SAND 95-2496C
CONF-951203--21 11-8-95

Near-Drift Thermal Analysis Including Combined Modes of Conduction, Convection, and Radiation

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I. Introduction

The performance of waste packages containing high-level nuclear wastes at underground repositories such as the potential repository at Yucca Mountain, Nevada, depends, in part, on the thermodynamic environment immediately surrounding the buried waste packages. For example, degradation of the waste packages can be caused by corrosive and microbial processes, which are influenced by both the relative humidity and temperature within the emplacement drifts. Gansemer and Lamont[1] cite a critical relative humidity of 70–75%, above which a water film may form on the container surface to initiate pitting and subsequent corrosion. Therefore, appropriate models of thermal and fluid transport near the waste package are necessary to predict the thermodynamic environment and performance of the waste packages. However, past models and simulations of the near-field at Yucca Mountain have made simplifying assumptions with regards to the thermal and fluid transport near the waste packages[2]. Convection in an empty drift is often ignored, and radiation from the waste packages to the drift wall is usually lumped into an effective thermal conductivity of the air surrounding the waste packages. In this paper, the effects of conduction, convection, and radiation are investigated for a heat-generating waste package in an empty drift. Simulations explicitly modeling radiation from the waste package to the drift wall are compared to simulations using only conduction. Temperatures, relative humidities, and vapor mass fractions are compared at various locations within the drift. In addition, the effects of convection on relative humidity and moisture distribution within the drift are presented.

II. Numerical Approach

The numerical code TOUGH2[3] (SNL Software Configuration Management v. 3.2) is used in the analyses. TOUGH2 is a multidimensional, multiphase, nonisothermal, porous media flow simulator that is used extensively in geothermal, environmental restoration, and nuclear waste management areas. The two-dimensional grid used in the analyses consists of a centralized element representing the waste package surrounded by elements representing the empty drift, all of which are bounded by elements representing a partially saturated tuffaceous rock (Figure 1). The heat output of the waste package is fixed at 1700 W, and its properties are specified to prevent advective and diffusive flux to or from the waste package. The drift elements surrounding the waste package have the properties of air and act as a capillary barrier to advective flux from the surrounding rock. The thermohydrologic properties of the tuffaceous rock elements are taken from reported values of the Topopah Springs welded unit at Yucca Mountain[2,4] (data from references [2] and [4] are unqualified). Boundary elements around the entire domain are maintained at a constant temperature of 20 °C, a relative humidity of 100%, and a zero permeability (no advective flux to or from the boundary). Initially, the system is set to a temperature of 20 °C and a relative humidity of 100%. The initial saturation of the tuff elements is set to 0.7.

A recent modification to TOUGH2[†] allows the code to model thermal radiation between any two connected elements. In order to model radiation from the waste package to the surrounding drift wall, additional connections had to be added between the waste package element and all of the tuff elements exposed to the waste package. Hottel's crossed-string method[5] was used to determine the configuration factors between each of the four radiating surfaces of the waste package element and the surfaces of the tuff elements facing the waste package. Only radiative heat transfer was allowed between these extra connections.

† The modified version of TOUGH2 that includes radiation is in the process of being entered into SNL Software Configuration Management

III. Results and Discussion

Simulations using the TOUGH2 model in Figure 1 were performed to compare the relative effects of conduction, convection, and radiation on the thermodynamic environment of the waste package for several years following emplacement. Simulations that explicitly modeled thermal radiation from the waste package to the drift wall showed lower and flatter temperature profiles within the empty drift when compared to simulations that used an effective thermal conductivity for the drift elements (Figure 2). This resulted in lower waste package temperatures but slightly higher relative humidities in the drift as a result of the lower temperatures. With regards to accuracy, the temperature profiles in the drift resulting from the thermal radiation simulations were more consistent than the conduction-only simulations when compared to analytical solutions of radiation through a non-participating medium with a low thermal conductivity. However, both simulations showed similar temperatures in the surrounding tuff elements (Figure 2). This similarity is a consequence of the relatively low thermal resistance of the drift elements as compared to the thermal resistance of the surrounding tuff elements. Since the properties and modes of heat transfer *of the tuff elements* were identical in the two simulations, the temperature profiles of the tuff elements were also similar.

The effects of buoyancy-driven gas-phase convection within the drift were investigated by specifying either a zero or a non-zero permeability of the drift elements. The simulations with a non-zero drift permeability (1×10^{-7} m^2)† showed that air convection lowered the temperatures slightly within the drift. Convection also increased the amount of water vapor within the drift by effectively redistributing the moisture from the adjacent tuff elements, in which vaporization was taking place, to the interior drift elements. These convective simulations resulted in significantly higher relative humidities near the waste package at early times (< 4 years) as a result of the lower temperatures and increased vapor mass fractions in the drift (Figure 3). However, when the

† Rigorously speaking, Darcy's law cannot be used to determine the velocity distribution caused by natural convection in an empty drift. Inertial terms in the full Navier-Stokes equation are neglected in Darcy's law and may play an important role in the velocity distribution. However, these effects are lumped into an effective permeability in this study to yield an approximate description of natural convection in the drift.

adjacent tuff elements that surrounded the drift dried ($S_l \rightarrow 0$), the relative humidities decreased dramatically to below "critical" levels, but still remained higher than those of the simulations without convection. The long-term trend of the relative humidity for the convective simulation is uncertain as a result of computational difficulties (small time steps) that inhibited the simulation at longer times.

IV. Conclusions

Simulations that explicitly modeled thermal radiation showed flatter and lower temperatures in the drift than simulations using an equivalent thermal conductivity. The use of thermal radiation models in this study can be readily extended to performance-assessment thermal calculations of the repository. Buoyancy-driven convection in the empty drift during early times (< 4 years following emplacement) resulted in high relative humidities near the waste package, but subsequent drying of the drift wall significantly reduced relative humidities to below "critical values".

Acknowledgments

This work was supported by the U.S. Department of Energy, Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project Office, under contract DE-AC04-94AL85000, WBS 1.2.5.4.6, WA-040, Rev. 2., QAGR 1.2.5.4.6 Rev. 00.

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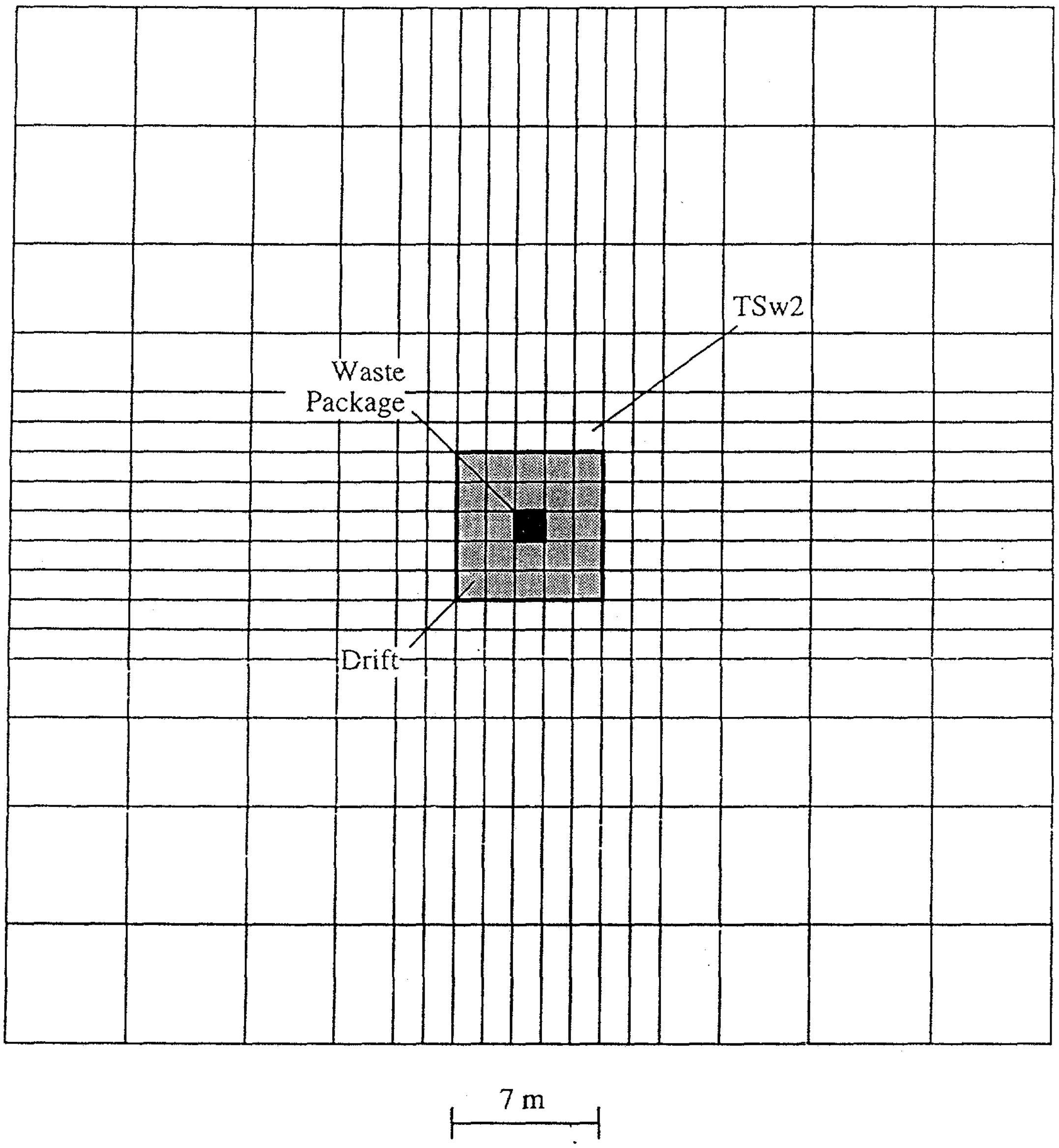
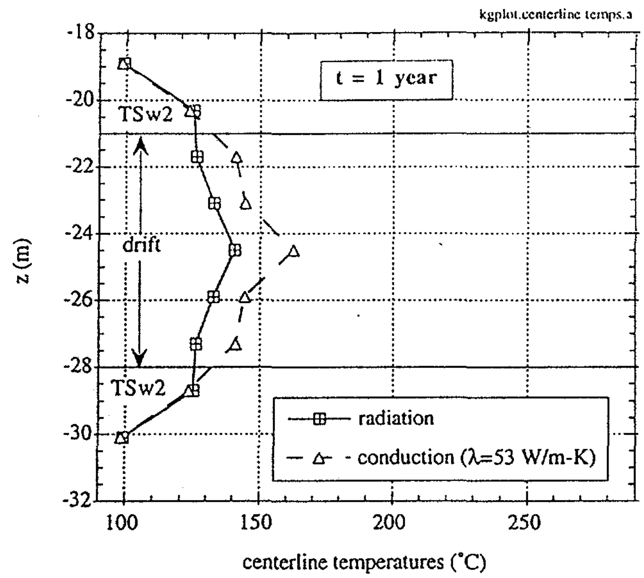
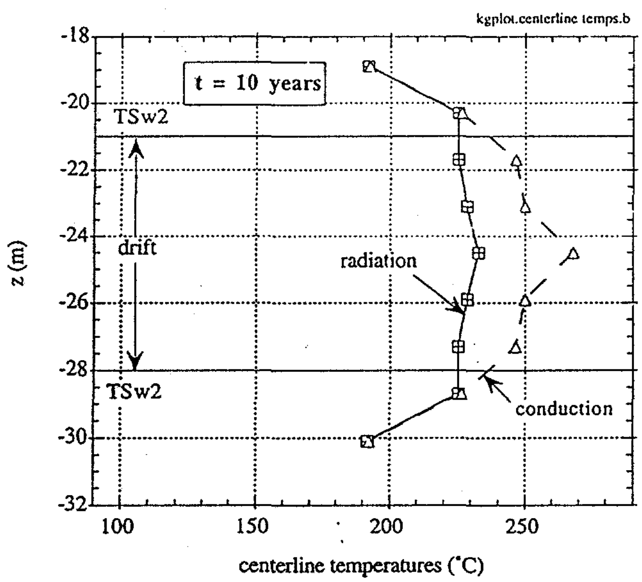


Figure 1. Near-drift thermal model. The boundaries of the domain are maintained at constant temperature, pressure, and air mass fraction. The output power of the waste package is 1700 W. The initial saturation of the TSw2 elements is 0.7, and the initial temperature is 20°C. The drift elements have the same properties of air.



(a)



(b)

Figure 2. Temperatures along a vertical transect through the waste package for simulations with radiation and conduction (no convection). An explicit radiation model is shown by the solid line, and an equivalent thermal conduction model is shown by the dashed line. The temperatures are given at a) 1 year and b) 10 years.

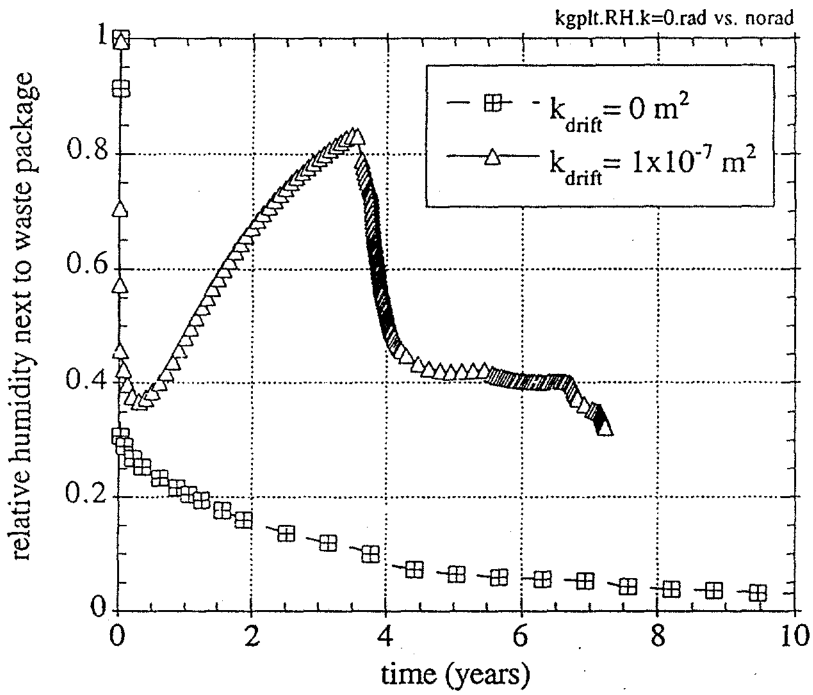


Figure 3. Relative humidity next to the waste package for simulations with and without convection in the drift (radiation and conduction exist). The sudden drop in relative humidity in the convection simulation corresponds to the dry-out of the element at the drift wall, which reduces the amount of water vapor available for recirculation by convection.

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