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# The Effects of Conduction, Convection, and Radiation on the Thermodynamic Environment Surrounding a Heat-Generating Waste Package



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## Abstract

The thermodynamic environment surrounding a heat-generating waste package can play an important role in the performance of a high-level radioactive waste repository. However, rigorous models of heat transfer are often compromised in near-drift simulations. Convection and radiation are usually ignored or approximated so that simpler conduction models can be used. This paper presents numerical simulations that explicitly model conduction, convection, and radiation in an empty drift following emplacement of a heat-generating waste package. Temperatures and relative humidities are determined at various locations within the drift. Comparisons are made between different models of heat transfer, and the relative effects of each heat transfer mode on the thermodynamic environment of the waste package are examined.

## 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 (1995) 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 heat 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 heat and fluid transport near the waste packages (Wilson et al., 1994). 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, which attempt to account for radiative heat transfer with an effective thermal conductivity. Temperatures and relative humidities 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.

## Numerical Approach

The numerical code TOUGH2 (Transport Of Unsaturated Groundwater and Heat; Pruess, 1991) (SNL Software Configuration Management v. 3.3) is used in the analyses. TOUGH2 is a multidimensional, multiphase, nonisothermal simulator that is used extensively in geothermal, environmental restoration, and nuclear waste management areas. Mass and energy balances are solved simultaneously using the integral finite difference method for air and water in porous media. The full details of the governing equations and the numerical code are given in Pruess (1987, 1991).

Simulations are performed to compare a TOUGH2 model that explicitly models radiation through the drift with a TOUGH2 model that uses only conduction in the drift. In addition, convection is turned on or off by specifying either a non-zero or zero permeability for the drift elements†. Table 1 summarizes the simulations that are performed in this study. The following sections describe the domain, the parameters, and some of the detailed pre-processing calculations required to run the different models.

### *Model Domain and Parameters*

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 (no backfill is assumed to exist in the drift in this study). The thermohydrologic properties of the tuffaceous rock elements outside of the drift are taken from reported values of the Topopah Springs welded unit at Yucca Mountain (Wilson et al.,1994; Pruess and Tsang, 1994; Incropera and DeWitt, 1985). Enhanced water vapor diffusion is assumed to exist in this region such that the product of the tortuosity, porosity, and gas phase saturation (used in the calculation of gas phase diffusion) is set equal to one. The rationale for the use of this constant is given in Jury and Letey

† Rigorously speaking, the use of a permeability in 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.

(1979). Boundary elements around the entire domain are maintained at a constant temperature of 20 °C, a relative humidity of 100%, a pressure of $1 \times 10^5$ Pa, and a zero permeability (no advective flux to or from the boundary). Initially, the system is set to a temperature of 20 °C, a relative humidity of 100%, and a pressure of $1 \times 10^5$ Pa The initial saturation of the tuff elements is set to 0.7. Table 2 summarizes the thermohydrologic parameters used in TOUGH2.

*View Factor Calculations for Radiation Simulations*

A recent modification to TOUGH2 allows the code to model blackbody thermal radiation between any two connected elements. The radiative heat transfer between two elements, $q_{rad}$, is given by the following equation:

$$q_{rad} = A_1 F_{1\text{-}2}\, \sigma (T_1^4 - T_2^4) \tag{1}$$

where $A_1$ is the area of the radiating surface, $F_{1\text{-}2}$ is a view factor that describes the fraction of emitted radiation from surface *1* that is received by surface *2*, $\sigma$ is the Stefan-Boltzmann constant ($5.67 \times 10^{-8}$ W/m$^2$-K$^4$), and $T_1$ and $T_2$ are the temperatures of surfaces 1 and 2, respectively.

Additional connections are added between the waste package element and all of the tuff elements exposed to the waste package to implement the radiative heat transfer in TOUGH2 (Runs 2 and 3). Hottel's crossed-string method (Siegel and Howell, 1981) is used to determine the view factors between the radiating surface of the waste package element and the surfaces of the tuff elements facing the waste package. Figure 2 shows an example of how the view factors are calculated for radiation between the right surface of the waste package element and the exposed surfaces of the surrounding tuff elements (symmetry is employed so only the top half of the drift is shown). The view factor for radiation between surface 1 (the waste package) and surface 2 (the exposed surface of one of the tuff elements) is calculated using Hottel's cross string method:

$$F_{1-2} = \frac{L_{ac} + L_{bd} - L_{ad} - L_{bc}}{2 A_1} \tag{2}$$

where $L$ is the distance between the two points designated by the subscripts (see Figure 2). Equation (2) conveniently expresses the view factor between any two elements as the sum of the "crossed strings" ($L_{ac} + L_{bd}$) minus the sum of the "uncrossed strings" ($L_{ad} + L_{bc}$) divided by twice the area of the radiating surface. Figure 2 shows the calculated view factors for five connections that can be used (as a result of symmetry) for all the connections between the waste package surfaces and the exposed tuff surfaces. Referring back to Figure 1, each of the four surfaces of the waste package element is exposed to (can "see") nine tuff elements. Therefore, 36 additional connections are added to the TOUGH2 input file to implement radiation exchange between the waste package and the tuff elements adjacent to the drift in Runs 2 and 3.

*Linearized Thermal Conductivity for Conduction-Only Simulations*

When radiation is not explicitly modeled (Run 1), a large effective radiative thermal conductivity is often assigned to the drift elements to represent the high heat transfer associated with radiation. The radiative thermal conductivity, $k_r$, is determined by linearizing equation (1) to express the radiative heat transfer as a function of a temperature difference rather than the difference between two temperatures to the fourth power:

$$q_{rad} = k_r (T_1 - T_2) / d \tag{3}$$

where

$$k_r = A_1 \sigma (T_1 + T_2)(T_1^2 + T_2^2) d \tag{4}$$

where $d$ is the distance between the radiating and receiving surfaces, and the view factor is set equal to one since we now consider the effective radiation from the entire waste package element to its surroundings. Equation (3) is in the same form as Fourier's law, so the total heat transfer through the drift can be modeled using conduction with the effective thermal conductivity of the drift elements being equal to the sum of the radiative thermal conductivity and the thermal conductivity of the drift elements. An inherent problem with this method is that the radiative thermal conductivity given by equation (4) is temperature dependent, making it a transient property. A rough approximation can be made by assuming a range of temperatures for the radiating and receiving surfaces and calculating an average radiative thermal conductivity using equation (4). For the purpose of calculating an average $k_r$, the average waste package temperature is assumed to be 473K and the temperatures of the tuff elements adjacent to the drift are assumed to vary between 293K and 473K, yielding an average radiative thermal conductivity of 53 W/m-K from equation (4). Since the thermal conductivity of the drift elements is small (~ 0.03 W/m-K for air), the effective thermal conductivity is approximately equal to the radiative thermal conductivity. This effective thermal conductivity is used in Run 1 where conduction is the only mode of heat transfer in the drifts. In Runs 2 and 3, where radiation is explicitly modeled, the thermal conductivity of air is used for the drift elements.

## Results

*Conduction-Only (Run 1) vs. Radiation (Run 2) (No Convection)*

Simulations that explicitly model thermal radiation from the waste package to the drift wall show lower and flatter temperature profiles within the empty drift when compared to simulations that use an effective thermal conductivity for the drift elements. Figure 3 shows the temperature profile along a vertical transect through the center of the waste package for the two models at one year and ten years following emplacement. Within the drift, the temperature gradient of the radiation model is very flat as a result of the efficient heat transfer from the waste package directly to the surrounding tuff elements that border the drift. Computationally, the radiative heat transfer bypasses the drift elements since connections are made directly between the waste package and tuff elements as shown in Figure 2 (the air in the empty drift is assumed to be a non-participating medium from a radiative standpoint). On the other hand, the conduction model requires heat to be conducted through the drift elements. Even though the thermal conductivity of the drift elements is quite large, the overall resistance to heat transfer is increased by the lower thermal conductivities of the waste package element and the tuff elements that border the drift. This causes sharp temperature gradients as shown in Figure 3 between the waste package element and the adjacent drift elements and between the outer drift elements and the bordering tuff (TSw2) elements.

It is also interesting to note that both models show similar temperatures in the surrounding tuff elements beyond the drift (Figure 3). 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. In both models, the heat transfer through the drift is enhanced by either radiation or (in the case of the conduction-only model) an effective thermal conductivity that attempts to account for radiation. Thus, from a global perspective, the heat transfer from the waste package is governed primarily by the thermal resistance of the tuff elements surrounding the drift. Since the properties and modes of heat transfer *of the tuff elements* are identical in both models, the temperature profiles in the tuff elements are also similar. This implies that when the effects of radiation are incorporated, either explicitly or approximately, both the conduction-only model and the radiation model yield similar temperature distributions in the tuff elements surrounding the drift as a result of the negligible resistance of the drift elements.

*The Effects of Convection (Run 3)*

The effects of buoyancy-driven gas-phase convection within the drift are investigated by specifying a non-zero permeability for the drift elements in Run 3. All three modes of heat transfer (conduction, convection, and radiation) are present in this model. The permeable drift elements allow natural convection to occur within the drift as shown in the plot of the gas-phase velocity vectors in Figure 4. Recall that the absolute values of the velocities may not be accurate as a result of the arbitrarily assigned permeability of the drift elements, but the general motion of the gas-phase should be well represented. Figure 5 shows that air convection lowers the temperatures slightly and produces more uniform temperatures within the drift than the results of the model without convection (Run 2). Note that the temperatures just below the waste package are depressed slightly below the temperatures just above the waste package. As warm air rises from the waste package, it cools as it circulates around the outside of the drift towards the bottom. Cooler air circulating back up towards the waste package therefore lowers the temperature in that region. However, the temperatures of the waste package and the surrounding tuff elements are nearly identical in the simulations with and without convection.

Convection also increased the amount of water vapor within the drift by effectively redistributing the moisture from the surrounding 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 6). However, when the tuff elements that bordered 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†. This implies that at early times, convection can substantially increase the relative humidity within the drift while liquid water is present in the adjacent tuffs.

## Conclusions

The thermodynamic environment surrounding a heat-generating waste package in an empty drift has been examined using different models of heat transfer. The major conclusions of this paper can be summarized as follows:

- Explicit modeling of radiative heat transfer (equation (1)) provides an effective means of heat transfer from the waste package to the drift wall. As a result, temperature gradients between the waste package and the drift wall tend to be small. Also, temperatures in the drift are generally lower than temperatures resulting from a conduction-only model.
- Both the equivalent conduction model, which approximates the effects of radiation, and the explicit radiation model yielded similar temperature profiles in the tuff surrounding the drift. This implies that the thermal resistance of the empty drift is negligible in both models when compared to the thermal resistance of the surrounding tuff. The use of the equivalent conduction model in larger site-scale models should therefore be suitable.
- Convection can significantly increase the relative humidity near the waste package at early times by redistributing moisture from the adjacent tuffs (where volatilization is occurring) to the waste package. When the drift wall dries, however, circulation and redistribution of the moisture are curtailed, significantly reducing the relative humidities to below "critical" levels.

† 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.

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Table 1. Summary of numerical simulations performed with TOUGH2.

| | Heat Transfer Modes in the Drift |
|---|---|
| Run 1 | Conduction Only† |
| Run 2 | Conduction and Radiation |
| Run 3 | Conduction, Convection, and Radiation |

†An effective thermal conductivity is used to approximate radiative heat transfer

Table 2. Thermohydrologic parameters used for each of the element materials in the TOUGH2 model (Wilson et al., 1994; Pruess and Tsang, 1994; Incropera and DeWitt, 1985; these data are unqualified).

| | heater | air | tuff (TSw2) |
|---|---|---|---|
| rock grain density ($kg/m^3$) | 8000 | — | 2480 |
| porosity ($m^3$ pore/$m^3$ total) | 0.0 | 1.0 | 0.139 |
| permeability ($m^2$) | 0.0 | 0.0 or $1x10^{-7}$ | $2.1x10^{-18}$ |
| wet thermal conductivity (S=1) (W/m-K) | 15.0 | 0.03 | 2.34 |
| dry thermal conductivity (S=0) (W/m-K) | 15.0 | 0.03 | 1.9 |
| specific heat (J/kg-K) | 475 | 1000 | 840 |

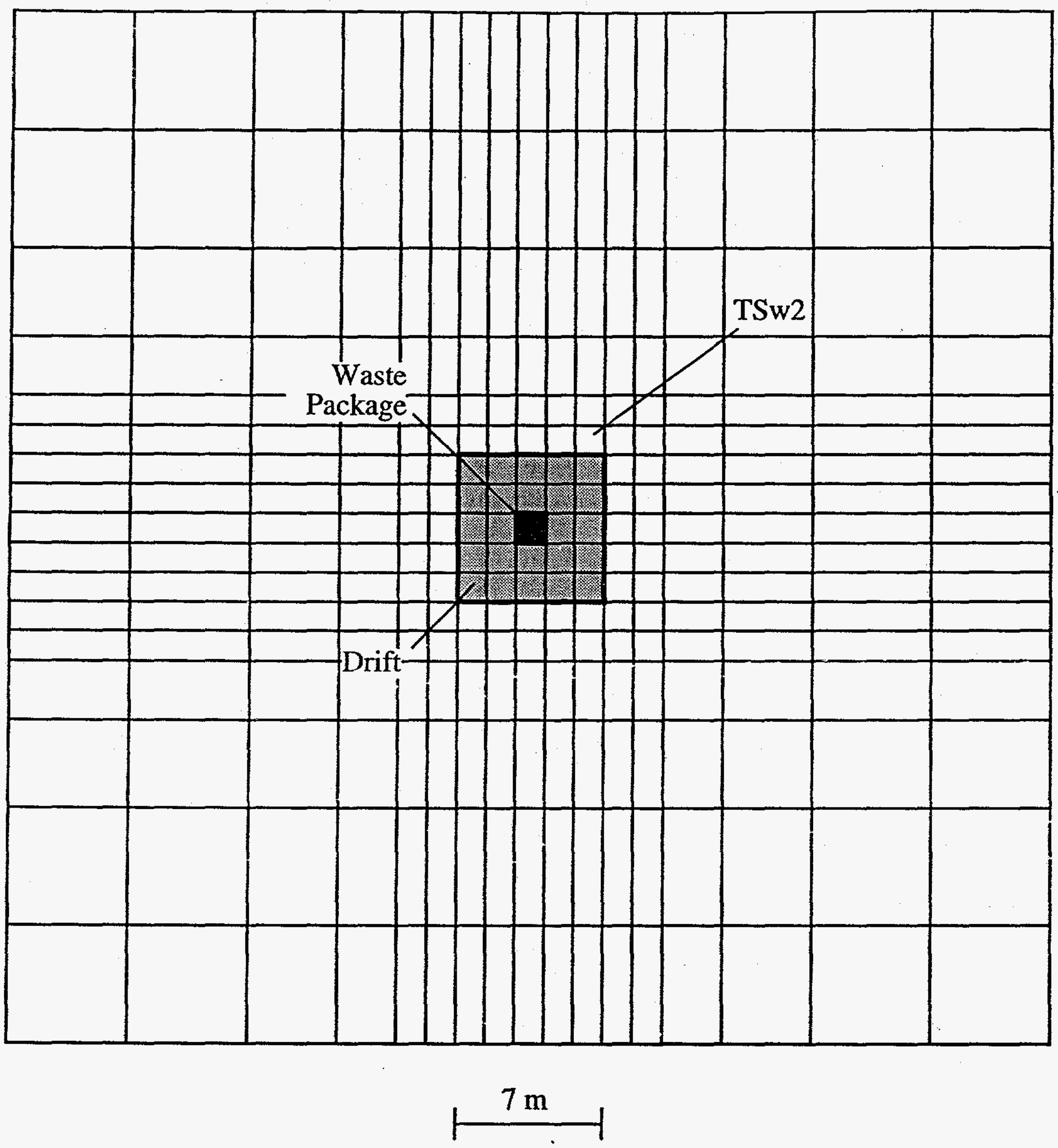


Figure 1. Grid used in TOUGH2 models. The boundaries of the domain are maintained at constant temperature, pressure, and air mass fraction. The output power of the waste package is 1700 W. The initial saturation of the TSw2 elements is 0.7, and the initial temperature is 20°C. The drift elements have the same properties of air.

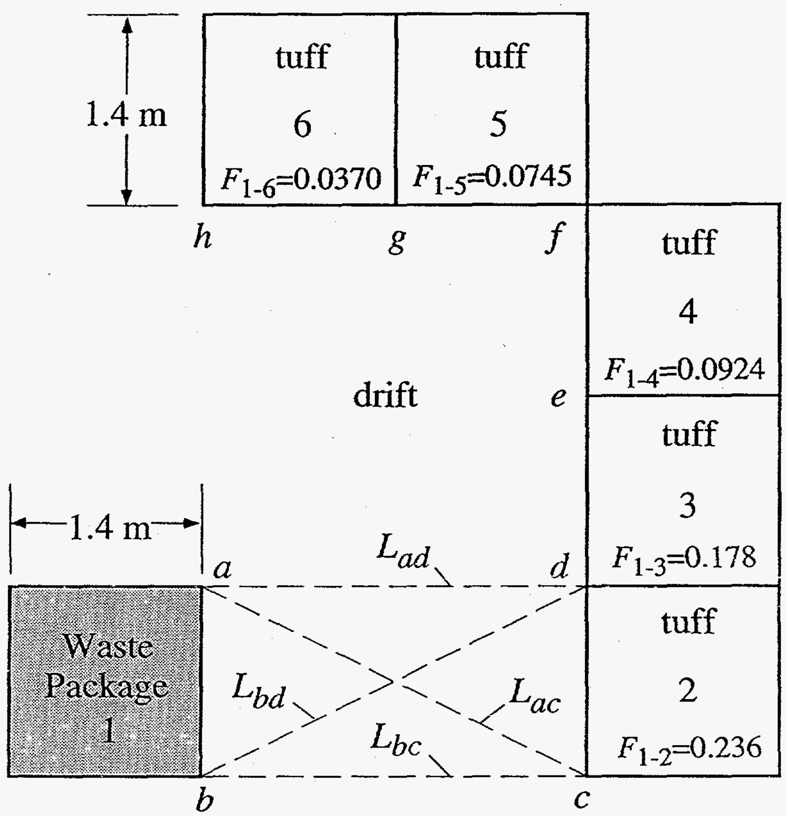


Figure 2. An expanded view of the upper-right quadrant of the drift. The view factor, $F_{1-2}$, for radiation exchange between elements 1 and 2 is calculated using equation (2). The remaining view factors are calculated in a similar fashion. By symmetry, all other view factors can be obtained from one of the five shown above.

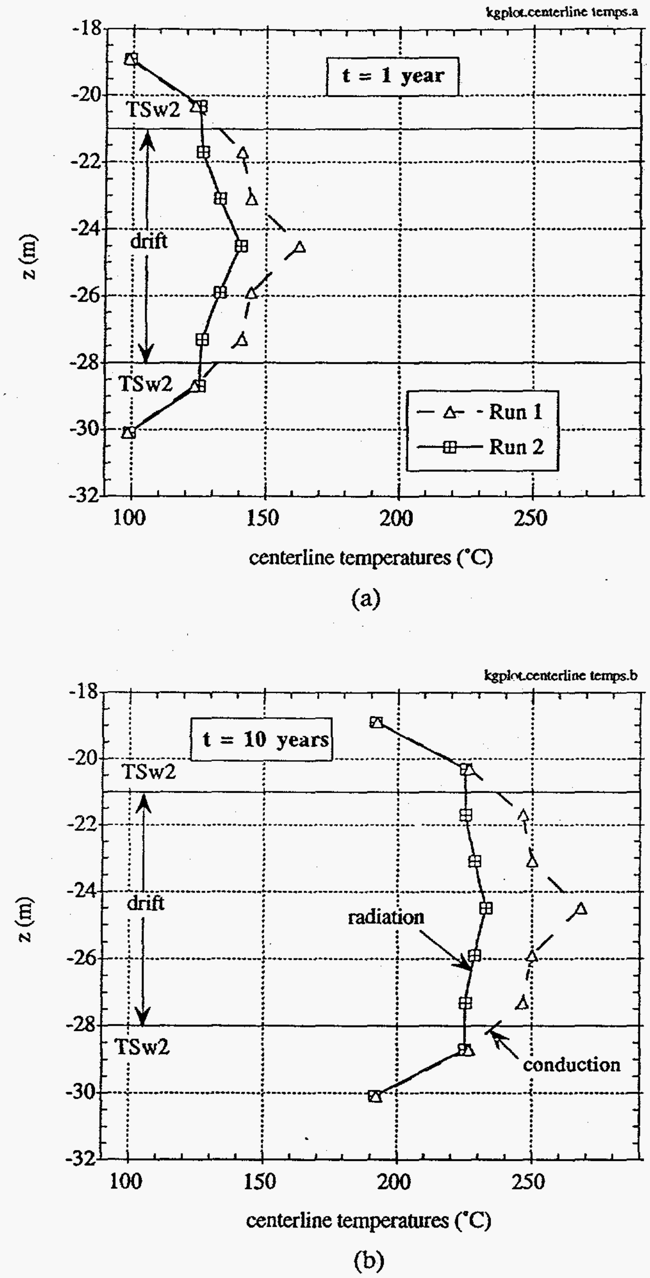


Figure 3. Temperatures along a vertical transect through the waste package for Runs 1 and 2. An explicit radiation model is shown by the solid line, and an equivalent thermal conduction model is shown by the dashed line. The temperatures are given at a) 1 year and b) 10 years following emplacement.

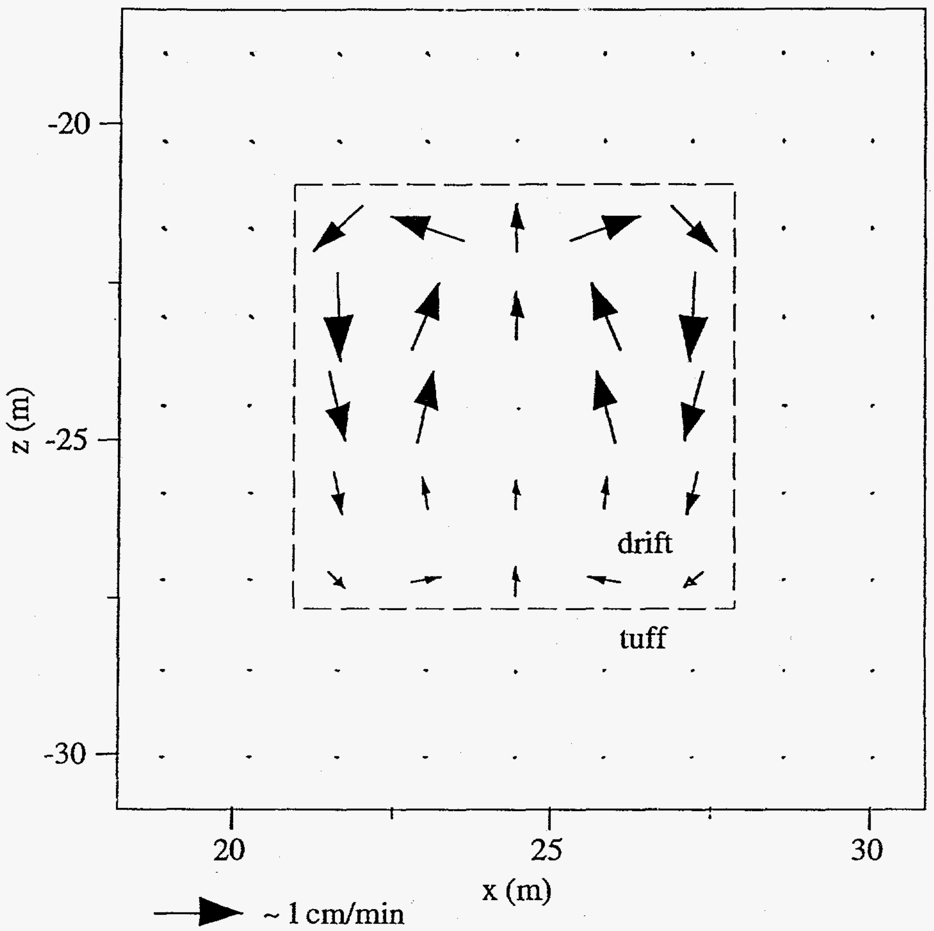


Figure 4. Gas-phase velocity vectors in and near the drift at one year following emplacement of a heat-generating waste package in the center of the drift. The outline of the drift is shown by a dashed line.

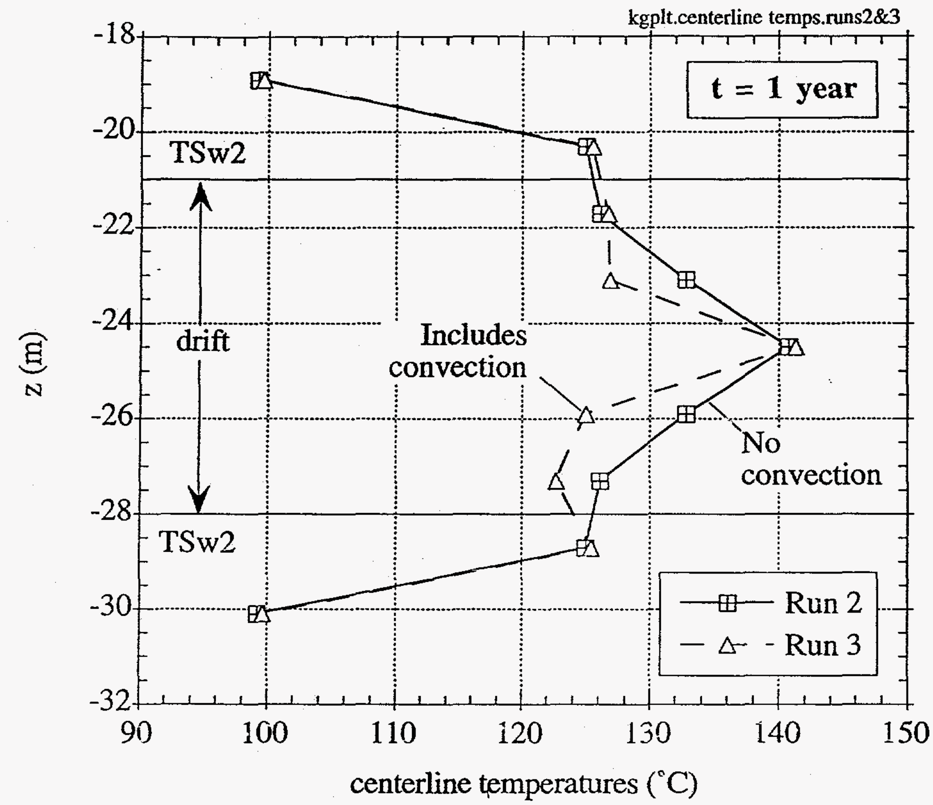


Figure 5. Temperatures along a vertical transect through the waste package for Runs 2 and 3 at one year following emplacement of a heat-generating waste package into an empty drift.

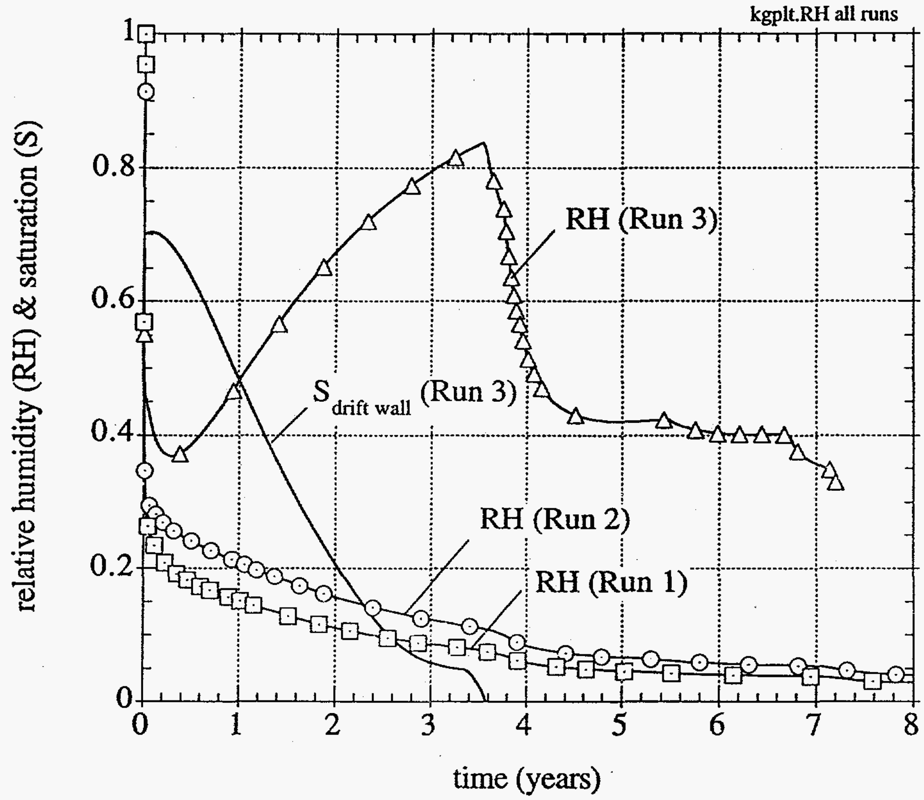


Figure 6. Relative humidities of the drift element just above the waste package element for Runs 1, 2, and 3. The saturation of the tuff element directly above the waste package element is also shown as a function of time for Run 3. Note the sharp decrease in the relative humidity of Run 3 when the drift wall dries.