Example Problem GT-1

Simulation of Countercurrent Flow and Heat Transport with Local Evaporation and Condensation (Natural Heat Pipe)

Abstract: *This heat pipe problem demonstrates the simulator's ability to model countercurrent aqueous and gas flow in variably saturated geologic media, including saturations below residual saturation. As posed, the problem involves one-dimensional horizontal flow and heat transport, but this classic multifluid subsurface flow and transport problem involves complex flow behavior, which is subtle to changes in soil properties. The user will first explore the effects of changes in soil thermal conductivity, specific heat, and enhanced vapor transport on the formation and temperature distribution for a horizontal one-dimensional heat pipe. After completing these investigations, the user is asked to design an input file for a two-dimensional problem involving dynamic heat pipe flow.*

Problem Description

Because of their ability to transport large quantities of heat over small temperature differences and surface areas, engineered heat pipes are commonly used in thermal engineering applications. Natural heat pipes can occur in partially saturated soils subjected to thermal gradients. The typical scenario for a natural heat pipe occurs when a heated engineered surface is in contact with the subsurface (e.g., nuclear waste repository containers, nuclear waste storage tanks, or in-situ soil heating). The general requirements for creating countercurrent hydrothermal (i.e., heat pipe) flow in geologic media are a heat source and heat sink separated by partially saturated porous media. The heat source causes pore water to evaporate, creating a locally elevated gas pressure and water vapor concentration. Evaporation of the pore water reduces the saturation near the heat source, which in turn elevates the local capillary pressure. The heat sink causes water vapor to condense, creating a locally reduced gas pressure and water vapor concentration. The condensing water vapor also increases the local saturation. The pressure and water vapor gradients in the gas phase produce a flow of water vapor and associated heat from the heat source to the heat sink. Conversely, the capillary draw created by the elevated capillary pressures near the heat sink produces flow of liquid water towards the heat source. This countercurrent flow of water vapor in the gas phase and liquid water in the aqueous phase yields a net flow of heat from the heat source to the heat sink. Because of the importance of heat pipe flow to the overall heat transfer of engineered geologic systems, the ability of the numerical simulator to accurately and efficiently predict these complex and multiple-phase flow structures is imperative. The heat pipe problem chosen for solution is a modified version of the problem posed and solved by Udell and Fitch (1985).

The heat pipe problem solved by Udell and Fitch involved a one-dimensional horizontal cylinder (2.25-m in length) of porous media, which was assumed to be perfectly insulated on the sides, subjected to a constant heat flux (100-W/m^2) on one end, and maintained at a constant temperature (70°C) on the other end. The heat flux end of the cylinder was sealed and the constant temperature end was maintained under total-liquid saturation conditions. Initial conditions for the porous media were a total-liquid saturation of 0.7, a temperature of 70°C, and an absolute gas pressure of 101,330 Pa. Initial conditions and boundary conditions are listed for reference in Table 1.

The constitutive functions used in this problem differ slightly from those used by Udell and Fitch. Soil-moisture retention was described using the van Genuchten formulation (van Genuchten 1980) with a modification to the residual saturation that allows aqueous saturation to fall below the residual saturation, as shown in Equations (1) and (2). The aqueous and gas relative permeabilities were described by the Fatt and Klikoff formulations, as shown in Equations (3) and (4), respectively. The effective thermal conductivity of the partially saturated porous media was described by the formulation of Sommerton (1974), according to Equation (5). Parameter values are shown in Table 1.

$$S_l = \left[1 + (\alpha\, h_{gl})^n \right]^{-m} \left[1 - \bar{S}_m \right] + \bar{S}_m = \bar{S}_l \left[1 - \bar{S}_m \right] + \bar{S}_m \tag{1}$$

$$\bar{S}_m = \left[1 - \frac{\ln(h_{gl})}{\ln(h_{od})} \right] S_m \tag{2}$$

$$k_{rl} = \bar{S}_l^{\,3} \tag{3}$$

$$k_{rg} = (1 - \bar{S}_l)^3 \tag{4}$$

$$k_e = k_{unsat} + \sqrt{S_l}\,(k_{sat} - k_{unsat}) \tag{5}$$

Table 1. Simulation Parameter Values

Parameter Description	Parameter Value
Unsaturated Thermal Conductivity	0.582 W/m K
Saturated Thermal Conductivity	1.13 W/m K
Intrinsic Permeability	10^{-12} m^2
Porosity	0.4
Grain Density	2650. kg/m^3
Grain Specific Heat	700. J/kg K
Tortuosity	0.5
van Genuchten α	1.5631 m^{-1}
van Genuchten n	5.4
Residual Saturation	0.15

The relatively high van Genuchten n parameter is representative of well-drained soils and is numerically difficult to resolve, as it yields a strongly nonlinear function between capillary head and saturation. To reduce convergence problems with this simulation, the time stepping was controlled using three execution periods over the 10,000-day span of the simulation. During the first 10-day period the maximum timestep was limited to 0.1 day. During the second execution period from day 10 to day 100 the maximum timestep was increased to 0.25 days, and during the final period from day 100 to day 10,000, the maximum timestep was increased to 1000 day. The simulation will execute without this manual time-stepping control, but the simulation suffers from numerous convergence errors and primary variable exceptions. Both of these errors are trapped by STOMP and result in a reduction in the current timestep.

Simulation results, in terms of profiles of temperature, aqueous saturation, and water vapor mass fraction at days 2, 5, 10, and 10,000 are shown in Figures 1 through 4, respectively. In these plots, the aqueous saturated boundary at 70 C is on the left side and the heated, flow-impermeable boundary is on the right. After 2 days (Figure 1), the temperature on the heated boundary has risen from 70 C to 89.8 C and water has started to imbibe from the saturated boundary. The water-vapor mass fraction in the gas phase is primarily a function of vapor pressure, which is a function of temperature. The water-vapor mass fraction profile, therefore, tracks the temperature profile. After 5 days (Figure 2), the heated boundary temperature reaches nearly 100 C and the soil moisture begins to evaporate. After 10 days, (Figure 3), the 100-C temperature point has nearly reached 1.8 m into the column and water is now being forced out the saturated boundary. At this point in time, the zone of countercurrent flow, (i.e., gas evaporating and moving toward the left and water being drawn back toward the right via capillary pressure) is still expanding. After 10,000 days (Figure 4), the simulation has reached steady-flow conditions and the column is exhibiting three heat transport regimes. In the left portion of the domain, heat transfer is via conduction, advection, and mass diffusion, as shown by the non-linear temperature profile; in the middle portion heat transfer is primarily via countercurrent advection and mass diffusion, as shown by the flat temperature profile; and in the right portion heat transfer is primarily by conduction as shown by the linear temperature profile. Under steady-flow conditions the right side of the column has aqueous saturations below the residual saturation and the gas phase comprises primarily water-vapor.

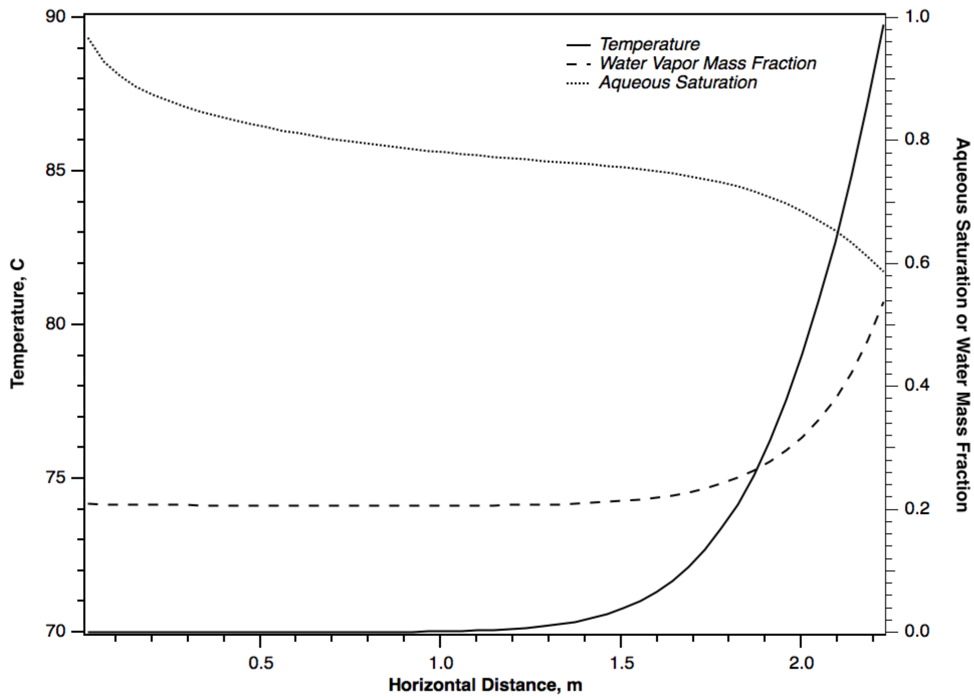

Figure 1. Temperature, Aqueous Saturation, and Water Vapor Mass Fraction Profiles at 2 Days

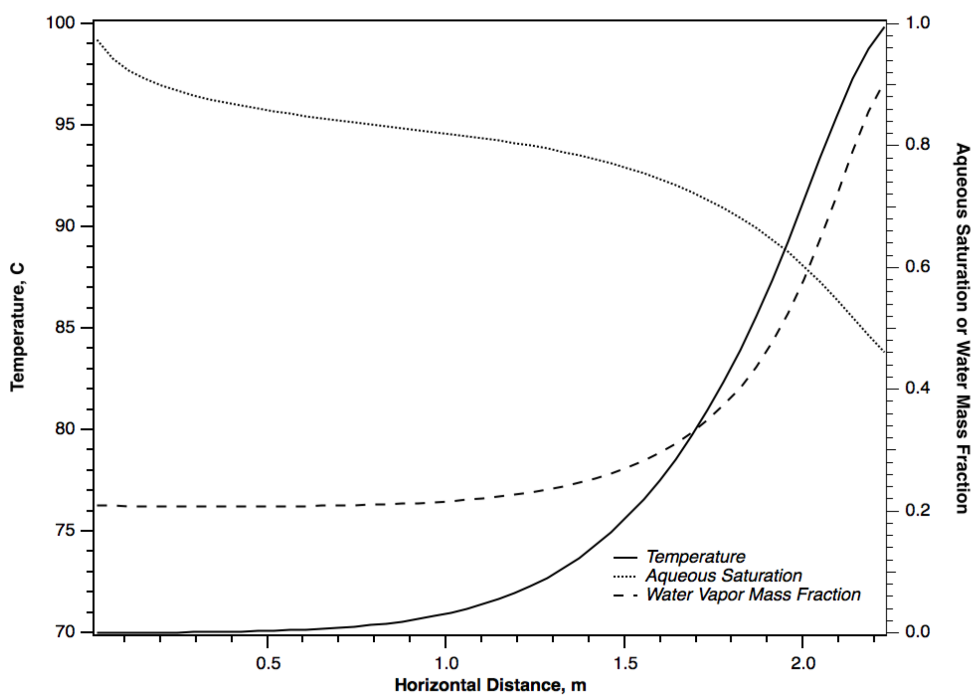

Figure 2. Temperature, Aqueous Saturation, and Water Vapor Mass Fraction Profiles at 5 Days

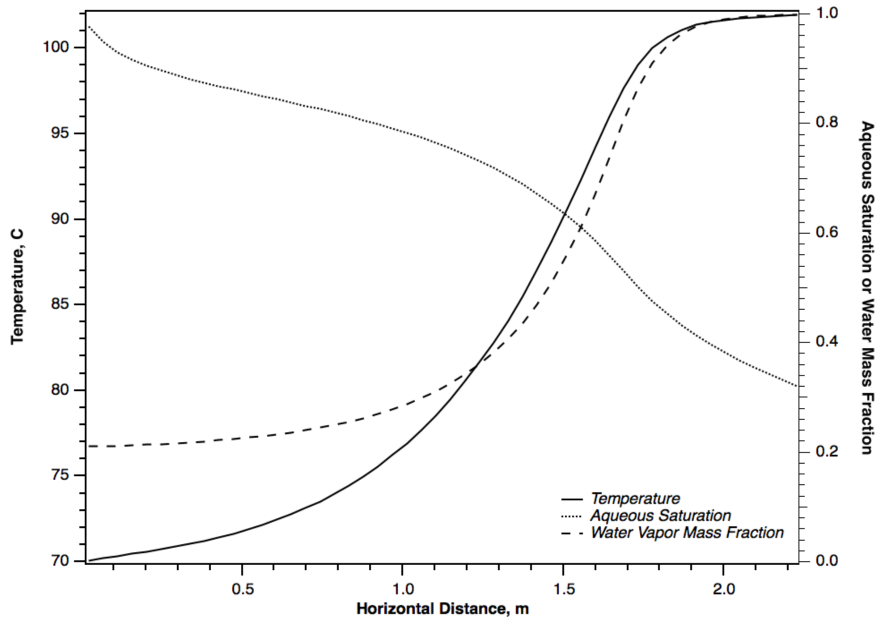

Figure 3. Temperature Aqueous Saturation, and Water Vapor Mass Fraction Profiles at 10 Days

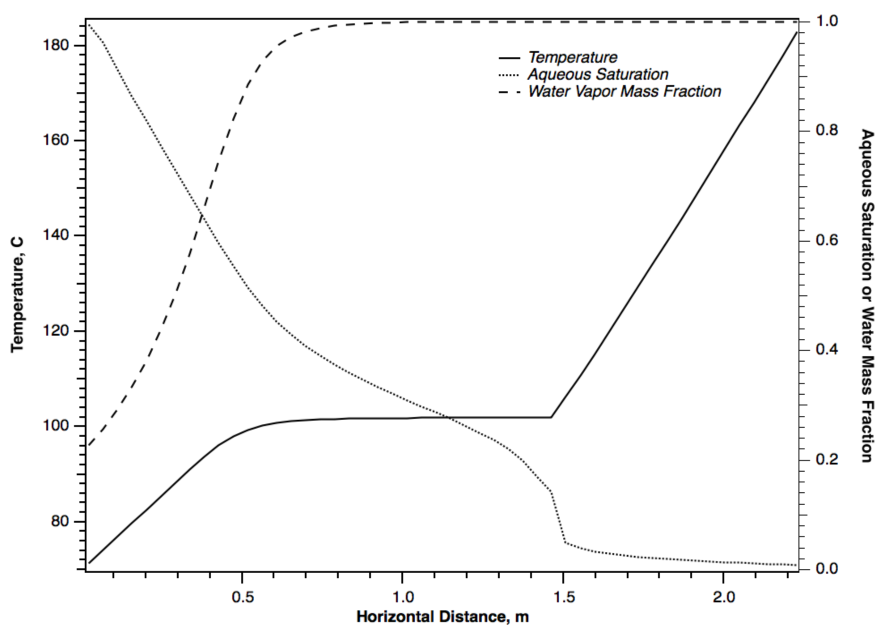

Figure 4. Temperature, Aqueous Saturation, and Water Vapor Mass Fraction

Profiles at 10,000 Days

The heat-pipe problem, which was solved using a semi-analytical approach by Udell and Fitch (1985), differs from the current problem in several aspects. First, the Udell and Fitch problem used constant physical properties, whereas the STOMP simulation included temperature and pressure dependent physical properties for the gas and aqueous phases. Second, nitrogen gas, instead of air, was used as the noncondensible in the Udell and Fitch problem. Third, the saturation-capillary function in the Udell and Fitch formulation used the Leverett function (Leverett 1941) without extensions below the residual saturation, whereas the STOMP simulation used a van Genuchten function which closely matched the Leverett function. In spite of these differences the results show good agreement between the solution of Udell and Fitch and the STOMP simulation for the steady-state conditions; the Udell and Fitch solution is valid only for the steady-state solution. Both results show temperature profiles with mixed conduction and advection/diffusion heat transport near the saturated boundary and nearly pure countercurrent gas and aqueous flow heat transport in the center portion of the heat pipe. The Udell and Fitch solution stops short of the dry-out region with the minimum saturation being the residual saturation level. The STOMP solution allows a region near the heated boundary to dry out, thus creating elevated temperatures, in comparison to the Udell and Fitch results.

References

Fayer, M.J., and C.S. Simmons. 1995. "Modified soil water retention function for all matric suctions." *Water Resources Research.* 31(5), 1233-1238.

Leverett, M.C. 1941. *Capillary behavior in porous solids*. AIME Transactions. 142-152.

Somerton, W.H., A.H. El-shaarani, and S.M. Mobarak. 1974. *High temperature behavior of rocks associated with geothermal type reservoirs*. Paper SPE-4897, presented at the 44th Annual California Regional Meeting of the Society of Petroleum Engineers, San Francisco, California.

Udell, K.S., and J.S. Fitch. 1985. *Heat and mass transfer in capillary porous media considering* *evaporation, condensation, and non-condensible gas effects*. In Proceedings of 23rd ASME/AIChE National Heat Transfer Conference, Denver, Colorado.

van Genuchten, M. Th. 1980. "A closed-form equation for predicting the hydraulic conductivity of unsaturated soils." *Soil Sci. Soc. Am. J.* 44:892-898.

White, M.D., and M. Oostrom. 2000. *STOMP Subsurface Transport Over Multiple Phases, Version 2.0, Theory Guide.* PNNL-12030. UC-2010. Pacific Northwest National Laboratory, Richland, Washington.

Exercises

1. (Basic) Repeat the one-dimensional horizontal column simulation changing the unsaturated and saturated thermal conductivities (*Thermal Properties Card*), grain density (*Mechanical Properties Card*) and grain specific heat (*Thermal Properties Card*). Compare the steady-flow temperature, aqueous saturation, and water-vapor mass fraction profiles against those reported herein.
2. (Intermediate) Repeat the one-dimensional horizontal column simulation using various time-stepping controls (*Execution Time Periods, Solution Control Card*). Check for differences in the simulation results at 2, 5, 10, and 10,000 days.
3. (Intermediate) Repeat the one-dimensional horizontal column simulation using the *Enhanced Gas Diffusion Option*, changing the clay mass fraction (*Solution Control Card*). Compare the steady-flow temperature, aqueous saturation, and water-vapor mass fraction profiles against those reported herein.
4. (Advanced) Design and execute a two-dimensional heat pipe simulation with heat emanating from an impermeable subsurface structure (e.g., pipe, nuclear waste canister, nuclear waste repository, heating element). Simulate the system with time varying heat source to form a dynamic heat pipe. Create a time sequence of temperature and aqueous saturation contours to visualize the dynamic heat pipe.

Input File

```
#-------------------------------------------------------
~Simulation Title Card
#-------------------------------------------------------
1,
STOMP Example Problem GT-1,
Mark White,
PNNL,
August 2018,
15:15,
4,
This application problem follows the heat-pipe problem solved
semi-analytically by Udell and Fitch. The soil moisture retention
function has been changed to a modified van Genuchten function to
allow saturations for all matric suctions.

#-------------------------------------------------------
~Solution Control Card
#-------------------------------------------------------
Normal,
Geothermal with isobrine,
3,
0,day,10,day,1,s,0.1,day,1.25,16,1.e-06,
10,day,100,day,0.1,day,0.25,day,1.25,16,1.e-06,
100,day,10000,day,0.25,day,1000,day,1.25,16,1.e-06,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

#-------------------------------------------------------
~Grid Card
#-------------------------------------------------------
Uniform Cartesian,
50,1,1,
4.5,cm,
10.0,cm,
10.0,cm,

#-------------------------------------------------------
~Rock/Soil Zonation Card
#-------------------------------------------------------
1,
Sand,1,50,1,1,1,1,

#-------------------------------------------------------
~Mechanical Properties Card
#-------------------------------------------------------
```

```
Sand,2650,kg/m^3,0.4,0.4,,,Constant,0.5,0.5,

#----------------------------------------------------
~Hydraulic Properties Card
#----------------------------------------------------
Sand,1.e-12,m^2,,,,,
#----------------------------------------------------
~Thermal Properties Card
#----------------------------------------------------
Sand,Somerton,0.582,W/m K,,,,,1.13,W/m K,,,,,700,J/kg K,

#----------------------------------------------------
~Saturation Function Card
#----------------------------------------------------
Sand,van Genuchten w/ Webb,1.563,1/m,5.4,0.15,,,

#----------------------------------------------------
~Aqueous Relative Permeability Card
#----------------------------------------------------
Sand,Fatt and Klikoff,

#----------------------------------------------------
~Gas Relative Permeability Card
#----------------------------------------------------
Sand,Fatt and Klikoff,

#----------------------------------------------------
~Initial Conditions Card
#----------------------------------------------------
Aqueous Saturation,Gas Pressure,
3,
Aqueous Saturation,0.7,,,,,,,1,50,1,1,1,1,
Gas Pressure,101330,Pa,,,,,,,1,50,1,1,1,1,
Temperature,70.0,C,,,,,,,1,50,1,1,1,1,

#----------------------------------------------------
~Boundary Conditions Card
#----------------------------------------------------
2,
West,Dirichlet Energy,Dirichlet Fluid Flow,BC1,Air Relative Saturation,Salt Relative Saturation,
1,1,1,1,1,1,1,
0,day,70,C,101330,Pa,1.0,0.0,
East,Neumann Energy,
50,50,1,1,1,1,1,
0,day,-70,W/m^2,,

#----------------------------------------------------
~Output Options Card
#----------------------------------------------------
2,
1,1,1,
50,1,1,
1,1,day,m,5,5,5,
6,
Temperature,,
```

```
Aqueous saturation,,
Phase condition,,
Water gas mass frac.,,
Aqueous pressure,,
Gas pressure,,
4,
2,day,
5,day,
10,day,
100,day,
6,
Temperature,,
Aqueous saturation,,
Phase condition,,
Water gas mass frac.,,
Aqueous pressure,,
Gas pressure,,
```

Solutions to Selected Exercises

Exercise 1

As thermal conductivity is a coefficient for heat transfer, we expect changes in thermal conductivity to change the transient and steady-flow profiles. Strong coupling between the thermal and hydrologic system, typical of heat-pipe flows, additionally makes us expect changes in both the temperature and saturation profiles with changes in the thermal conductivity. The Somerton model for calculating the effective thermal conductivity of partially saturated soils is dependent on the aqueous saturation and the saturated and unsaturated thermal conductivity of the soil. We, therefore, expect changes in the transient and steady-flow profiles with changes in both the unsaturated and saturated thermal conductivities. The effect of increasing the saturated thermal conductivity and decreasing the unsaturated thermal conductivity are shown in Figures 5 and 6, respectively. Increasing the saturated thermal conductivity (Figure 5) lessens the slope in the temperature profile in the regions of higher saturation (i.e., left-hand side). Consequentially, this shifts the region of countercurrent flow toward the heated side (i.e., right-hand side), eliminating the region of saturation values below residual. Decreasing the unsaturated thermal conductivity (Figure 6) has little effect on the steady-flow profiles in the regions of higher saturations (i.e., right-hand side).

The slope of the temperature profile in the unsaturated region is steeper, resulting in higher peak temperatures and slight increases in soil drying in the unsaturated region (i.e., left-hand side). The grain density and grain specific heat are variables that only appear in the thermal storage term of the energy conservation equation. Under steady-flow conditions the thermal storage term is zero; therefore, changing the grain density and specific heat has no effect on the steady-flow profiles.

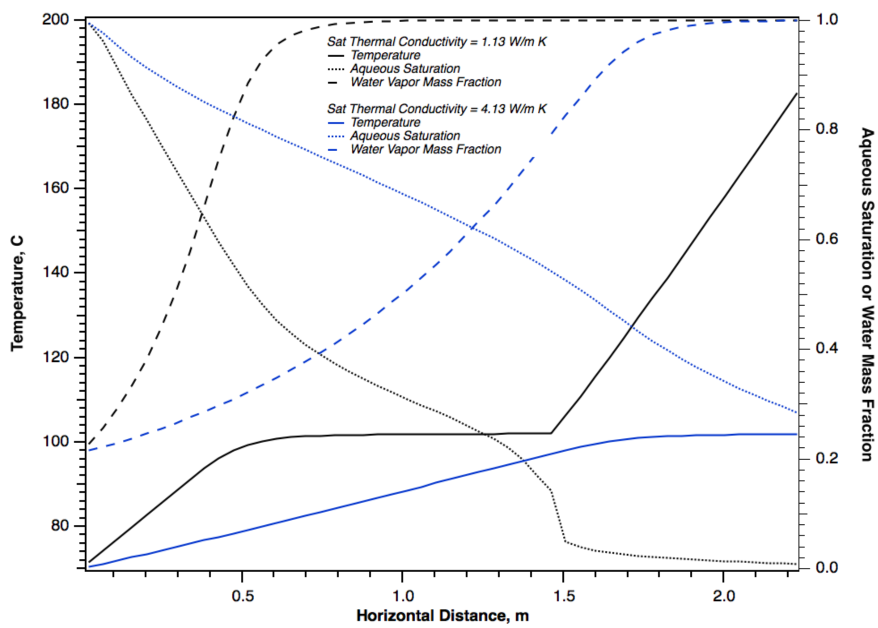

Figure 5. Temperature, Aqueous Saturation, and Water Vapor Mass Fraction Profiles Under Steady-Flow Conditions for Different Saturated Thermal Conductivities

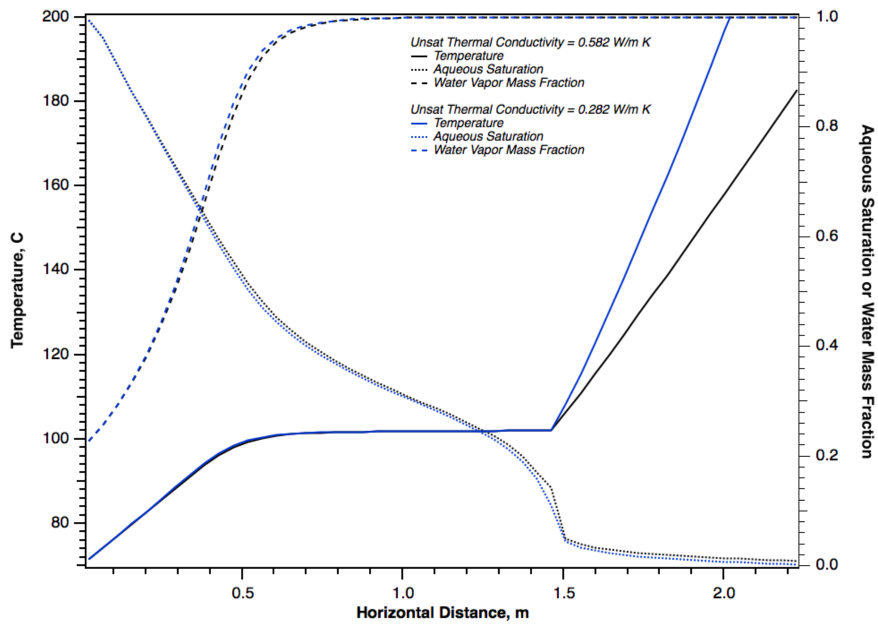

Figure 6. Temperature, Aqueous Saturation, and Water Vapor Mass Fraction Profiles Under Steady-Flow Conditions for Different Unsaturated Thermal Conductivities

Exercise 2

The original *Solution Control Card* used three execution periods that controlled the maximum timestep (i.e., 0.1 day for the first 10 days, 0.25 day from 10 to 100 days, and 1000 days from 100 to 10,000 days). The time-step controlled simulation required 543 timesteps to reach steady-flow conditions at 10,000 days. The effect of no timestep control can be seen by executing the simulation with the following simpler *Solution Control Card* as shown below.

```
#-----------------------------------------------------
~Solution Control Card
#-----------------------------------------------------
Normal,
Geothermal with isobrine,
1,
0,day,10000,day,100,s,5000,day,1.25,16,1.e-06,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,
```

Whereas, the simulation reached steady-flow conditions at 10,000 days after 176 timesteps, the transient portion of the simulation required forced time-step reductions because of convergence failures. Although no differences in results are apparent in the profiles of temperature, aqueous saturation and water-vapor mass fraction at steady-flow conditions, there are differences in these profiles at 10 days, as illustrated in Figure 7. Theoretically, the simulator will produce more accurate solutions, to a point, using smaller timesteps. There is, however, a dimensioning return on increased accuracy with smaller and smaller timesteps. It is the onus of the user to select time-stepping schemes that achieve the desired accuracy at minimal computational effort. An effective approach for achieving the appropriate time-stepping scheme is to systematically reduce the timesteps until no further change in the results are noticed.

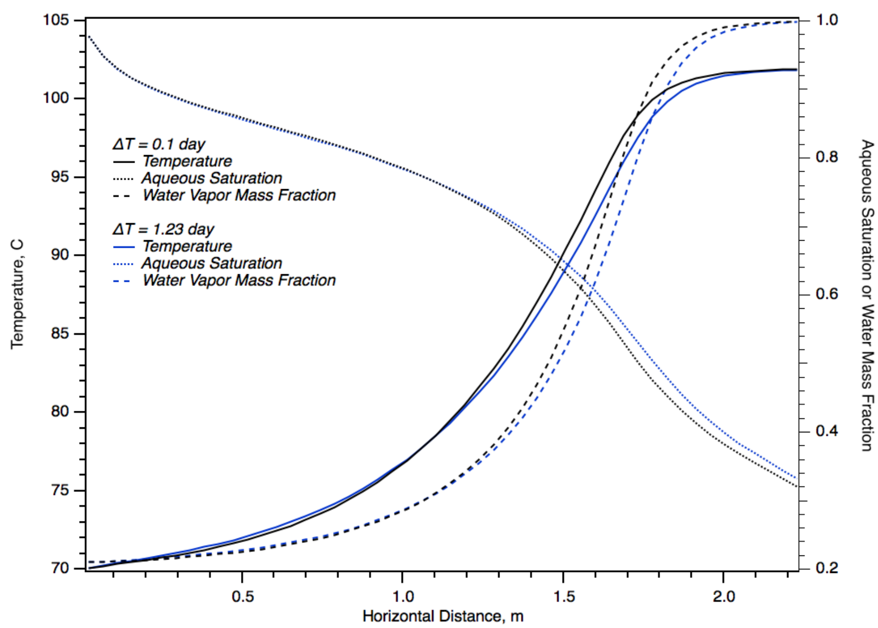

Figure 7. Temperature, Aqueous Saturation and Water-Vapor Mass Fraction Profiles at 10 Days, with Different Time-Step Control

Exercise 3

Water-vapor diffusion in the gas phase in porous media occurs at rates greater than those in free gas. This affect is often referred to as enhanced vapor diffusion. Enhanced vapor diffusion can be simulated in the STOMP simulator through the *Enhanced Gas Diffusion Option* and specifying a clay mass fraction for the soil. This can be done by modifying the *Solution Control Card* as shown below:

```
#-------------------------------------------------------
~Solution Control Card
#-------------------------------------------------------
Normal,
Geothermal with isobrine,
1,
0,day,10000,day,100,s,5000,day,1.25,16,1.e-06,
1000,
Variable Aqueous Diffusion,
Enhanced Gas Diffusion, 0.1,
```

The effect of using a clay mass fraction of 0.1 to enhance the water-vapor mass diffusion is apparent in the steady-flow profiles of temperature, aqueous saturation and water-vapor mass fraction, shown in Figure 8. The enhanced water-vapor diffusion has a significant impact on all profiles at steady-flow conditions. The flat temperature profile in the countercurrent flow region is replaced with a sloped temperature profile caused by the gradient in water-vapor mass fraction in this region. The aqueous saturation profile is shifted toward the left, yielding an increased region below residual saturation and the enhanced water-vapor diffusion allows air to exist in the drier regions (i.e., right-hand side).

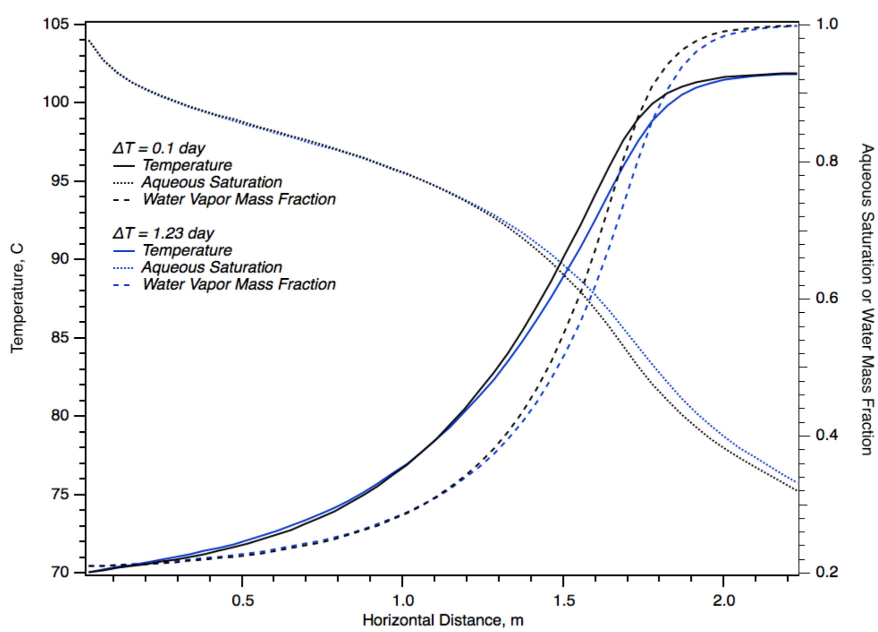

Figure 8. Temperature, Aqueous Saturation, Water-Vapor Mass Fraction Profiles at Steady-Flow Conditions with Different Clay Mass Fractions