuff. A permeability of 10^{-8} cm^2 is used for the Paintbrush nonwelded unit.

The heat source (power output) is treated as a function of time[5]. We assume that the spent fuel is 30 years old at the beginning of the calculation and the waste is emplaced at a constant rate evenly over a 25-year period. The initial heat source density was uniformly over the initial repository area as 57 kw/acre. Because the waste is 30 years old when emplacement begins, the repository area is less than the 5.7 km^2 used in previous studies[1,10] which assumed emplacement of 57 kw/acre of 10-year-old waste.

Carbon-14 particle travel times are calculated for a mathematical particle that is not affected by diffusion or dispersion. These processes would affect a particle of carbon-14 or any other contaminant and cause some spreading in the distribution of travel times. However, the spreading of travel times caused by the geometry of the mountain and the gas flow field is so large that diffusion and dispersion can safely be ignored. The calculated transient gas flow field is used for particle trajectory and travel time calculation by the TRACK code using the semianalytical method.[8]

To prevent the results from being biased by a non-random selection of particle origins, particle starting locations are selected using a simple analogue of the Latin Hypercube method[9]. In each of the three cross sections, the repository is divided into 30-meter intervals and one particle origin is chosen randomly within each interval. In all, travel times from the repository to the surface are calculated for 260 points. This method gives less statistical noise and avoids clustering of starting points compared to having the same number of particles randomly and independently located. In this study we assume all 260 particles are released at the same time.

Because the travel times vary with particle release time, we conduct particle tracking analysis at nineteen different release times ranging from 1,000 to 19,000 years in increments of 1,000 years.

Figures 3a through 3d are travel time histograms that combine the results of all three cross sections. Figures 4a through 4d illustrate calculated temperature fields at 1,000, 5,000, 10,000, and 15,000 years for one of the three cross sections. Figure 3a shows travel times when the carbon-14 inventory is released at 1,000 years after waste emplacement. At this early time, temperatures near the repository are high (Figure 4a) due to the large heat output. Gas velocities near the repository area are larger than in the far field. The calculated carbon-14 travel times range from 200 to 600 years.

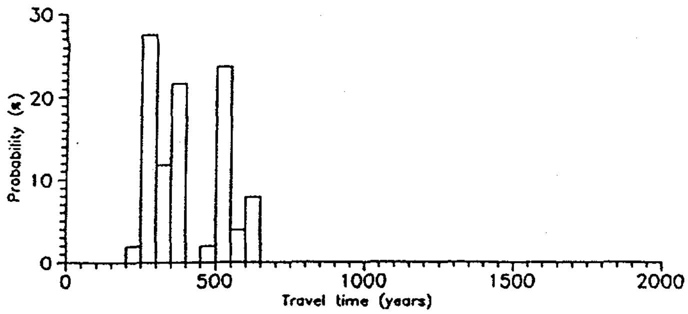

Figure 3a - Retarded travel times of ^{14}C particles from the repository to the atmosphere with particles released at 1000 years.

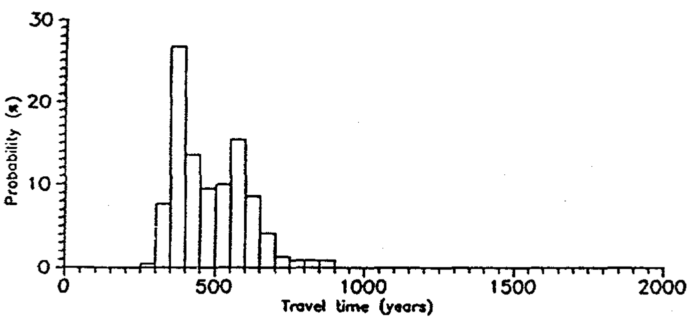

Figure 3b - Retarded travel times of ^{14}C particles from the repository to the atmosphere with particles released at 5000 years.

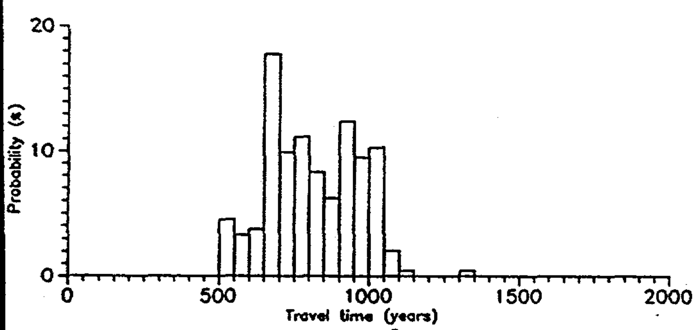

Figure 3c - Retarded travel times of ^{14}C particles from the repository to the atmosphere with particles released at 10000 years.

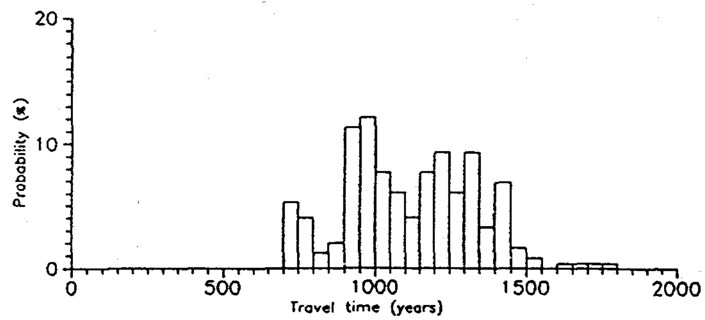

Figure 3d - Retarded travel times of ^{14}C particles from the repository to the atmosphere with particles released at 15000 years.

At 5,000 years, the heat spreads outward and temperature gradients become smaller within the mountain (Figure 4b). Note that the hot area moves upward from the repository toward the mountain surface as a result of convective heat flow. Particles released at this time travel through the mountain in 300 to 900 years (Figure 3b).

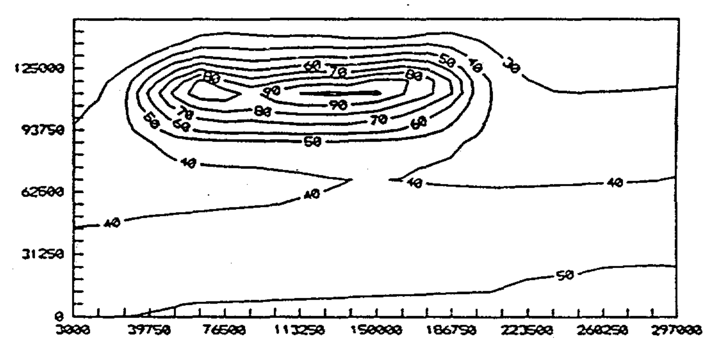

Figure 4a - Calculated temperature field at Yucca Mountain at 1000 years for cross section N765000. The unit for the temperature is °C.

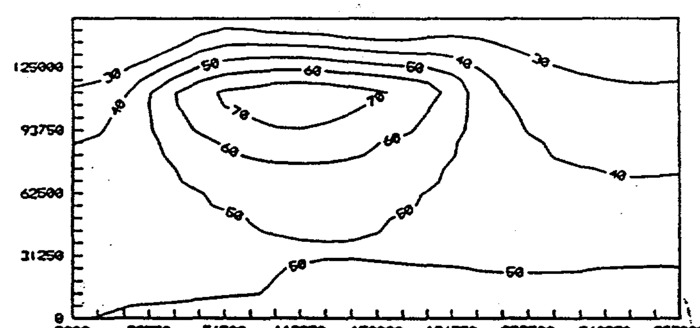

Figure 4b - Calculated temperature field at Yucca Mountain at 5000 years.

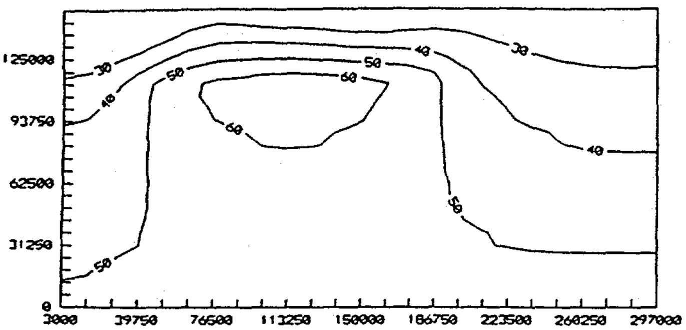

Figure 4c - Calculated temperature field at Yucca. Mountain at 10000 years.

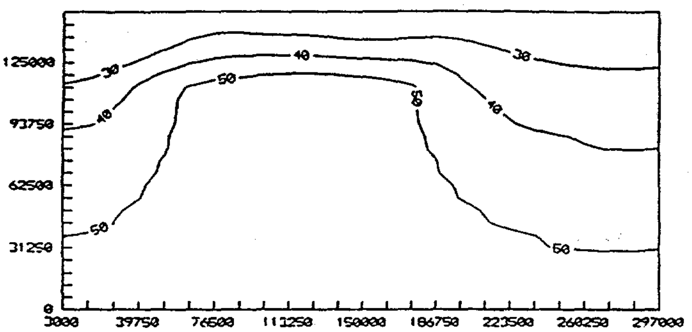

Figure 4d - Calculated temperature field at Yucca Mountain at 15000 years.

As the time reaches 10,000 years, the temperature field within the mountain becomes smoother (Figure 4c) and temperature gradients are smaller than at earlier times. Carbon-14 particles released at this time travel slower than particles released earlier. Travel times range from 500 to 1,200 years (Figure 3c)

Finally, we present the results when the waste has been emplaced 15,000 years. Less heat is being released from the repository, and the temperature and gas flow fields become more linearly distributed (Figure 4d). As time passes, gas velocity and temperature decrease and their magnitudes are much smaller than that at the earlier time. Particle travel times are slower and some of the particles can travel as long as 1,800 years before they escape from the mountain (Figure 3d).

The travel times calculated for later times are faster than those previously calculated.[10] This is due to the assumed emplacement of older waste at the same initial power density, leading to a larger mass density of waste in the repository. The heat output at late times depends on the mass density of the waste; thus, heat output and temperatures at these times are greater than in previous calculations.

CONCLUSIONS

The results from both verification and simulations show that TGIF2 is a reliable predictive model for mountain scale heat transfer and gas flow simulation. Both temperature and gas flow fields change dynamically through the simulation time. The thermal regime is found to be dominated by conduction in the early phase of the repository (several hundred years). As time passes, mountain-scale gas flow becomes more pronounced. After several thousand years, it starts to decline. During this active period, carbon-14 particles can move quickly through the mountain. The simulations indicate that carbon-14 travel time is on the order of several hundred to one or two thousand years, which is less than the 10,000-year regulatory period and the 5720-year half life of carbon-14.

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