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TITLE  Simulation of Heat Transfer in the Unsaturated Zone

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Simulation of Heat Transfer in the Unsaturated Zone

George Zyvoloski

Introduction

It is well known that heat transfer can play an important role in fluid flow near the emplacement site of high-level nuclear waste (Pruess and Wang, 1987). Heat transfer effects on far-field flow have received much less attention. The effects, though less dramatic than near-field effects, nevertheless can be important in understanding net moisture fluxes above the repository zone. Weeks (1987) described two wells at the Yucca Mountain site that produce air at high flow rates in winter. It was postulated that convection in the unsaturated zone was responsible for this movement. If this is so, then the convection could provide a mechanism for drying the rock above the repository zone and thus provide a buffer for heavy rainfall events. In addition, the convection would increase the movement of gaseous radionuclides such as $^{14}$CO$_2$, tritiated water vapor, and $^{129}$I (Weeks, 1987). Because of the complexity of the problem, numerical models were required to calculate gas flow and vapor transport at the site.

Kipp (1987) previously modeled this problem using the code LIST3D. This code represents the flow of a single-phase fluid with both heat-and mass-transfer effects included. Water density and partial pressure effects are accounted for by the virtual temperature method [List (1966)]. In this paper, the problem was simulated using the code FEHMN, a finite-element heat-and mass-transfer code being developed for the Yucca Mountain Project at Los Alamos National Laboratory. Besides aiding in the understanding of the problem described above, the work described in this paper was done in preparation of the upcoming problem to be formulated for the Performance Assessment Calculation Exercise (PACE).

The Model

FEHMN models the flow of heat and mass in a saturated or unsaturated porous media. The conservation of mass is expressed by the equation
\[
\frac{\partial A_m}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{F_m} + q_m = 0 ,
\]

where the mass per unit volume, \(A_m\), is given by

\[
A_m = \phi(S_v \rho_v + S_\ell \rho_\ell) ,
\]

and the mass flux \(\overrightarrow{F_m}\) is given by

\[
\overrightarrow{F_m} = \rho_v \overrightarrow{V_v} + \rho_\ell \overrightarrow{V_\ell} .
\]

Here \(\phi\) is the porosity of the rock matrix, \(S_v\) and \(S_\ell\) are the phase saturations, \(\rho_v\) and \(\rho_\ell\) are the phase densities, and \(\overrightarrow{V_v}\) and \(\overrightarrow{V_\ell}\) are the phase velocities. The subscripts \(v\) and \(\ell\) refer to the vapor and liquid phases respectively. The source or sink terms are represented by \(q_m\). The conservation of energy is expressed by the equation

\[
\frac{\partial A_\varepsilon}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{F_\varepsilon} + q_\varepsilon = 0 ,
\]

where the energy per unit volume is given by

\[
A_\varepsilon = (1 - \phi)\rho_r u_r + \phi(S_v \rho_v u_v + S_\ell \rho_\ell u_\ell) ,
\]

and the energy flux \(F_\varepsilon\) can be written as

\[
F_\varepsilon = \rho_v h_v \overrightarrow{V_v} + \rho_\ell h_\ell \overrightarrow{V_\ell} + K \overrightarrow{\nabla} T .
\]

Here \(T\) is the temperature; \(u_r, u_v,\) and \(u_\ell\) are specific internal energies; and \(h_v\) and \(h_\ell\) are specific enthalpies. In addition to the subscripts previously mentioned, \(r\) refers to the rock matrix. The energy contributed from sources is given by \(q_\varepsilon\). \(K\) is the effective thermal conductivity. This parameter is difficult to establish as it depends not only on rock type and porosity, but also on the saturation value. A major assumption used in the energy equation is thermal equilibrium between the phases and the rock. The slow flow rates justify this assumption. In addition to the total mass and energy conservation equations, an air conservation equation is also required. This equation may be written as
where the air mass per unit volume, \( A_c \), is given by

\[
A_c = \phi(S_v \eta_v \rho_v + S_t \eta_t \rho_t)
\]  

and the air mass flux is given by

\[
\overline{F}_c = \rho_v \eta_v \overline{V}_v + \rho_t \eta_t \overline{V}_t
\]

where \( \eta_v \) and \( \eta_t \) are the mass fractions of air in the vapor and liquid phases respectively. The source term for air is given by \( q_c \). For the present analysis, we have neglected vapor-air diffusion and Knudsen effects, which can be important in other applications. Darcy's law provides the momentum equations to complete the description of the mass and energy flows:

\[
\overline{V}_v = \frac{k R_v}{\mu_v} (\nabla P_v + \rho_v \vec{g})
\]

and

\[
\overline{V}_t = \frac{k R_t}{\mu_t} (\nabla P_t + \rho_t \vec{g})
\]

Here \( k \) is the intrinsic rock permeability, \( R_v \) and \( R_t \) the relative phase permeabilities, \( \mu_v \) and \( \mu_t \) the phase viscosities, \( \rho_v \) and \( \rho_t \) the phase pressures, and \( \vec{g} \) is the acceleration of gravity. The phase pressures are related by the capillary pressure, \( P_{cap} \):

\[
P_v = P_t + P_{cap}
\]

Substituting the velocity expression into the conservation equations, a set of diffusion-like equations is obtained. It is these equations that are solved in FEHM-N.

The conservation equations contain many terms that require constitutive relationships. The rules governing the mixtures of air and water vapor will not be covered here, the reader is referred to Zyvoloski (1988) for details. The water properties themselves
are obtained by rational polynomial fits to National Bureau of Standards (NBS) steam table data. Air properties were represented by polynomials and the perfect gas law. The capillary pressure and the relative permeabilities are usually strongly nonlinear functions of the saturation. In this study, however, we allow only the gas phase to flow, so at least for now, the functional dependence of the capillary pressure and the relative permeabilities are irrelevant.

The conservation equations are discretized with a nodal-based finite-element method and are formulated with an implicit time-stepping scheme. A Preconditioned Conjugate Gradient method is used to solve the equations. For details on the numerical procedures, the reader is referred to Zyvoloski (1988).

The code also has provisions to model tracer transport with velocities provided by the flow portion of the code. In this study, no transport calculations were made. The reader will find a brief description of the transport capability of FEHM in Zyvoloski (1988).

Simulation Studies

Weeks (1987) presents a cross section of the region of interest in Yucca Mountain. This is reproduced in Fig. 1. Evident in the figure are the two wells, UZ-6 and UZ-6S. These wells have been observed to flow at 3 m/s in the winter. With these air velocities and using the observed exit air temperature of 18°C, UZ-6 and UZ-6S were discharging 560 l/d and 125 l/d respectively of water. An idealized 2-D model of the shaded region in Fig. 1 is shown in Fig. 2 where the left boundary is the side of the mountain.

The grid in the figure is similar to that used by Kipp (1987). It contains 400 nodes. The input parameters for the 2-D calculation are shown in Table 1. The boundary temperatures shown in Table 1 were season averages and were taken from Kipp.

Figure 3 shows the result of the 2-D simulation without a borehole. The pattern of flow for summer and winter are similar to those obtained by Kipp. The maximum velocities obtained by Kipp were several times larger than those obtained in this study. The spring and fall velocities were at least an order of magnitude smaller than summer and winter velocities. The flow patterns for spring and fall were qualitatively different than Kipp's results. These seasons produce pressure distributions along the mountain face similar to
Fig. 1. Cross section of Yucca Mountain in the vicinity of wells UZ-6 and UZ-6S. (Reprinted with permission from AGU monograph 42.)

Specified T,P

Specified Heat Flow

Fig. 2. Idealized 2-D model of Yucca Mountain for numerical computations.
Fig. 3. Velocity vector field for 2-D simulation with no wellbore. A vector 50 m long is equivalent to $10^{-3}$ m/s.
TABLE I. Input Parameters for 2-D Calculation

Geometry:
- Reservoir Size: 500m (x), 150m (y)
- 20 nodes x direction (graded)
- 20 nodes y direction (graded)

Rock Properties:

<table>
<thead>
<tr>
<th></th>
<th>Soil Layer</th>
<th>Welded Tuff</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability</td>
<td>1.e-11 m²</td>
<td>1.e-10 m²</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.25</td>
<td>0.10</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>1000. kj/kg/K</td>
<td>1000. kj/kg/K</td>
</tr>
<tr>
<td>Density</td>
<td>2000. kg/m³</td>
<td>1300. kg/m³</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.75 W/m/K</td>
<td>2.25 W/m/K</td>
</tr>
</tbody>
</table>

Fluid Properties:
- Water: Given by rational polynomial fits to NBS steam table data
- Air: Polynomial fits perfect gas law, Henry's law

Boundary Conditions:
- Specified temperature and pressure on surface A
  - Spring: \( T = 20°C, p = 0.085 \text{Mpa} + \text{hydrostatic} \)
  - Summer: \( T = 30°C, p = 0.085 \text{Mpa} + \text{hydrostatic} \)
  - Fall: \( T = 20°C, p = 0.085 \text{Mpa} + \text{hydrostatic} \)
  - Winter: \( T = 10°C, p = 0.085 \text{Mpa} + \text{hydrostatic} \)
- Heat Flux: 0.075 W/m² on surface B
- No fluid or heat flow on surface C

Initial Conditions:
- Pressure is hydrostatic
- Temperature varies as 0.03° k/m
- Saturation: 0.1 (irreducible)

those inside the mountain. Small differences in density, resulting from the different ways in which the saturated air densities are calculated, could produce the different character of flow in the two studies. This discrepancy is currently being investigated. The temperature contours are given in Fig. 4. The contours reflect the seasonal temperature boundary conditions. The small hump on the \( T = 24°C \) contour is a numerical artifact of the small
zoning in that region. An additional 2-D model run was made with a crude model of a wellbore the size of UZ-6. It was placed 60 m from the left boundary. While it is difficult to represent a wellbore in the 2-D cartesian grid (we are averaging across the mountain), we can still get some idea of the induced upward velocity due to the implacement of a well. Using the expected 3-m/s wellbore velocity, appropriate air properties, 1.8 Pa/m pressure drop for turbulent flow [reported by Weeks (1987)], and equivalent darcy permeability of $2 \times 10^{-5}$ m$^2$ was obtained. This large permeability produced numerical difficulties (i.e., smaller time steps) so $10^{-6}$ was used instead. The seasonal velocity vector plots are presented in Fig. 5. In addition to the increased velocities in the wellbore region, the wellbore appears to curtail vapor movement interior to the wellbore. Maximum velocity occurred in the wellbore was $10^{-2}$ m/s upward flow in the winter. If the permeability were increased to the proper value, this velocity would likely increase to order $10^{-1}$ m/s, still an order of magnitude slower than the observed rate. Temperature changes induced by the wellbore were only slight and are not shown.

The 2-D model lacks information on the lateral flow from the side of Yucca Mountain as well as any 3-D flow effects. To help understand these phenomena, a simple 3-D representation of the region around wells UZ-6 and UZ-6S was constructed. This is shown in Fig. 6. There were 3740 nodes in this problem: 20 in the $z$ direction, 11 in the $y$ direction, and 17 in the $z$ direction. The boundary and initial conditions are the same as for the 2-D calculations with the exception that the pressure and temperature boundary conditions are applied to three sides and the top instead of just the left face and the top as in the 2-D calculations. The results for the 3-D run without a wellbore is presented in Fig. 7. Shown in the figure is a vertical slice of Yucca Mountain in the center of the calculation region. Comparing Fig. 7 with Fig. 3, it can be seen that the 3-D results are qualitatively different than the 2-D results. While the 2-D results show much of the gas exiting the side of the mountain during the spring, summer, and fall, the 3-D results show the flow going toward the center of the mountain. The temperature results given in Fig. 8 show smoother contours than the corresponding 2-D case (even taking into account the differing scales of the two figures). Introducing a wellbore the size of UZ-6 into the grid (with a permeability of $10^{-7}$ m$^2$) produced some very interesting results. The results are
Fig. 4. Temperature contours for the 2 D simulation with no wellbore.
Fig. 5. Velocity vector field for the 2-D simulation with a wellbore. A vector 50 m long is equivalent to $10^{-3}$ m/s.
Fig. 6. Idealized 3-D model of Yucca Mountain for numerical computations.
Fig. 7. Velocity vector field for an \( z \) \( z \) slice in center of simulation region. A vector 50 m long is equivalent to \( 10^{-5} \) m/s.
Fig. 8. Temperature contours for the 3-D simulation.
Fig. 9. Velocity vector field for an $x-z$ slice in the center of the simulation region. A vector 50 m long is equivalent to $10^{-2}$ m/s.
presented in Fig. 9 show that the effect of the wellbore was quite dramatic. Velocities in the wellbore during winter were $2 \times 10^{-5}$ m/s. As with the 2-D simulation, a smaller permeability was used for the numerical calculations. Increasing the permeability to the wellbore value of $2 \times 10^{-5}$ would likely produce velocities of $\sim 0.5$ m/s. Once again the 3-D flows were qualitatively different than the 2-D flows. As expected, the winter flows were more evenly spread throughout the mountain with the 3-D model than with the 2-D model.

Remarks

1. While the runs presented here did not produce the observed flow rates, they did come close. It was noticed that by making the ratio of horizontal-to-vertical permeability larger, more gas would enter the wellbore. This would occur at Yucca Mountain if the wellbores intersected large, nearly horizontal fractures. Simulations of this phenomena are presently being performed.

2. Due to the deep circulation patterns observed in the simulation, an expansion of the grid in the vertical direction is warranted.

3. As the model is capable of simulating multiple-phase flow, rainfall can also be included. The interaction of convection and moisture movement could be evaluated.

4. Moisture fluxes from the top of Yucca Mountain will be evaluated in the future as well as temperatures inside the well.

5. The 3-D simulation (3 unknowns/node, 3470 nodes, 219 timesteps) took about 50 minutes of CPU time on the CRAY XMP computer.

Conclusions

A numerical model capable of describing the flow of heat, mass and air in a variably saturated porous and fractured media has been described. Simplified 2-D and 3-D simulations of the gas flow near the wells UZ 6 and UZ 6S were run. The 2-D results matched those of Kipp, and the 3-D results provided insight into the real gas flow in Yucca Mountain. The simplified model was not able to closely match the observed flow in well UZ 6. Simulations with more realistic geometries and properties are needed to evaluate the effect of convection as a moisture barrier and a transport mechanism for gaseous radionuclides.
Acknowledgement.

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The software documented in this report was not verified, validated, or otherwise subjected to the controls of a Yucca Mountain Project Office-approved quality program.

References


