STUDIES OF NON-ISOTHERMAL FLOW IN SATURATED AND PARTIALLY SATURATED POROUS MEDIA

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ABSTRACT

Physical and numerical experiments have been performed to investigate the behavior of non-isothermal flow in two-dimensional saturated and partially saturated porous media. The physical experiments were performed to identify non-isothermal flow fields and temperature distributions in fully saturated, half-saturated, and residually saturated two-dimensional porous media with bottom heating and top cooling. Two counter-rotating liquid-phase convective cells were observed to develop in the saturated regions of all three cases. Gas-phase convection was also evidenced in the unsaturated regions of the partially saturated experiments. TOUGH2 numerical simulations of the saturated case were found to be strongly dependent on the assumed boundary conditions of the physical system. Models including heat losses through the boundaries of the test cell produced temperature and flow fields that were in better agreement with the observed temperature and flow fields than models that assumed insulated boundary conditions. A sensitivity analysis also showed that a reduction of the bulk permeability of the porous media in the numerical simulations depressed the effects of convection, flattening the temperature profiles across the test cell.

I. INTRODUCTION

Coupled thermal and hydrologic flow processes in unsaturated fractured rock are important in the evaluation of Yucca Mountain as a potential repository for high level nuclear waste. High temperatures induced by the waste can mobilize the liquid and vapor phases either towards or away from the heated regions. Since the possibility of radionuclide release is potentially enhanced if mobile water contacts the radioactive waste\(^1\), understanding the behavior of these thermally
induced flows is of particular importance. While the physics of thermally induced flow in saturated systems is reasonably well understood, the behavior of thermally induced two-phase flow has only recently been considered.\textsuperscript{2}

Several models and numerical codes such as TOUGH\textsuperscript{2}\textsuperscript{3} have been used to investigate two-phase thermohydrologic conditions near potential nuclear waste repositories.\textsuperscript{4,5,6,7} However, very few of these models have been compared with laboratory or field scale studies. Reda\textsuperscript{8} performed natural convection experiments in a liquid saturated cell that were later modeled by Moridis and Pruess\textsuperscript{9} using TOUGH, but flow fields were not identified. Green et al.\textsuperscript{10} performed two-dimensional, partially saturated, non-isothermal flow experiments with a simulated fracture within the porous matrix, but they were unable to replicate the experimental results with TOUGH simulations.

Well-controlled experimental studies of non-isothermal flow in porous media in the laboratory and in the field are required to 1) identify processes important to thermal and hydrologic transport and 2) test the validity of existing models at the given experimental scale. Such studies should be conducted in a variety of materials ranging from non-fractured to fractured porous media and should span a variety of scales and dimensions. Currently, preparations for a field scale experiment are in progress near Yucca Mountain in a large fractured block of Topopah Spring Tuff.\textsuperscript{11} Complementary laboratory scale experiments within the same material are also being planned. As a preliminary to these experiments in fractured tuff, we begin fundamental numerical and physical experimentation in a simple non-fractured system composed of a vertical, two dimensional, thin sand slab heated from below and cooled at the top. Combined physical and numerical experimentation in simple systems such as this allows development of experimental techniques and understanding that aids in the design of more complicated experiments that will be conducted in fractured tuff.\textsuperscript{12}

In this paper we first present the results of a saturated non-isothermal flow experiment in uniform sand. Comparisons with numerical simulations assuming either insulated or heat-loss boundary conditions show the importance of including heat loss from the test cell to properly model the physical experiment. Further numerical analyses also reveal the sensitivity of the results to changes in bulk permeability as well as heat losses. The results of two additional experiments conducted in our system under unsaturated conditions are also presented. These experiments indicate that convective cells form in the partially saturated regions as well as the saturated regions of the experiment. Finally, conclusions and a brief description of future work are presented at the end of this paper.
II. EXPERIMENTAL APPROACH

A schematic of the experimental apparatus is shown in Figure 1. A square "two-dimensional" test cell (26 cm high x 26 cm wide x 1.3 cm deep) was constructed with clear Lexan plates. The front and back of the cell consisted of Lexan panels 1.3 cm thick bordering the entire face of the cell. The left and right sides of the cell were bordered by 1.3 cm thick Lexan spacers (each approximately 3 cm wide) positioned between the front and back panels. The bottom of the cell consisted of a thin aluminum strip placed directly above a heating element to provide a constant hot temperature boundary condition. The top of the cell was maintained at a cool temperature by a heat exchanger composed of an aluminum manifold through which cool tap water flowed. The manifold also acted as a lid which could be removed for the emplacement of sand. Ports were located at the top and bottom of the cell, serving as filling and draining points for water. Three horizontal rows of ten K-type thermocouples were spaced equally (2.54 cm apart) along the bottom (0.64 cm), middle (13 cm), and top (26 cm) of the test cell. Each thermocouple was inserted to touch the inner surface of the cell and was mounted with epoxy. Four K-type thermocouples were also spaced equally along the length of the top heat exchanger and bottom electrical heating element. Midway between each thermocouple on the front face of the test cell a dye port was drilled and filled with silicone. Dye was injected through these ports so that flow patterns could be observed as the dye propagated from the point of injection.

Following calibration of the thermocouples in a water bath, the test cell was filled with 14-20 mesh sand (mean particle diameter ~ 1 mm). The cell was then filled from the bottom to fully saturate the system with de-ionized water. The bottom heater was set to achieve a temperature of 90 °C, and the top heat exchanger was maintained at an ambient temperature near 23 °C. The data acquisition system recorded thermocouple voltages at 1 minute or 5 minute intervals. The system was allowed to reach steady-state conditions, which were determined to exist when constant temperature profiles were attained. Blue dye was then injected manually into the dye ports with a hypodermic needle (gauge 25) starting with the outermost ports on a row and moving inward to the central port. The needle was inserted until it hit the far face and then withdrawn approximately half way. Approximately 2 minutes were required to inject the dye in an entire row. After the dye was injected, 35 mm photographs were taken at periodic intervals to trace the movements of the concentrated dye solute and calculate approximate flow velocities. Subsequent to the saturated test, two unsaturated tests following the same procedure were conducted.

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III. NUMERICAL APPROACH

The numerical code TOUGH2 was used to simulate the non-isothermal flow behavior observed in the saturated experiment. TOUGH2 (Transport Of Unsaturated Groundwater and Heat) is a numerical code developed by Pruess\textsuperscript{3} to model the coupled transport of air, water, vapor, and heat in porous media. It is quite similar to its predecessor, TOUGH\textsuperscript{13}, and includes additional transport modeling capabilities as well as automated mesh generating features. The mathematical formulation used in TOUGH2 can be found in Pruess\textsuperscript{3} and will not be presented here.

A critical step in interpreting thermally induced flow experiments conducted in the laboratory is to determine the boundary conditions of the experiment. The design of a truly two-dimensional experimental system for both heat and fluid-phase transport that allows measurement of temperature, saturation, and velocity fields is non-trivial. Heat loss from "two-dimensional" system boundaries can create three-dimensional behavior which obscures proper interpretation. Although we are ultimately interested in non-isothermal flow behavior in two-phase systems, we only attempt to simulate our designed experimental system under saturated conditions since the physics of thermally induced saturated flow are less ambiguous. Once the effects of heat loss and other system parameters are well understood, simulations of the partially saturated experiments will be performed.

To evaluate the effects of heat loss through the boundaries of the experimental apparatus, three grids have been used in the numerical simulations. The first, shown in Figure 2(a), assumes insulated conditions on all sides of the apparatus, resulting in a two-dimensional model. The second grid allows for heat loss through the left and right sides of the apparatus, as shown in Figure 2(b), but the front and back faces remain insulated. In the third grid shown in Figure 2(c), heat loss is allowed through all boundaries, resulting in a three-dimensional model. The sand elements in the 'heat loss' models are bordered by Lexan elements simulating the frame of the apparatus. Adjacent to the Lexan elements are air elements which represent a boundary layer that buffers the heat loss to the surrounding ambient boundaries. The thickness of the "air" elements (0.5 cm) were chosen to yield an effective heat flux from the Lexan elements based on a correlation for natural convection from a heated vertical plane with air as the buoyant fluid.\textsuperscript{14} Note that Figure 2(c) shows only half of the test domain (the back half) due to the assumed symmetry of the test cell. As initial conditions, the temperature of the domain was taken to be uniform at an ambient temperature of 23 °C, and the pressure distribution was specified according to hydrostatic conditions. For times greater than zero, the temperature of the upper and lower boundaries were maintained at 23 °C and 90 °C, respectively. The properties of the different elements used in the grids are summarized in Table 1 and were obtained experimentally unless otherwise noted.
IV. RESULTS AND DISCUSSION

A. Physical and Numerical Experiments: Saturated Case

1. Experimental Results

Figures 3(a)-(d) show the movement of the dye following injection into the middle row of ports of the test cell after steady-state, saturated, non-isothermal flow conditions were attained. Figure 4 shows a qualitative sketch of the flow field as determined by the movement of the dye. From this sketch it is apparent that two counter-rotating convective cells existed in the saturated sand. (Tewari17 also found two convective cells to be the dominant mode of convection in similar experiments). Lower density liquid moves upward at the center of the chamber after being heated near the bottom. As this liquid moves toward the heat exchanger at the top of the chamber, it cools and its density increases, causing it to move downward along both the left and right sides. As the liquid reaches the bottom heating element, it heats up again and the convective cycle repeats. Steady-state temperature fields are shown in Figure 5. The elevated temperatures at the center of each row confirm the upward convective flow of liquid.

Figures 3(a) and 3(b) were used to approximate the steady-state flow velocity at each of the seven locations shown in Figure 3(a). The coordinates of each dye 'blob' (using the approximate center of mass) were determined from the two 35 mm photographs corresponding to Figures 3(a) and 3(b), and velocities were calculated based on the time elapsed between the photographs. Table 2 shows the velocity magnitudes and directions (angles were measured counterclockwise from the positive x-axis) at each of the seven positions shown in Figure 3(a).

<table>
<thead>
<tr>
<th>position</th>
<th>velocity magnitude (mm/min)</th>
<th>direction angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.78</td>
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<tr>
<td>2</td>
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<td>3</td>
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<td>6</td>
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<td>-53°</td>
</tr>
<tr>
<td>7</td>
<td>1.1</td>
<td>-70°</td>
</tr>
</tbody>
</table>
2. Results of the Insulated 2-D Model

The steady-state flow and temperature fields resulting from the insulated 2-D TOUGH2 simulation (see grid in Figure 2(a)) are shown in Figure 6 (steady-state conditions were assumed to exist in the numerical model when negligible changes occurred in the temperature field—after approximately 1 day of simulated bottom heating). Three counter-rotating convective cells were predicted to develop in the test cell, whereas only two convective cells were experimentally observed as shown in Figures 3 and 4. The reason for the discrepancy is postulated as follows.

In physical systems, heat loss through the boundaries of the experiment influence the convective flow behavior. For example, heat loss through the left and right Lexan borders of the experiment act as sinks for heat flow. Heated liquid that pushes upwards will therefore tend to cool and flow downwards along the left and right sides of the test cell—forming two counter-rotating cells as shown in Figures 3 and 4. However, since the boundaries of this numerical simulation were insulated, the instabilities that triggered the onset of convection resulted only from round-off and truncation errors in the code. As a result, no guarantee of a unique solution in TOUGH2 exists if these perturbations are not identical in each simulation. Slight variations of round-off or truncation caused by different time steps (TOUGH2 continuously changes the time step as required for convergence) are sufficient to alter the steady-state direction and number of convective cells resulting from the insulated model.

Figure 7 shows the temperature distribution of this simulation along a horizontal transect of the test cell corresponding to the location of the middle row of thermocouples. The simulated temperature profile is significantly different than the observed temperatures (also shown in Figure 7). This was expected since the number and direction of the convective cells predicted by the insulated TOUGH2 model did not match those of the experiment. In addition, the magnitudes of the predicted temperatures are significantly higher than the measured temperatures, suggesting that heat loss may have been significant in the experimental system.

Only the middle row of temperatures are shown for comparison in Figure 7 since the locations of the top and bottom rows of thermocouples did not correspond to the locations of the top and bottom rows of elements used by the models. The thermocouples were placed very near the top and bottom boundaries of the test cell, whereas the temperatures obtained along the top and bottom rows of elements represented temperatures that were 1 cm away from the top and bottom boundaries of the test cell.
3. Results of the 2-D Model with Side Heat Loss

The steady-state flow and temperature fields resulting from the 2-D numerical model with side heat loss (Figure 2(b)) are shown in Figure 8. The flow field reveals two steady-state counter-rotating convective cells, qualitatively similar to the flow field experimentally observed in Figures 3 and 4. The heat loss through the left and right sides were therefore sufficient to influence the flow and provide a unique solution, as opposed to the non-unique solutions of the insulated model where numerical perturbations were the only modes of instability.

The calculated velocities from this numerical simulation at positions 1 and 4 (shown in Figure 3(a)) were 5.4 mm/min (at an angle of 90° from the positive x-axis) and 13 mm/min (at an angle of 87° from the positive x-axis), respectively. These values are nearly an order of magnitude larger than the corresponding observed velocities given in Table 2. In addition, Figure 7 shows that although the profiles are qualitatively similar, the predicted temperatures along the middle row of the test cell are still significantly higher than the measured temperatures. A 57% difference exists between the predicted and measured temperatures at the center of the test cell. The high convective velocities in this simulation also yield large predicted gradients in the temperature distribution along a horizontal transect of the test cell. The difference between the temperature at the center and outside edges of the middle row was predicted to be approximately 27 °C while the actual temperature difference was seen to be only 13 °C.

3. Results of the 3-D Model

The 3-D model allowed heat losses through all the boundaries of the apparatus as shown in Figure 2(c). The resulting steady-state flow field shown in Figure 9 reveals two counter-rotating convective cells which qualitatively match the observed flow field shown in Figures 3 and 4. The calculated velocities taken from the numerically predicted flow field at positions 1 and 4 (shown in Figure 3(a)) were 3.6 mm/min (at an angle of -115° from the positive x-axis) and 3.3 mm/min (at an angle of 83° from the positive x-axis), respectively. The magnitudes and directions of these velocities are seen to be in better agreement with the observed values shown in Table 2.

The predicted steady-state temperatures along the middle row of the test cell are shown in Figure 7. The temperatures resulting from this model along the middle row of the test cell are seen to be in closer agreement with the experimental results, indicating that heat losses from the apparatus have a significant effect of lowering the magnitude of the steady-state temperatures in the saturated case. In addition, these reduced temperatures produce smaller density gradients, thereby reducing the driving potential for convective flow as evidenced by the reduced velocities predicted by the 3-D model.
4. Sensitivity to Bulk Permeability

Additional numerical simulations were performed to investigate the sensitivity of the saturated non-isothermal flow behavior to the bulk permeability of the sand. It has already been shown that simulated heat losses act to reduce the temperatures and convective velocities in the saturated sand. However, another parameter that could affect the experimental system in a similar manner is the bulk permeability of the sand. A lower permeability, possibly due to entrapped air or packing methods, could inhibit the convective flow, thereby depressing the temperature profile. On the other hand, a higher bulk permeability could increase the convective flow and temperature gradients. In order to verify these effects, the bulk permeability was varied in the three-dimensional model shown in Figure 2(c). Two simulations were made with bulk permeabilities that were approximately 30% lower (5.6x10^-10 m^2) and 30% higher (9.5x10^-10 m^2) than the measured bulk permeability of 7.3x10^-10 m^2.

Both simulations revealed two counter-rotating convective cells similar to the experimentally observed results. The predicted temperatures along the middle row of the test cell are shown in Figure 10 for both simulations. For reference, the experimental values and the predicted values using the measured bulk permeability are also shown in Figure 10. A significant effect of reducing the bulk permeability is the reduction of convective flow. This is evidenced by the flattened temperature profiles shown in Figure 10 resulting from lower bulk permeabilities. The change in temperature profiles here is slightly different than the change resulting from the addition of 3-D heat losses shown in Figure 7. Although both act to reduce the temperatures near the center of the test cell, the addition of heat losses lowers the temperatures uniformly across the entire cell, whereas the reduction of the bulk permeability tends to flatten the temperature profile near the center as a result of the reduced convective velocities.

B. Physical Experiments: Partially Saturated Cases

Following the saturated experiment, water was drained from the bottom of the test cell until the level of the visible saturated zone dropped to half the total height of the cell (the water level was at the middle row of thermocouples). Due to the coarseness of the sand, the capillary fringe is small. The top and bottom boundary temperatures were again set to near 23 °C and 90 °C, respectively, and the system was allowed to equilibrate. The steady-state flow field is shown in Figure 11, and the steady-state temperature profiles along the three horizontal rows of thermocouples are shown in Figure 12. Two counter-rotating convective cells similar to the fully saturated case are seen to develop in the saturated bottom half of the test cell as evidenced by the movement of the injected dye. The temperatures along the middle and top rows of thermocouples are elevated in the center of the test cell, indicating the motion of heated liquid or vapor upward in the center of the test cell.
Although only liquid movement was visible in the test cell via dye tracking, the elevated temperatures near the center of the middle row of thermocouples indicated that gas phase convection may also have been taking place in the unsaturated upper-half of the test cell. Other possible transport mechanisms of evaporation, vapor phase diffusion, and condensation could not be identified.

Following the half-saturated case, water was drained from the bottom of the test cell for half a day. Since suction was not applied to the bottom of the cell, the bottom 3-4 cm remained tension saturated due to capillary forces. The top and bottom boundary temperatures were set to near 23 °C and 90 °C, respectively, and allowed to equilibrate. Figure 13 shows the steady-state flow field for this residually saturated case. Based on the dye movements in the test cell, two counter-rotating convective cells were observed in the visibly wet region extending only a few centimeters above the bottom of the test cell. No bulk liquid movement was readily apparent in the unsaturated region above the convective liquid cells. However, based on the elevated temperatures along the middle row of the test cell shown in Figure 14, gas-phase convection cells apparently existed in the unsaturated region. It is hypothesized that heated water vapor and air pushed upward in the center, elevating the temperatures in the middle region of thermocouples along the middle row. Then, the moist air was cooled as it neared the top heat exchanger, where the moist air either condensed or flowed outward toward the left and right ends of the test cell. The downward return of the moist air would then lower the temperatures at the left and right boundaries of the middle row as evidenced in Figure 14.

V. CONCLUSIONS AND FUTURE WORK

Physical experiments have demonstrated the effects of various saturation levels on non-isothermal flow in porous media composed of coarse sand heated at the bottom and cooled at the top. Fully saturated, half-saturated, and residually saturated conditions were investigated in a square, two-dimensional, sand-filled test chamber heated from below. Results showed that in all three cases two counter-rotating convective cells developed in the saturated region, but no bulk liquid movement was evident in the unsaturated regions during the time scales of these experiments. However, gas-phase convection in the unsaturated regions of the experiments was evidenced by elevated temperatures near the center of the chamber, corresponding to the upward flow of convective moist air.

Numerical simulations of the saturated experiment were made using TOUGH2. Comparison of a 2-D model assuming insulated boundaries and a 3-D model with heat losses showed the importance of including heat losses in modeling our physical experiment. The insulated model
(Figure 2(a)) produced non-unique solutions that were sensitive to numerical perturbations of round-off and truncation. The introduction of heat losses through the left and right boundaries of the model (Figure 2(b)) influenced the flow so that unique solutions were rendered, but the predicted temperatures were still significantly higher than the measured temperatures. Finally, the three-dimensional model that allowed heat losses through all boundaries yielded temperatures and flow fields that were in better agreement with the observed values. Sensitivity analyses also revealed that reducing the bulk permeability of the sand in the model depressed the convective velocities in the test cell, thereby lowering the temperature gradients across the test cell. The lowering of temperatures in the center of the test cell was similar to the behavior resulting from the addition of heat losses, but in the latter case the temperatures were reduced uniformly across the test cell.

Experiments in the near future will incorporate light transmission digital imaging techniques to measure two-dimensional liquid saturation and dye concentration fields for more exact comparisons with numerical simulations. This will allow a more quantitative analysis of fluid flow within the unsaturated zone. Systematic variations in physical parameters such as particle size, boundary temperatures, and liquid saturations will also be performed in the next set of experiments to gain a more complete understanding of non-isothermal flow in homogeneous porous media. Concurrent numerical simulation of the physical experiments will assist in understanding the flow processes in each case.

To fulfill model validation requirements for the Yucca Mountain project, investigation of effective continuum models used under non-isothermal conditions for heterogeneous fractured rock must also be accomplished. Subsequent to our work in homogeneous, non-fractured systems we will consider discrete heterogeneities introduced into our numerical and physical experiments to determine critical permeability ratios for non-isothermal flow behavior. In addition, experiments are being designed in collaboration with other Yucca Mountain project participants to investigate non-isothermal flow behavior in thin slabs of fractured tuff where x-ray imaging capabilities can quantify two-dimensional saturation fields.

ACKNOWLEDGMENTS

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Table 1. Element properties in TOUGH2 grid (numbers in parentheses refer to references; all other parameters were experimentally determined.

<table>
<thead>
<tr>
<th>Element Material</th>
<th>Density (kg/m$^3$)</th>
<th>Total porosity</th>
<th>Bulk Permeability (m$^2$)</th>
<th>Thermal Conductivity (W/m-K)</th>
<th>Specific Heat (J/kg-K)</th>
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<td>2.5 (15)</td>
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</tr>
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<td>0</td>
<td>0.195 (16)</td>
<td>1260 (16)</td>
<td>—</td>
</tr>
<tr>
<td>Air</td>
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<td>0</td>
<td>0.03 (14)</td>
<td>1000 (14)</td>
<td>—</td>
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<td>0</td>
<td>2.5 (15)</td>
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<td>Zero volume; P&gt;P$_{matrix}$; T=23 °C</td>
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<tr>
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<td>0.41</td>
<td>0</td>
<td>2.5 (15)</td>
<td>717 (15)</td>
<td>Zero volume; P&gt;P$_{matrix}$; T=90 °C</td>
</tr>
</tbody>
</table>
Figure 1. Two-dimensional non-isothermal experimental apparatus.
Figure 2. Grids used in TOUGH2 simulations of the non-isothermal experiment: a) 2-D model assuming insulated boundaries b) 2-D model with side heat loss only c) 3-D model with heat loss through all boundaries.
Figure 3. Sketches of the dye movement at a) 8 minutes b) 23 minutes c) 53 minutes and d) 2 hours 9 minutes following injection into a saturated sand pack. The top and bottom boundaries are maintained near 20 °C and 90 °C, respectively.
Figure 4. Sketch of the steady-state flow field in the fully saturated case as evidenced by the movement of the injected dye. The top and bottom boundaries are maintained near 23 °C and 90 °C, respectively.
Figure 5. Experimentally measured steady-state temperatures along horizontal transects located at the bottom, middle, and top of a saturated test cell heated from below (90 °C) and cooled at the top (23 °C).
Figure 6. Steady-state flow and temperature fields resulting from the insulated 2-D TOUGH2 model of the fully saturated case. The top and bottom boundaries are maintained at 23 °C and 90 °C, respectively. All other boundaries are insulated.
Figure 7. Experimentally measured (symbols) and numerically simulated (lines) temperatures along the middle row of the test cell.
Figure 8. Steady-state flow and temperature fields resulting from the 2-D TOUGH2 model of the fully saturated case with heat loss through the left and right boundaries. The top and bottom boundaries are maintained at 23 °C and 90 °C, respectively.
Figure 9. Steady-state flow and temperature fields resulting from the 3-D TOUGH2 model of the fully saturated case. The top and bottom boundaries are maintained at 23 °C and 90 °C, respectively. Heat loss occurs through all other boundaries.
Figure 10. Temperatures along the middle row of the test cell as predicted by TOUGH2 using different bulk permeabilities, $k$, of the sand.
Figure 11. Sketch of the steady-state flow field in the half saturated case as evidenced by the movement of the injected dye. The top and bottom boundaries are maintained near 23 °C and 90 °C, respectively.
Figure 12. Experimentally measured steady-state temperatures along horizontal transects located at the bottom, middle, and top of a half-saturated test cell heated from below (90 °C) and cooled at the top (23 °C).
Figure 13. Sketch of the steady-state flow field in the residually saturated case as evidenced by the movement of the injected dye. The top and bottom boundaries are maintained near 23 °C and 90 °C, respectively.
Figure 14. Experimentally measured steady-state temperatures along horizontal transects located at the bottom, middle, and top of a residually-saturated test cell heated from below (90 °C) and cooled at the top (23 °C).
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