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1 ROLE OF NONEQUILIBRIUM WATER VAPOR DIFFUSION IN GEOTHERMAL

2 ENERGY STORAGE SYSTEMS IN THE VADOSE ZONE

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6 **Abstract:** Although siting of geothermal energy storage systems in the vadose zone may be
7 beneficial due to the low heat losses associated with the low thermal conductivity of unsaturated
8 soils, water phase change and vapor diffusion in soils surrounding geothermal heat exchangers
9 may play important roles in both the heat injection and retention processes that are not considered
10 in established design models for these systems. This study incorporates recently-developed
11 coupled thermo-hydraulic constitutive relationships for unsaturated soils into a coupled heat
12 transfer and water flow model that considers time-dependent, nonequilibrium water phase change
13 and enhanced vapor diffusion to study the behavior of geothermal energy storage systems in the
14 vadose zone. After calibration of key parameters using a tank-scale heating test on compacted silt,
15 the ground response during 90 days of heat injection from a vertical geothermal heat exchanger

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16 followed by 90 days of ambient cooling was investigated. Significant decreases in degree of
17 saturation and thermal conductivity of the ground surrounding the vertical geothermal heat
18 exchanger were observed during the heat injection period that were not recovered during the
19 cooling period. This effect can lead to a greater amount of heat retained in the ground beyond that
20 estimated in conduction-based design models.

21 **INTRODUCTION**

22 An important challenge facing society is the storage of energy collected from renewable
23 sources. One such application is the storage of heat collected from solar thermal panels in the
24 subsurface so that it can be harvested later (Claesson and Hellström 1981; Nordell and Hellström
25 2000; Chapuis and Bernier 2009). A practical mode of heat injection into the subsurface involves
26 circulation of a heated carrier fluid through a closely-spaced array of closed-loop geothermal heat
27 exchangers in boreholes to reach ground temperatures ranging from 35 to 80 °C (Sibbitt et al.
28 2012; Başer et al. 2016a; McCartney et al. 2017). Unsaturated soils in the vadose zone are ideal
29 thermal energy storage media because low heat losses can be expected due to the low thermal
30 conductivity of unsaturated soils (McCartney et al. 2013). The mode of heat transfer during
31 injection of heat into unsaturated soils is complex as it may be coupled with thermally-induced
32 water flow in either liquid or vapor forms along with latent heat transfer associated with phase
33 change. However, most design models for geothermal heat storage systems focus on ground
34 temperature changes during heating and do not consider coupled heat transfer and water transport
35 (Claesson and Hellström 1981; Eskilson 1987). Although some recent studies on geothermal
36 energy storage systems highlighted the importance of considering coupled heat transfer and water
37 flow in their performance evaluation (Catolico et al. 2016; Moradi et al. 2016), the impact of water
38 vapor diffusion and phase change in unsaturated soils during heat injection on the heat retention

39 during a subsequent ambient cooling phase is an important topic that has not been investigated.
40 This paper presents simulations of the response of a low-permeability, low activity,
41 incompressible, unsaturated silt layer surrounding a single geothermal heat exchanger to
42 understand the impacts of considering water vapor diffusion and water phase change on the
43 transient heat injection and retention processes. Comparison of the simulation results from the
44 coupled heat transfer and water flow model with a simpler heat transfer model without water vapor
45 diffusion or phase change permits an evaluation of the importance of these heat transfer
46 mechanisms in simulating geothermal energy storage systems in the vadose zone.

47 **BACKGROUND**

48 Most models of heat transfer from geothermal heat exchangers employ analytical solutions to
49 the heat equation assuming conduction is the primary mechanism of heat transfer, using constant
50 thermal properties that do not consider the effects of changes in degree of saturation expected
51 during heat transfer in unsaturated soils (e.g., Kavanaugh 1985; Eskilson 1987). Analytical
52 solutions have been developed for geothermal heat exchanger geometries including the infinite
53 line source (Ingersoll and Plass 1948; Beier et al. 2014), finite line source (Acuña et al. 2012;
54 Lamarche and Beauchamp 2007), hollow cylinder source (Ingersoll et al. 1954; Gehlin 2002),
55 finite plate source (Ciriello et al. 2015), and one- and two-dimensional solid cylinder sources (Tarn
56 and Wang 2004). Although numerical simulations of geothermal heat exchangers have also been
57 performed, most have also considered conduction as the primary mechanism of heat transfer
58 (Ozudogru et al. 2015; Welsch et al. 2015; Başer et al. 2016a). While these conduction-based
59 analytical models and numerical simulations may be practical for the design of geothermal heat
60 exchangers in dry or saturated low permeability soils, they may not be practical for design of those
61 in unsaturated soils due to the potential for convective heat transfer associated with thermally-

62 induced liquid water or water vapor flow, which may result in irreversible changes in behavior
63 during cyclic heat injection and extraction (or ambient cooling). Further, the thermal properties of
64 unsaturated soils are highly dependent on the degree of saturation, even when conduction is
65 assumed to be the primary mode of heat transfer (e.g., Farouki 1981; Côté and Konrad 2005; Smits
66 et al. 2013; Lu and Dong 2015). Conduction-only models may also not be practical for use in
67 saturated soils with high permeability due to the potential for thermally-induced convection of
68 water from buoyancy effects (Catolico et al. 2016).

69 Because the properties of water in liquid and gas forms are dependent on temperature, heat
70 transfer in the unsaturated soils in the vadose zone leads to thermally induced water flow through
71 soil. Specifically, temperature dependency of the density of liquid water ρ_w (Hillel 1980), dynamic
72 viscosity of liquid water μ_w (Lide 2001), surface tension of soil water σ (Saito et al. 2006), relative
73 humidity at equilibrium $R_{h,eq}$ (Philip and de Vries 1957), saturated vapor concentration in the gas
74 phase $c_{v,sat}$ (Campbell 1985), vapor diffusion coefficient in air D_v (Campbell 1985), and the latent
75 heat of water vaporization L_w (Monteith and Unworth 1990) may lead to thermally-induced water
76 flow through unsaturated soils. The movement of water in soil caused by thermal and hydraulic
77 gradients and the associated impacts on heat transfer have been studied experimentally for more
78 than 100 years (Bouyoucos 1915; Lewis 1937; Smith 1943; Gurr et al. 1952; Baladi et al. 1981;
79 Shah et al. 1983; Ewen 1988; Gens et al. 1998, 2007, 2009; Cleall et al. 2011; Smits et al. 2011;
80 Moradi et al. 2015, 2016; Başer et al. 2016b). Some general observations from these studies are:
81 (1) heat transfer occurs in unsaturated porous media by conduction, convection in both liquid and
82 gas phases, and latent heat transfer associated with water phase change; (2) water movement due
83 to a temperature gradient is controlled by both vaporization/condensation processes as well as
84 development of suction gradients caused by changes in water properties with temperature (i.e.,

85 density, viscosity, solid-liquid contact angle) and drying effects; (3) vapor diffusion may occur at
86 greater rates than predicted by Fick's law, (4) the magnitude of thermally induced water flow
87 depends on the initial degree of saturation; and (5) the times required to reach steady-state
88 distributions in degree of saturation and temperature may be different depending on the coupling
89 between the thermal and hydraulic properties of a given soil.

90 The governing equations for coupled heat transfer and flow of water in liquid and vapor forms
91 have been investigated for unsaturated porous media in nondeformable conditions (Philip and de
92 Vries 1957; Ewen and Thomas 1989; Thomas and King 1991; Thomas and Sansom 1995; Thomas
93 et al. 2001; Smits et al. 2011), deformable conditions (Thomas and He 1996; Thomas et al. 1996),
94 and in the presence of pore fluids containing salts or chemicals (Cleall et al. 2007; Olivella et al.
95 1996; Guimaraes et al. 2007, 2013). Most models for coupled heat transfer and water flow in liquid
96 and vapor forms in nondeformable unsaturated soils are based on the model of Philip and de Vries
97 (1957), who proposed the "liquid island" theory as an explanation for observations from studies
98 like Gurr et al. (1952) that vapor diffusion occurred at a faster rate than predicted by Fick's law.
99 Their theory is a pore-scale explanation where local thermal gradients is assumed to be higher
100 across microscopic air-filled pores than the global thermal gradient across a soil element, and
101 where water vapor diffusion is enhanced by evaporation and condensation from water held
102 between soil particles by capillarity (liquid islands), effectively increasing the area available for
103 vapor diffusion through a soil element. They implemented their pore-scale theory on a
104 macroscopic scale by extending the vapor diffusion theory of Penman (1940) through inclusion of
105 a soil-specific enhancement factor to correct the vapor diffusion rate calculated from Fick's law.
106 Cass et al. (1984) found that the enhancement factor approaches 1.0 (no enhancement) for dry soils
107 and increases significantly with increasing degree of saturation. Although the model of Philip and

108 de Vries (1957) has been used in many coupled heat transfer and water flow problems in
109 nondeformable soils, their model does not account for convective transport in the gas or liquid
110 water phases, nonequilibrium phase change, vapor dispersion, or sensible heat dispersion in the
111 liquid phase (Smits et al. 2011). Of these issues, consideration of nonequilibrium phase change in
112 the model is expected to lead to more accurate identification of the appropriate vapor enhancement
113 factor for a given soil (Smits et al. 2011). Lozano et al. (2008) observed that phase change may
114 become the process limiting evaporation at low saturations rather than vapor diffusion as
115 classically believed.

116 In the model of Philip and de Vries (1957), it is assumed that the water in liquid and gas phases
117 are in equilibrium, which means that phase change occurs instantaneously in response to a change
118 in vapor pressure. However, experimental studies have identified that time is required for liquid
119 water to volatilize in response to a change in vapor pressure in a pore resulting from vapor diffusion
120 in response to gradients in vapor pressure and/or temperature (Bénet and Jouanna 1982; Armstrong
121 et al. 1994; Chammari et al. 2008, Bénet et al. 2009). To account for this in a model of coupled
122 heat transfer and water flow, a source term for the liquid/gas phase change rate is added to the
123 mass balance equations of liquid and vapor that is based on irreversible thermodynamics, first
124 order reaction kinetics, or the kinetic theory of gases and contains a fitting coefficient that can
125 calibrated for a given soil (Bénet and Jouanna 1982; Bixler 1985; Zhang and Datta 2004). Smits
126 et al. (2011) adopted the source term of Bixler (1985) because it was derived from the kinetic
127 theory of gases and is thus inherently temperature dependent. In the model of Bixler (1985), the
128 vaporization rate is proportional to the difference between local equilibrium vapor pressure and
129 local partial vapor pressure and the difference between the local degree of saturation and residual
130 saturation. Smits et al. (2011) compared predictions of coupled heat transfer and water flow from

131 equilibrium and nonequilibrium models, and found major differences in the early stages of the
132 flow process, with greater differences for soils with initially lower degrees of saturation. Smits et
133 al. (2011) and Trautz et al. (2015) also found that nonequilibrium models provide a better match
134 to experimental data from column tests involving evaporation from fine sand with a heated surface
135 than the model of Philip and de Vries (1957), indicating that the nonequilibrium assumption for
136 phase change may better capture the transient process of thermally-induced drying.

137 **MODEL CALIBRATION**

138 **Model Description**

139 A non-equilibrium, non-isothermal, and coupled heat transfer and water flow numerical model
140 developed by Smits et al. (2011) and extended by Moradi et al. (2016) was used to consider the
141 behavior of an unsaturated soil layer during heating and cooling of a single vertical geothermal
142 heat exchanger. The governing equations and primary variables used in the formulation are given
143 in Table 1. Calibration of the model requires soil-specific quantification of the parameters for the
144 thermo-hydraulic constitutive relationships governing water retention, hydraulic conductivity,
145 thermal conductivity, and volumetric heat capacity, as well as estimates of parameters a and b in
146 Equations (4) and (5) that govern the rates of vapor diffusion and phase change, respectively.

147 The model used in the simulations incorporates recently-developed thermo-hydraulic
148 constitutive relationships for unsaturated soils (Lu and Dong 2015; Baser et al. 2016c). The
149 experimental approach used by Lu and Dong (2015) was used to obtain the data for calibration of
150 these coupled thermo-hydraulic constitutive relationships. Lu and Dong (2015) used a modified
151 form of the transient-release and imbibition method (TRIM) of Wayllace and Lu (2012) that
152 included a dual-needle thermal probe to measure the thermal conductivity and volumetric heat
153 capacity during monotonic drying of different unsaturated soils under isothermal conditions.

154 TRIM uses an inverse analysis to estimate the parameters of the soil-water retention curve (SWRC)
 155 and hydraulic conductivity function (HCF) given by van Genuchten (1980). These parameters
 156 include α_{vG} , which represents the inverse of the air entry suction in the SWRC, N_{vG} , which
 157 represents the pore size distribution in the SWRC, and k_{sw} , which is the hydraulic conductivity of
 158 saturated soil. The value of k_{sw} obtained from a test at room temperature can be used to calculate
 159 the intrinsic permeability κ in Equation (1). Although the saturation-dependent relative
 160 permeability to water (the HCF) was assumed not to vary with temperature, the hydraulic
 161 conductivity of the unsaturated soil will vary with temperature because the dynamic viscosity and
 162 density of water vary with temperature according to the relationships presented in Lide (2001) and
 163 Hillel (1980), respectively. The relative permeability to gas was not measured in this study, but
 164 was assumed to equal $k_{rg}=1-k_{rw}$. The temperature-dependent surface tension σ relationship
 165 presented by Saito et al. (2006) was used in the temperature correction for capillary pressure of
 166 Grant and Salehzadeh (1996), given as follows:

$$P_c(T) = P_c(T_{ref})[\sigma(T)/\sigma(T_{ref})] \quad (7)$$

167 where σ is the surface tension (N/m), T is the temperature (K), and T_{ref} is the initial reference
 168 temperature of 293.15 K.

169 Lu and Dong (2015) defined a thermal conductivity function (TCF) that can capture transitions
 170 in the thermal conductivity in the capillary, funicular, and pendular water retention regimes of the
 171 SWRC, given as follows:

$$\frac{\lambda - \lambda_{dry}}{\lambda_{sat} - \lambda_{dry}} = 1 - \left[1 + \left(\frac{S_{rw}}{S_f} \right)^m \right]^{1/m-1} \quad (8)$$

172 where λ_{dry} and λ_{sat} are the thermal conductivities of dry and saturated soil specimens, respectively,
 173 S_f is a parameter representing the degree of saturation at the onset of the funicular regime, and m

174 is a parameter related to the pore fluid network connectivity. Lu and Dong (2015) correlated the
 175 parameters of the TCFs and SWRCs of several soils and found that the m parameter in the TCF is
 176 related to the pore-size parameter N_{vG} in the SWRC model of van Genuchten (1980), and can be
 177 estimated to be $3.0-0.2N_{vG}$. Evaluation of the form of Equation 8 indicates that the thermal
 178 conductivity will not reduce to the value of λ_{sat} when $S_e=1$, so Lu and Dong (2015) treated λ_{sat} as
 179 a fitting parameter. Although Smits et al. (2013) observed that the TCF may vary with temperature,
 180 this temperature dependency is likely due to vapor diffusion and phase change that was not
 181 accounted for in their simulations. Because the simulations in this study account for vapor
 182 diffusion and phase change explicitly, the TCF and VCHF measured at 20 °C were used in the
 183 coupled heat transfer and water flow simulations.

184 Başer et al. (2016c) presented trends in the volumetric heat capacity of compacted silt during
 185 monotonic drying and found that it also depends on the degree of saturation in a similar manner to
 186 the thermal conductivity, and defined a volumetric heat capacity function (VCHF) that has the
 187 same form as the THF of Lu and Dong (2015), as follows:

$$\frac{C_v - C_{v\text{dry}}}{C_{v\text{sat}} - C_{v\text{dry}}} = 1 - \left[1 + \left(\frac{S_{rw}}{S_f} \right)^m \right]^{1/m-1} \quad (9)$$

188 where $C_{v\text{dry}}$ and $C_{v\text{sat}}$ are the volumetric heat capacities of dry and saturated soil, respectively, and
 189 are similarly treated as fitting parameters, and S_f and m are the same parameters as in Equation (8).
 190 Başer et al. (2016c) found that this model and the assumptions regarding the parameters provided
 191 a good match to the volumetric heat capacity data measured in the TRIM tests on different soils
 192 performed by Lu and Dong (2015) that were not reported in their paper due to its focus on the
 193 thermal conductivity.

194

195 **Calibration of Thermo-Hydraulic Constitutive Relationships**

196 The soil investigated in this study is Bonny silt, which is classified as ML (inorganic silt)
197 according to the Unified Soil Classification System (USCS), and has a specific gravity of 2.65.
198 Silt was selected for this evaluation because it is not expected to deform significantly during
199 changes in temperature or degree of saturation, and its low activity of 0.33 (plasticity index of 4
200 divided by clay size fraction of 12%) indicates that it will not have significant diffuse double layer
201 effects which could complicate thermo-hydraulic analyses. The silt specimens used in the
202 calibration process were prepared using compaction at a gravimetric water content of 13.7% to a
203 dry unit weight of 14.0 kN/m^3 , which correspond to an initial degree of saturation of 0.42 and a
204 porosity of 0.46. For reference, the optimum water content and the maximum dry unit weight
205 corresponding to the standard Proctor compaction effort are 13.6% and 16.3 kN/m^3 respectively.

206 The SWRC and HCF (in terms of the relative permeability to water) obtained from the
207 modified TRIM test on compacted Bonny silt are shown in Figure 1(a) along with the model
208 parameters. The shape of the SWRC indicates that an appreciable amount of water will be retained
209 in the soil several meters above the water table under hydrostatic conditions. The compaction
210 conditions for these curves are the same as those mentioned above, even though Lu and Dong
211 (2015) report a different porosity due to a lower value of G_s used in their calculations. An intrinsic
212 permeability of $1.27 \times 10^{-14} \text{ m}^2$ was calculated from the hydraulic conductivity of saturated soil of
213 $1.24 \times 10^{-7} \text{ m/s}$ and the values of water viscosity and density at $20 \text{ }^\circ\text{C}$ (293.15 K). The TCF and
214 VHCF for Bonny silt are shown in Figure 1(b), along with the TCF and VHCF parameters in
215 Equations (8) and (9). The value of $m = 2.62$ measured in the experiment for Bonny silt was used
216 in the simulations, which is lower than the value of 2.68 obtained from the correlation between m
217 and N_{vG} of Lu and Dong (2015). The experimental value still reflects the coupling between the

218 thermo-hydraulic properties as they were defined in the same test. The thermal conductivity ranges
219 from 1.25 to 0.37 W/mK for saturated to dry conditions, respectively, while the volumetric heat
220 capacity ranges from 2.75 to 1.30 MJ/m³K for saturated to dry conditions, respectively. The
221 variations in these parameters with degree of saturation indicate that changes in heat retention
222 within a storage volume may occur if a soil experiences drying during heat injection.

223 **Calibration of Vapor Diffusion and Phase Change Parameters**

224 To define the parameters a and b , a tank-scale heat injection experiment was performed in an
225 instrumented layer of compacted Bonny silt, which was then simulated using the parameters from
226 the thermo-hydraulic constitutive relationships defined in Figure 1. A schematic of the
227 experimental setup is shown in Figure 2. Bonny silt was compacted in 9 lifts in a cylindrical
228 aluminum container having a diameter of 550 mm and a height of 477 mm. A 215 mm-long
229 cylindrical cartridge heater having a diameter of 10 mm was used as the heating source. During
230 heat injection, a temperature control unit was used to impose a constant temperature boundary
231 condition of 60 °C on the heating rod. To monitor changes in temperature and degree of saturation
232 during heating of the soil, ten 5TM dielectric sensors manufactured by Decagon Devices of
233 Pullman, WA were placed at the locations shown in Figure 2. After all the lifts and sensors were
234 placed, the top of the soil layer was covered with several layers of plastic wrap to minimize loss
235 of water vapor to the laboratory air. The top and sides of the tank were then wrapped in insulation,
236 and thermocouples were used to monitor the temperatures of the boundaries of the tank. The soil
237 had an initial temperature of 23.5 °C and an initial degree of saturation of 0.42.

238 In the simulations of the tank-scale tests, no mass flux boundary conditions were applied for
239 both liquid water and vapor flow for all boundaries of the tank. The top boundary was thermally
240 insulated, convective heat flux boundaries were defined for the side boundaries to consider heat
241 loss from the tank, a constant temperature boundary condition was used for the heating rod, and a

242 constant temperature of 18 °C was applied at the bottom of tank. The system of partial differential
243 equations in Table 1 was solved simultaneously using COMSOL Multiphysics software. Results
244 from the numerical analyses were then compared with the experimental results to calibrate the
245 parameters a and b . Comparisons of predicted and measured time series of temperature and degree
246 of saturation inferred from dielectric sensor #3 are shown in Figures 3(a) to 3(d). Sensor #3 was
247 selected as the primary location for calibration of the model as it is near the center of the heating
248 rod and is relatively close to the heat exchanger. The predicted time series in these figures include
249 curves for different values of the fitting parameters a and b . The parameters are observed to have
250 a greater effect on the change in degree of saturation as they control the rates of vapor diffusion
251 and water phase change. Simulations from a model where no vapor diffusion or phase change is
252 considered (hereafter referred to as the “no vapor” case) are also shown in Figures 3(a) and 3(b),
253 which indicate slower increases in temperature to lower magnitudes at this location as well as a
254 negligible change in degree of saturation. Values of $a = 30$ and $b = 5 \times 10^{-7} \text{ s/m}^2$ were found to best
255 fit the Bonny silt data based on visual inspection, a similar approach used by Smits et al. (2011).

256 To evaluate the calibration, the spatial distributions of temperature and degree of saturation
257 along Transects B and A at the end of the heating from the numerical simulations and the
258 experiments are shown in Figures 4(a) through 4(d). In most of the cases, the predicted profiles
259 show good agreement with the measured data, except in the case of the degree of saturation
260 measured by the sensor nearest the edge of container in Figure 4(b). This sensor may have
261 malfunctioned due to the compaction process. Overall, the comparisons between model predictions
262 and experimental results in Figures 3 and 4 indicate that the calibrated values of a and b can be
263 assumed to be representative of Bonny silt under these compaction conditions.

264 **EVALUATION OF VAPOR DIFFUSION AND PHASE CHANGE AROUND A FIELD-** 265 **SCALE GEOTHERMAL HEAT EXCHANGER**

266 **Scenario Considered**

267 The main goal of this study is to use the calibrated parameters to understand the changes in the
268 behavior of a layer of unsaturated Bonny silt surrounding a geothermal heat exchanger during a
269 heating and cooling cycle representative of geothermal energy storage systems. Although
270 geothermal heat storage systems typically involve an array of geothermal heat exchangers with
271 spacings as close as 1.5 m (Baser et al. 2016a), this study focuses on the changes in soil behavior
272 around a single geothermal heat exchanger. This choice simplifies the boundary conditions and
273 permits evaluation of the relative effects of the different heat transfer mechanisms. It is possible
274 that the close spacing between geothermal heat exchangers may lead to different distributions in
275 temperature and degree of saturation than those observed in this evaluation due to interactions
276 between heat exchangers, but the simpler scenario of a single vertical geothermal heat exchanger
277 is evaluated in this paper to help establish the impact of a heating-cooling cycle on the distributions
278 in temperature and degree of saturation in the surrounding unsaturated silt layer.

279 The vertical geothermal heat exchanger investigated in this study has a length of 25 m and a
280 radius of 0.04 m, embedded at a depth of 1 m from the surface. The embedment is consistent with
281 the practice of installing geothermal heat exchangers below the frost depth. Even though this
282 scenario could be investigated using an axisymmetric analysis, a 3D simulation was performed for
283 a rectangular domain so that the domain could be modified to incorporate additional geothermal
284 heat exchangers in future studies. The quarter domain having a height of 30 m and a width of 10 m
285 with the geothermal heat exchanger along one edge is shown in Figure 5. The entire domain was
286 assumed to be uniform and isotropic, and the soil was discretized into 101,073 elements (394,394

287 degrees of freedom) with finer elements around the heat exchanger. The hydraulic and thermal
288 boundary conditions for the models are also shown in Figure 5. For liquid water and gas flow,
289 Neumann boundary conditions (no mass flux) were assumed for all boundaries except the bottom
290 boundary, which was set to be a constant head boundary condition corresponding to the water
291 table. For heat transfer, a constant temperature that represents an average mean subsurface soil
292 temperature of 21 °C was applied at the bottom while at the outer boundaries the temperature
293 varied with depth. No flux boundary conditions were applied to the planes of symmetry. The size
294 of the domain was selected to be large enough that a constant temperature and zero fluid flux could
295 be assumed on the outer vertical boundaries.

296 The initial conditions are shown in the color bars in Figure 5. The initial ambient temperature
297 of the domain was assumed to be a function of depth until a certain depth of 9 m from surface, and
298 this initial temperature profile is a representative of early summer months in San Diego
299 (specifically May 2015). A hydrostatic initial condition was assumed, so the soil along the length
300 of the heat exchanger is unsaturated with initial degrees of saturation ranging from 0.50 to 0.21
301 depending on the height from the water table. Two locations of interest that will be investigated
302 further are noted in Figure 5(b) having different initial degrees of saturation.

303 During heat injection, a constant heat flux of 50 W/m² was applied to the outer boundary of
304 the geothermal heat exchanger. This heat flux was converted to a volumetric heat source to obtain
305 the value of Q in Equation (6). Although the magnitude of heat flux used in this study is
306 representative of average value in geothermal energy storage systems (Acuña et al. 2012; Welsch
307 et al. 2015; McCartney et al. 2017), a constant heat flux is not expected in a system where solar
308 thermal panels are the heat source. In these cases, the input temperature from the solar thermal
309 panels will remain relatively constant, which means that the heat flux will decrease with time as

310 the subsurface warms (Welsch et al. 2015). Although use of a constant heat flux will lead to greater
311 increases in ground temperature than those expected when using solar thermal panels as the heat
312 source, it provides a simple boundary condition for evaluating the roles of different heat transfer
313 mechanisms in unsaturated soils.

314 **Heat Transfer and Water Flow Evaluation**

315 The temperature time series at a distance of 0.05 m from the geothermal heat exchanger and a
316 depth of 8.5 m from the surface (i.e., $S_{r0} = 0.25$) is shown in Figure 6(a). After the 90-day heat
317 injection period, the ground temperature reached a maximum value of 45.6 °C at this location. For
318 comparison, the temperature time series from the model where no vapor diffusion or phase change
319 is considered (the no vapor case) is also shown in Figure 6(a). In addition to showing a slower rate
320 of increase in temperature, a lower maximum temperature of 36.3 °C was observed for the no
321 vapor case. After the heating injection period, the heat flux was set to 0 W/m² and the soil was
322 allowed to cool ambiently. After 180 days from the start of the simulation (90 days after the end
323 of heat injection), the temperature decreased to 22.8 °C for the model with vapor diffusion and
324 phase change and to 21.8 °C for the no vapor case. Although the gradients for heat loss are higher
325 in the model with vapor diffusion and phase change, more heat is retained at this location after the
326 180-day cooling period due to the decrease in degree of saturation of the soil during heat injection
327 due to vapor diffusion and latent heat transfer observed in Figure 6(b). Specifically, at the end of
328 the heat injection period, a decrease in degree of saturation of 0.14 at this depth was observed for
329 the model with vapor diffusion and phase change, while a negligible decrease in degree of
330 saturation of 0.01 was observed for the no vapor case. The greater decrease in the degree of
331 saturation for the model with vapor diffusion and phase change led to a decrease in thermal
332 conductivity according to the TCF (from 0.84 to 0.49 W/mK), which will be assessed in more

333 detail later. Another interesting observation from Figure 6(b) is that at the end of the 90-day
334 cooling period, only 16.5% of the decrease in degree of saturation observed during heat injection
335 was recovered, indicating that the drying near the heat exchanger was permanent from a practical
336 point of view. This may have an impact on subsequent heat injection and cooling cycles, and may
337 be one of the reasons that an increase in the ground temperature is observed after several cycles of
338 heat injection and extraction in practice (Sibbitt et al. 2012).

339 Radial distributions in temperature at a depth of 8.5 m from the surface at the ends of the heat
340 injection and cooling periods are shown in Figure 7(a). Heat injection led to a notable change in
341 temperature up to a distance of about 3 m from the heat exchanger. The temperature at the location
342 of the heat exchanger was nearly 10 °C greater when vapor diffusion and latent heat transfer was
343 considered than the case when it was not, and the temperature at the end of the ambient cooling
344 period was greater throughout the zone of influence. A decrease in degree of saturation was only
345 observed within approximately 1 m from heat exchanger for the model with vapor diffusion and
346 phase change, as shown in Figure 7(b). A slight decrease in degree of saturation was observed near
347 the heat exchanger for the no vapor case due to thermally-induced liquid flow. The zone of
348 influence for temperature changes is greater than the zone of influence for degree of saturation
349 changes for the conditions evaluated. For Bonny silt, this indicates that an overlap in the effects of
350 different heat exchangers may be observed for the typical geothermal heat exchanger spacing of
351 1.5 m in geothermal energy storage systems.

352 Profiles of temperature with depth at horizontal distances of 0.05 m and 0.20 m from the heat
353 exchanger at the end the 90-day heat injection period are shown in Figure 8(a). The temperature
354 profiles varied nonlinearly with depth and had a maximum value at a depth of 4.5 m from the
355 surface. For comparison, the temperature profiles for the no vapor case show more uniform

356 distributions in temperature with depth at the end of the heat injection period. The difference in
357 temperature observed with depth in both models is due to the thermo-hydraulic properties with
358 depth associated with the variations in initial degree of saturation with depth shown in Figure 5. A
359 significant decrease in the in degree of saturation with depth is observed at both horizontal
360 distances for the model with vapor diffusion and phase change in Figure 8(b), while only a slight
361 decrease was observed for the no vapor case. Profiles of temperature after the ambient cooling are
362 shown in Figure 8(c), with the profiles at horizontal distances of 0.05 m and 0.20 m overlapping.
363 Although most of the heat injected has dissipated away from the heat exchanger, a greater amount
364 of heat was retained in the soil close to the heat exchanger for the model with vapor diffusion and
365 phase change. The profiles of degree of saturation at the end of the cooling period shown in Figure
366 8(d) only show slight increases from the profiles observed in Figure 8(b).

367 The impact of the initial degree of saturation on heat transfer and water flow can be investigated
368 by evaluating the transient response at different depths in the soil profile, which have different
369 initial degrees of saturation. Time series of temperature at depths of 8.5 m and 24.5 m from the
370 surface at a horizontal distance of 0.05 m from the heat exchanger corresponding to initial degrees
371 of saturation of 0.25 and 0.50 are shown in Figure 9(a). Increases in temperature of 45.6 and
372 42.3 °C at the end of the heat injection period were observed when the initial degree of saturation
373 was doubled from 0.25 to 0.50. However, decreases in degree of saturation of 0.14 and 0.35 were
374 observed at the end of the heat injection period for the same depths, as shown in Figure 9(b). The
375 greater decrease in degree of saturation for the initially wetter soil is likely due to the availability
376 of water to evaporate from the region near the heat exchanger. The horizontal zone of influence of
377 the change in temperature is similar for the two depths as shown in Figure 9(c), but the horizontal
378 zone of influence of the change in degree of saturation was greater at the depth of 8.5 m as shown

379 in Figure 9(d). This is consistent with observations that dryer initial conditions lead to greater
380 zones of influence of vapor diffusion (e.g., Smits et al. 2011). The soil with $S_{r0}=0.50$ also shows a
381 slight wetting front due to the movement of water away from the heat exchanger.

382 **Assessment of Heat Transfer Mechanisms and Effects of Coupled Flow**

383 Profiles of thermal conductivity and volumetric heat capacity that correspond to the profiles of
384 degree of saturation in Figure 8(b) are shown in Figures 10(a) and 10(b), respectively. Despite the
385 nonlinear decrease in degree of saturation along the length of the heat exchanger, a comparatively
386 uniform decrease of approximately 0.3 W/mK is observed at 0.05 m from the heat exchanger. A
387 more nonlinear decrease in thermal conductivity is observed further away from the heat exchanger
388 at 0.20 m. The shapes of the profiles of the volumetric heat capacity are the same as those for the
389 thermal conductivity due to the same parameters used in Equations (8) and (9), but because of the
390 range of the two relationships for Bonny silt the volumetric heat capacity decreased by as much as
391 25% while the thermal conductivity decreased by as much as 70%. This is a positive finding for
392 geothermal energy storage in similar soil deposits, as it means that lower heat losses can be
393 expected without a significant reduction in the quantity of heat stored.

394 The vapor diffusion and latent heat transfer that results in the drying around the heat exchanger
395 also leads to a suction gradient that may result in liquid water flow back toward the heat exchanger.
396 Horizontal profiles of suction profiles at a depth of 8.5 m ($S_{r0}=0.25$) at different times are shown
397 in figure 11(a). Large increases in suction are observed within 0.6 m from the heat exchanger, with
398 decreases in suction beyond that point. Despite the large gradient associated with the suction
399 distribution at the end of the heating period, the suction did not return to its original distribution
400 during the ambient cooling period. This may have been due to the order of magnitude decrease in

401 the hydraulic conductivity (adjusted for temperature effects) shown in Figure 11(b), indicating that
402 more time may be needed for liquid flow to occur than permitted in the 90-day cooling period.

403 Vapor concentrations (kg/m^3) near the heat exchanger normalized by the equilibrium vapor
404 concentration (kg/m^3) are shown in Figure 12(a) for Bonny silt with initial degrees of saturation
405 of 0.25 and 0.50 (depths of 8.5 and 24.5 m). When the normalized vapor concentration is greater
406 or equal to 0.75, the phase change in the soil can be assumed to be near equilibrium (Lozano et al.
407 2008). For an initial degree of saturation of 0.25, the normalized vapor concentration soon after
408 the start of heating was smaller than this limit. The normalized vapor concentration decreased to
409 0.63 at the end of the heating period, indicating that use of the nonequilibrium model was justified.
410 For an initial degree of saturation of 0.5, the normalized vapor concentration was 0.82 soon after
411 the start of heating and remained above 0.75 indicating that an equilibrium phase change
412 assumption may be valid for initially wetter soils. The time series in Figure 12(a) indicate that the
413 phase change process did not reach steady state conditions by the end of the heat injection period.
414 Horizontal profiles of the normalized vapor concentrations at the end of heating shown in Figure
415 12(b) indicate that lower vapor concentrations were present near the heat source and had a similar
416 zone of influence to the degree of saturation in Figure 7(b). Despite the higher magnitudes of
417 normalized vapor concentration, greater changes in normalized vapor concentration with
418 horizontal distance are observed for the initially wetter soil ($S_{r0}=0.5$), which may be the reason for
419 the greater change in degree of saturation at this location. Vertical profiles of normalized vapor
420 concentration at the end in Figure 12(c) are similar to those for the degree of saturation in Figure
421 8(b). A higher vapor concentration was observed close to the surface because of the lower initial
422 degrees of saturation and higher temperatures and because of upward movement of water vapor
423 due to buoyancy effects.

424 Horizontal profiles of the latent heat transfer rate, calculated as the product of $L_w R_{gw}$ in
425 Equation (6), at the end of heat injection for soil at depths corresponding to initial degrees of
426 saturation of 0.25 and 0.50 are shown in Figure 13(a). While a positive latent heat transfer rate was
427 higher near the heat source indicating evaporation, a very slight value less than zero was observed
428 at a distance about 1 m away from the heat exchanger. This indicates that condensation is occurring
429 in the soil at lower temperatures further from the heat source. A comparison between the total
430 thermal energy injected into the geothermal heat exchanger and the total latent heat (i.e., the total
431 energy associated with phase change calculated by integrating the product of $L_w R_{gw}$ over the
432 volume of the domain and over time) is shown in Figure 13(b). The total energy associated with
433 phase change at the end of 90 days was 44 MJ, which is approximately 24% of the total heat
434 injected into the system of 180 MJ. This indicates that an appreciable amount of the thermal energy
435 injected into the system leads to phase change and further justifies the need to accurately account
436 for nonequilibrium phase change effects in unsaturated soils. The total latent heat appears to have
437 stabilized over the heat injection period, which may be because of the decrease in degree of
438 saturation and reduction in availability of water to change phase near the heat exchanger.

439 **CONCLUSIONS**

440 A model that includes a recently-developed set of thermo-hydraulic constitutive relationships
441 was used to understand the roles of vapor diffusion and phase change on the coupled heat transfer
442 and water flow in a fine-grained, non-deformable unsaturated silt layer initially under hydrostatic
443 conditions surrounding a vertical geothermal heat exchanger during heat injection and ambient
444 cooling. In general, the modeling results confirm the importance of considering vapor diffusion
445 and water phase change in simulations of geothermal heat exchangers in unsaturated soils, as well
446 as the relevance of considering nonequilibrium phase change in initially drier soil layers. Although

447 quantitative conclusions from the simulations are specific to the given soil and geometry
448 investigated, several conclusions can be drawn regarding the use of geothermal heat exchangers
449 in geothermal energy storage systems in unsaturated soils, including:

- 450 • A greater rate of increase in temperature and greater magnitude of temperature change were
451 observed in the soil near the heat exchanger during heat injection in a model that includes
452 enhanced vapor diffusion and phase change. This conclusion indicates that conduction-only
453 design models may underestimate the heat injection response of geothermal energy storage
454 systems in the vadose zone.
- 455 • The heat retained in the soil near the heat exchanger during an ambient cooling period was
456 greater when considering vapor diffusion and phase change, despite the greater thermal
457 gradient compared to a model with no vapor. This was found to be due to the decrease in
458 thermal conductivity associated with drying during heat injection. The drying during heat
459 injection can be considered permanent for practical purposes within the time frame of ambient
460 cooling considered. This may partially be due to the decrease in hydraulic conductivity due to
461 thermally-induced drying, leading to a negligible amount of liquid water flow back toward the
462 heat exchanger during ambient cooling.
- 463 • Although reductions in both thermal conductivity and volumetric heat capacity are observed
464 during thermally induced drying of the soil near the geothermal heat exchanger, the percentage
465 reductions in thermal conductivity were greater. This indicates that the greater amount of heat
466 retention can be expected in unsaturated soils during ambient cooling, but the maximum
467 possible heat stored will not decrease by as large of an amount.
- 468 • The zone of influence of changes in temperature was observed to be greater than the zone of
469 influence of changes in degree of saturation for the silt under investigation, but both zones of

470 influence are appreciable enough that overlap is expected in geothermal energy storage
471 systems with closely-spaced geothermal heat exchangers (i.e., 1.5 to 2.0 m).

- 472 • The normalized vapor concentrations in the initially drier soil near the ground surface were
473 below the limit at which nonequilibrium phase change is expected to occur, justifying the use
474 of this more advanced modeling approach. The vapor concentration gradient was greater in the
475 initially wetter soil deeper in the profile
- 476 • The initial degree of saturation was observed to influence both heat transfer and water flow in
477 the model with vapor diffusion and phase change, with the greatest change in the degree of
478 saturation occurring for soil with initially higher degrees of saturation.

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663

664

TABLE 1. Equations used in the numerical analyses

Equation	Number	Reference
<p><i>Nonisothermal liquid flow governing equation:</i></p> $nS_{rw} \frac{\partial \rho_w}{\partial t} + n\rho_w \frac{dS_{rw}}{dP_c} \frac{\partial P_c}{\partial t} + \nabla \cdot \left[\rho_w \left(-\frac{k_{rw} \kappa}{\mu_w} \right) \nabla (P_w + \rho_w g z) \right] = -R_{gw}$ <p>n=porosity (m³/m³), S_{rw}=degree of water saturation (m³/m³), ρ_w=temperature-dependent density of water (kg/m³) (Hillel 1980), t=time(s), P_c=P_w-P_g=capillary pressure (Pa), P_w=pore water pressure (Pa), P_g=pore gas pressure (Pa), k_{rw}=relative permeability function for water (m/s); κ=intrinsic permeability (m²); μ_w=temperature-dependent water dynamic viscosity (kg/(ms)) (Lide 2001), g=acceleration due to gravity (m/s²) R_{gw}=Phase change rate (kg/m³s)</p>	(1)	(Bear 1972; Moradi et al. 2016)
<p><i>Nonisothermal gas flow governing equation:</i></p> $nS_{rg} \frac{\partial \rho_g}{\partial t} + n\rho_g \frac{dS_{rg}}{dP_c} \frac{\partial P_c}{\partial t} + \nabla \cdot \left[\rho_g \left(-\frac{k_{rg} \kappa}{\mu_g} \right) \nabla (P_g + \rho_g g z) \right] = R_{gw}$ <p>S_{rg}=degree of gas saturation (m³/m³), ρ_g=temperature-dependent density of gas (kg/m³) (Smits et al. 2011), k_{rg}=relative permeability function for gas (m/s); μ_g=temperature-dependent gas dynamic viscosity (kg/(ms))</p>	(2)	(Bear 1972; Moradi et al. 2016)
<p><i>Water vapor mass balance equation:</i></p> $n \frac{\partial (\rho_g S_{rg} w_v)}{\partial t} + \nabla \cdot (\rho_g u_{gv} - D_e \rho_g \nabla w_v) = R_{gw}$ <p>D_e=D_vτ=effective diffusion coefficient (m²/s), D_v=diffusion coefficient of water vapor in air (m²/s) (Campbell 1985), w_v=mass fraction of water vapor in the gas phase (kg/kg), τ=n^{1/3}S_{rg}^{7/3}η=tortuosity (Millington and Quirk 1961)</p>	(3)	(Smits et al. 2011)
<p><i>Enhancement factor for vapor diffusion, η:</i></p> $\eta = a + 3S_{rw}^{-(a-1)} \exp \left\{ - \left[\left(1 + \frac{2.6}{\sqrt{f_c}} \right) S_{rw} \right]^3 \right\}$ <p>a=empirical fitting parameter, f_c= clay content</p>	(4)	(Cass et al. 1984)
<p><i>Nonequilibrium gas phase change rate, R_{gw} (kg/m³s):</i></p> $R_{gw} = \left(\frac{bS_{rw} RT}{M_w} \right) (\rho_{veq} - \rho_v)$ <p>b=empirical fitting parameter (s/m²), R=universal gas constant (J/molK), ρ_{veq}=c_{v,sat}R_{h,eq}=equilibrium vapor density (kg/m³), T=Temperature (K), ρ_v=ρ_gw_v=vapor density (kg/m³), M_w=molecular weight of water (kg/mol)</p>	(5)	(Bixler 1985; Zhang and Datta 2004; Moradi et al. 2016)
<p><i>Heat transfer energy balance:</i></p> $(\rho C_p) \frac{\partial T}{\partial t} + \nabla \cdot ((\rho_w C_{pw}) u_w T + (\rho_g C_{pg}) u_g T - (\lambda \nabla T)) = -L_w R_{gw} + Q$ <p>ρ=total density of soil (kg/m³), C_p=specific heat of soil (J/kgK), C_{pw}=specific heat capacity of water (J/kgK), C_{pg}=specific heat capacity of gas (J/kgK), λ=thermal conductivity (W/mK), L_w=latent heat of water vaporization (J/kg), u_w=water velocity (m/s), u_g=gas velocity (m/s), Q=heat source term (W/m³)</p>	(6)	(Whitaker 1977; Moradi et al. 2016)

666 **LIST OF FIGURE CAPTIONS**

667 **FIG. 1.** Hydraulic and thermal constitutive relationships and relevant parameters for Bonny silt:

668 (a) SWRC and HCF; (b) TCF and VHCF

669 **FIG. 2.** Cross-sectional elevation view of the experimental setup for model calibration with

670 dielectric sensor locations

671 **FIG. 3.** Predicted and measured time series from the tank-scale heating test: (a) Soil temperatures

672 for different values of a ; (b) Changes in degree of saturation for different values of a ; (c)

673 Soil temperatures for different values of b ; (d) Changes in degree of saturation for different

674 values of b

675 **FIG. 4.** Simulated and observed temperatures and changes in degree of saturation: (a) Horizontal

676 temperature profile; (b) Horizontal change in degree of saturation profile; (c) Vertical

677 temperature profile; (d) Vertical change in degree of saturation profile

678 **FIG. 5.** Initial and boundary conditions on the quarter domain model for a field-scale geothermal

679 heat exchanger: (a) Thermal; (b) Hydraulic

680 **FIG. 6.** Comparisons of the effects of heat transfer mechanisms and heat flux for a 90-day heat

681 injection period followed by cooling: (a) Temperature time series; (b) Degree of saturation

682 time series

683 **FIG. 7.** Effects of including vapor flow in the coupled analysis; (a) Radial profiles of temperature

684 at a depth of 9.5 m (an initial degree of saturation of 0.25) at the end of heating and cooling;

685 (b) Radial profiles of degree of saturation profiles before and after heating

686 **FIG. 8.** Vertical profiles for comparison of different heat transfer mechanisms: (a) Temperature at

687 the end of a 90-day heat injection period; (b) Degree of saturation at the end of a 90-day

688 heat injection period; (c) Temperature at the end of a 90-day cooling period; (d) Degree of
689 saturation at the end of a 90-day cooling period

690 **FIG. 9.** Effect of initial degree of saturation: (a) Time series of temperature; (b) Time series of
691 degree of saturation; (c) Radial temperature profiles; (d) Radial degree of saturation
692 profiles

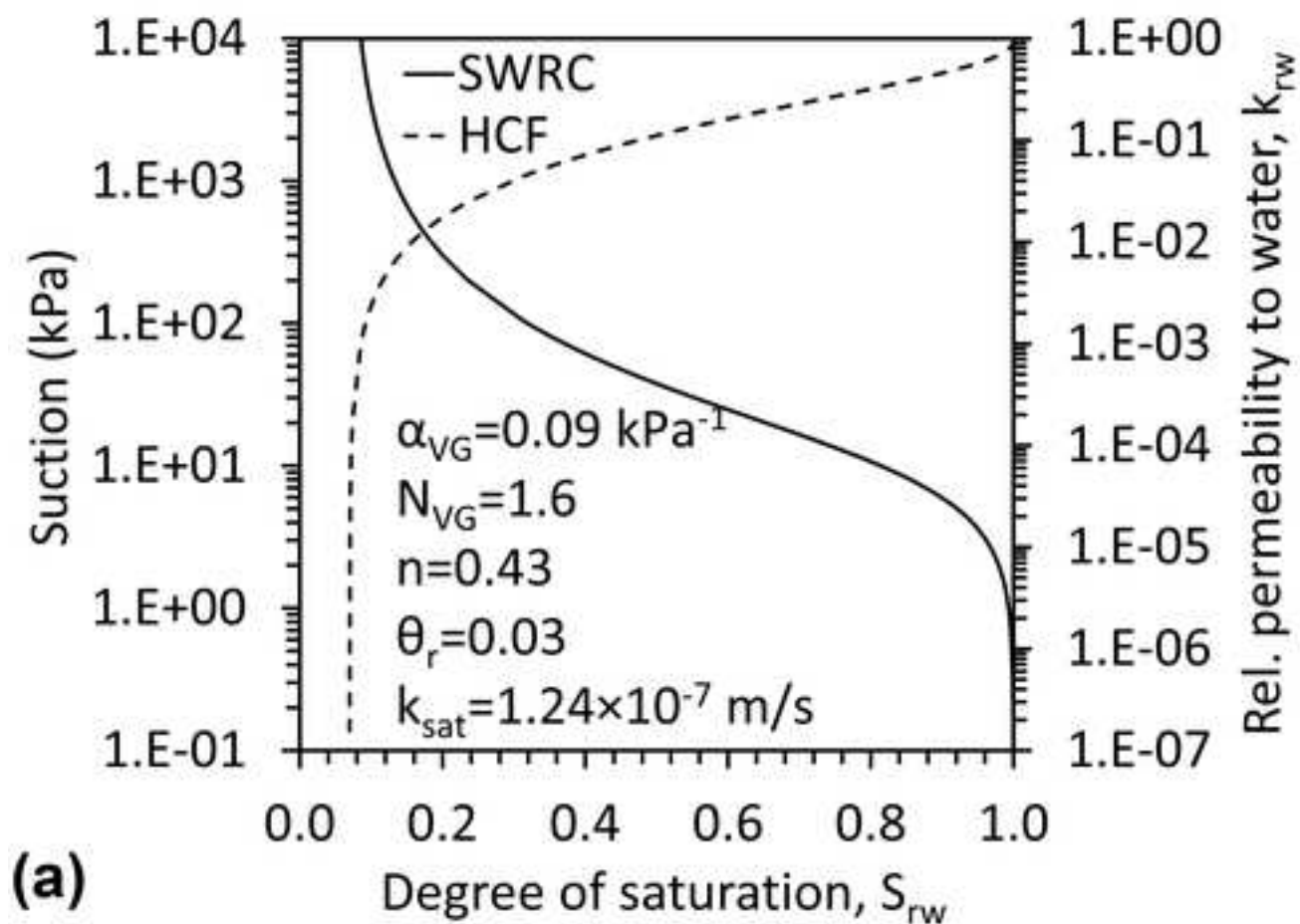
693 **FIG. 10.** Thermal property evaluation at the end of heat injection: (a) Thermal conductivity
694 profiles; (b) Volumetric heat capacity profiles

695 **FIG. 11.** Liquid water flow evaluation: (a) Horizontal profiles of suction at different times;
696 (b) Horizontal profiles of hydraulic conductivity at different times

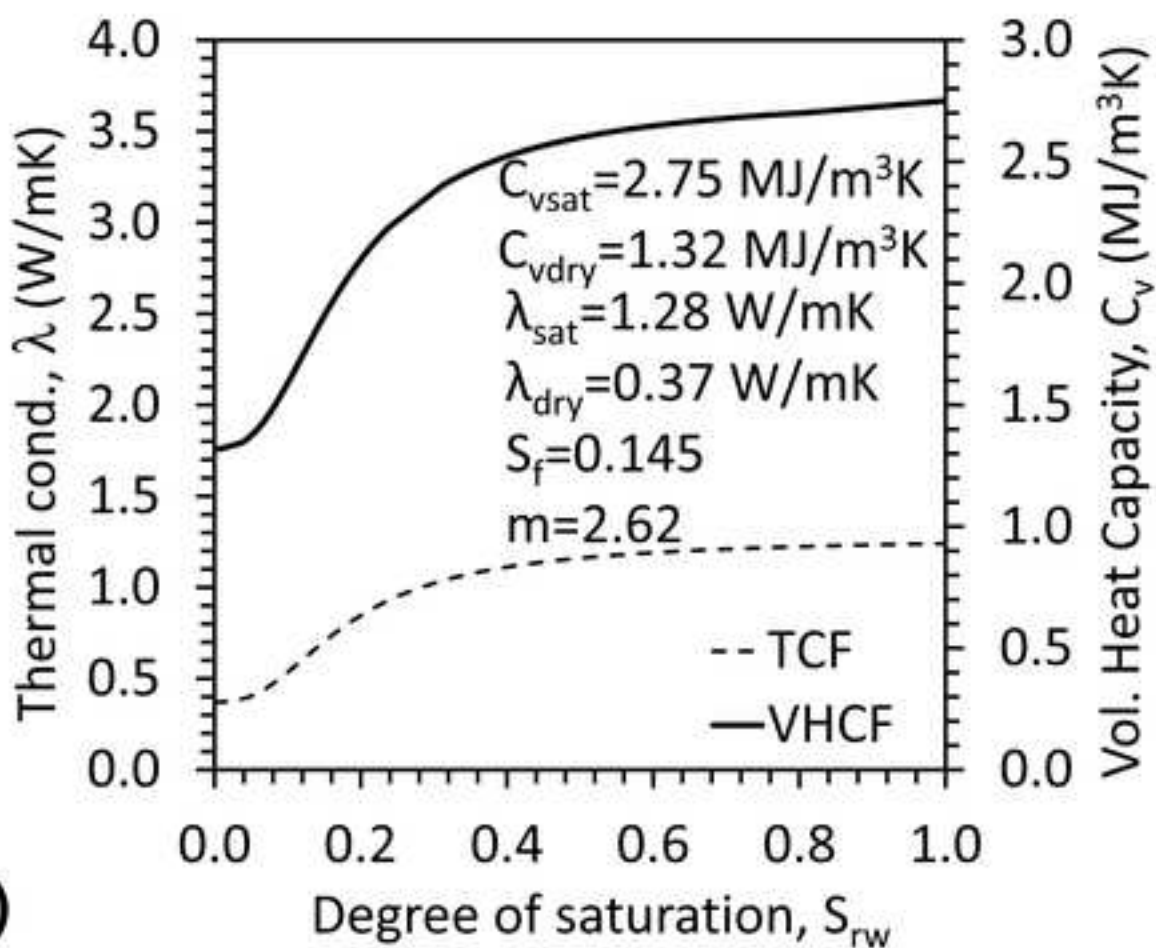
697 **FIG. 12.** Vapor concentrations normalized by the equilibrium vapor concentration: (a) Time
698 series; (b) Horizontal profiles at the end of heating; (c) Vertical profiles at the end of
699 heating

700 **FIG. 13.** (a) Distributions of latent heat transfer rate at depths corresponding to initial degrees of
701 saturation of 0.25 and 0.50; (b) Comparison of the total heat injected with the energy due
702 to phase change

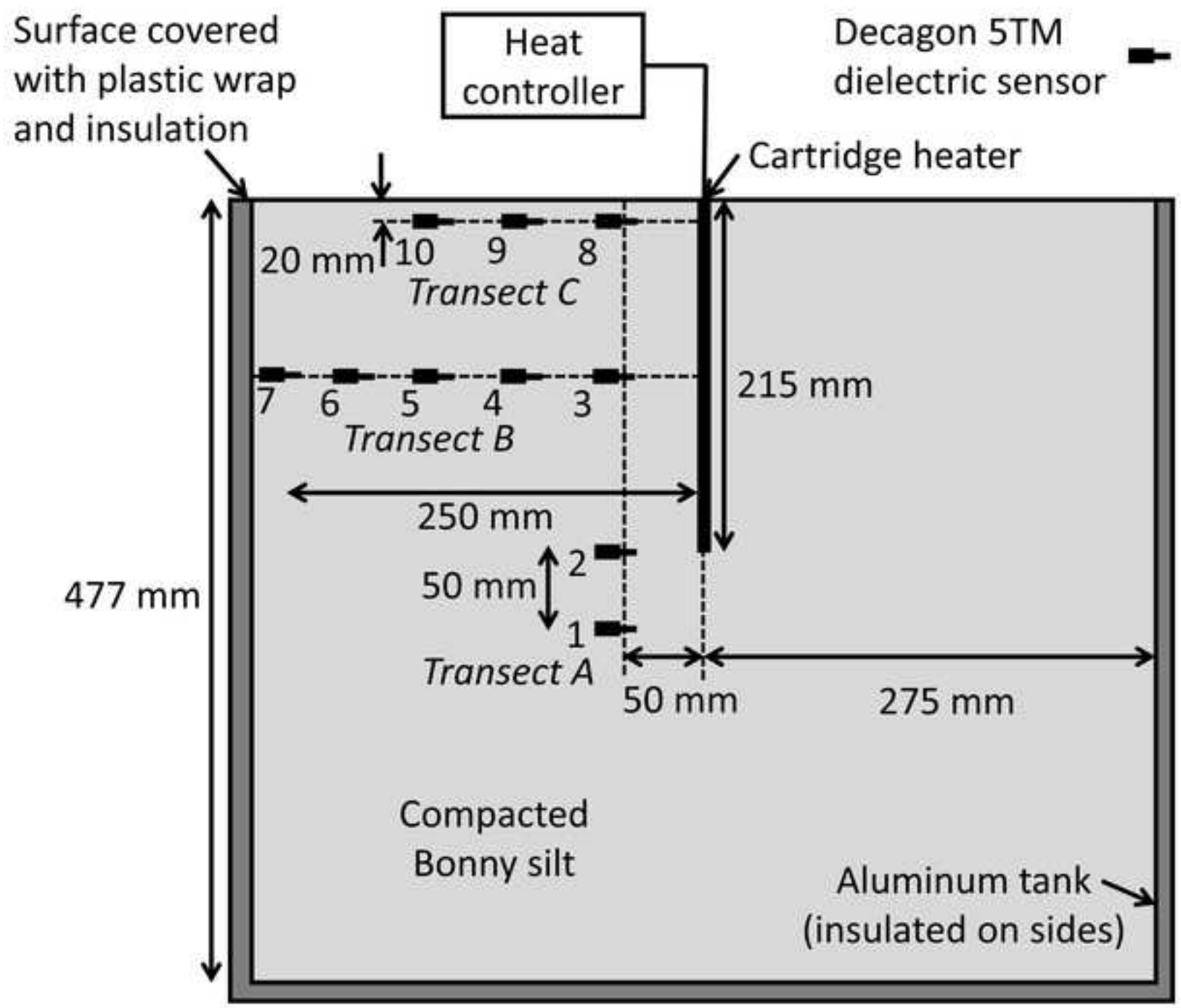
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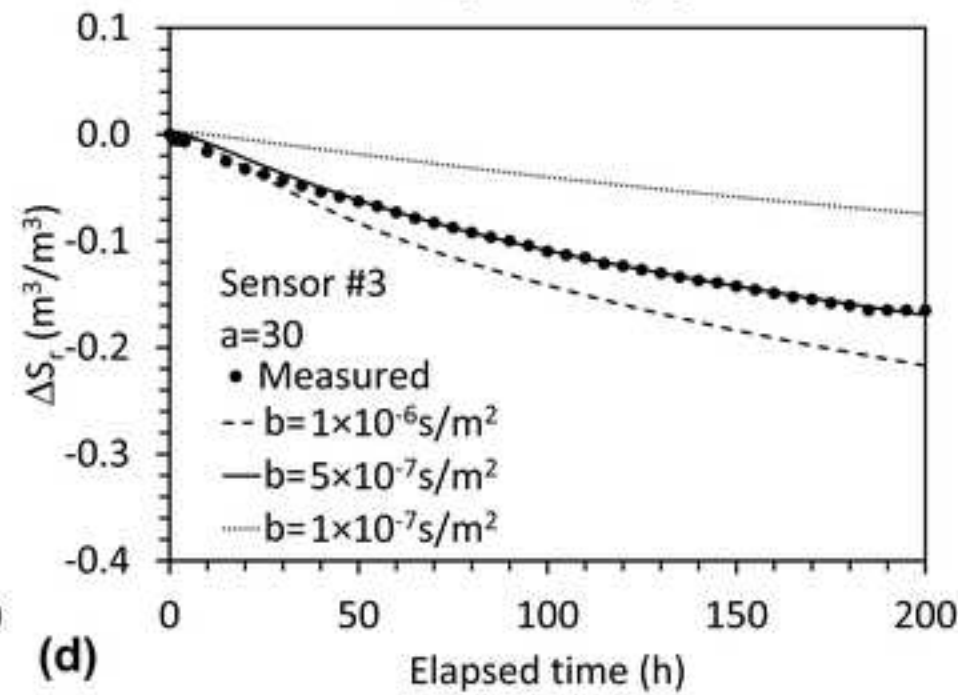
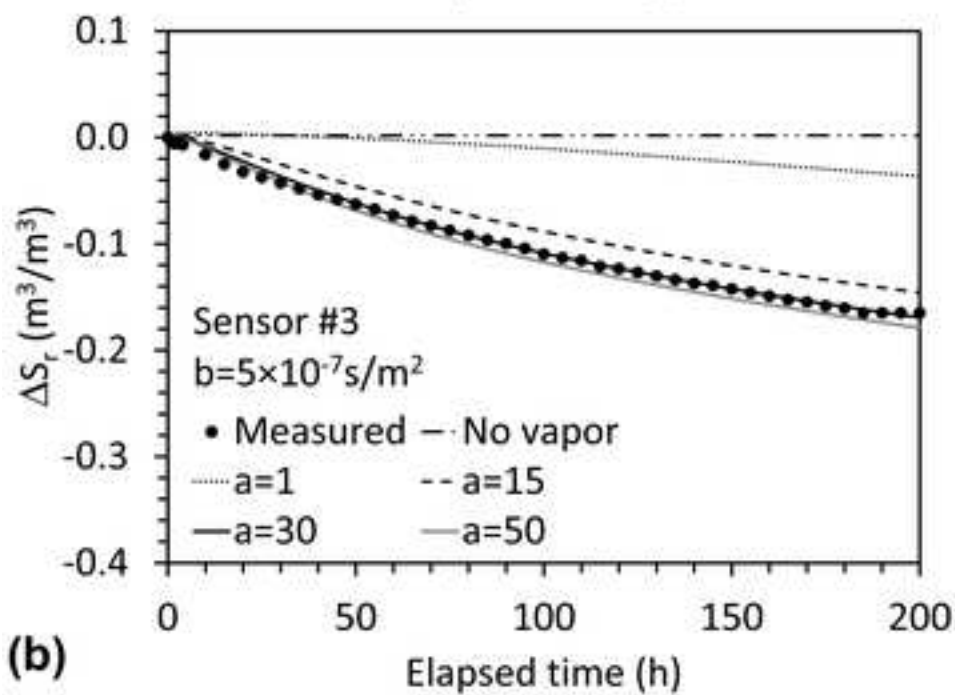
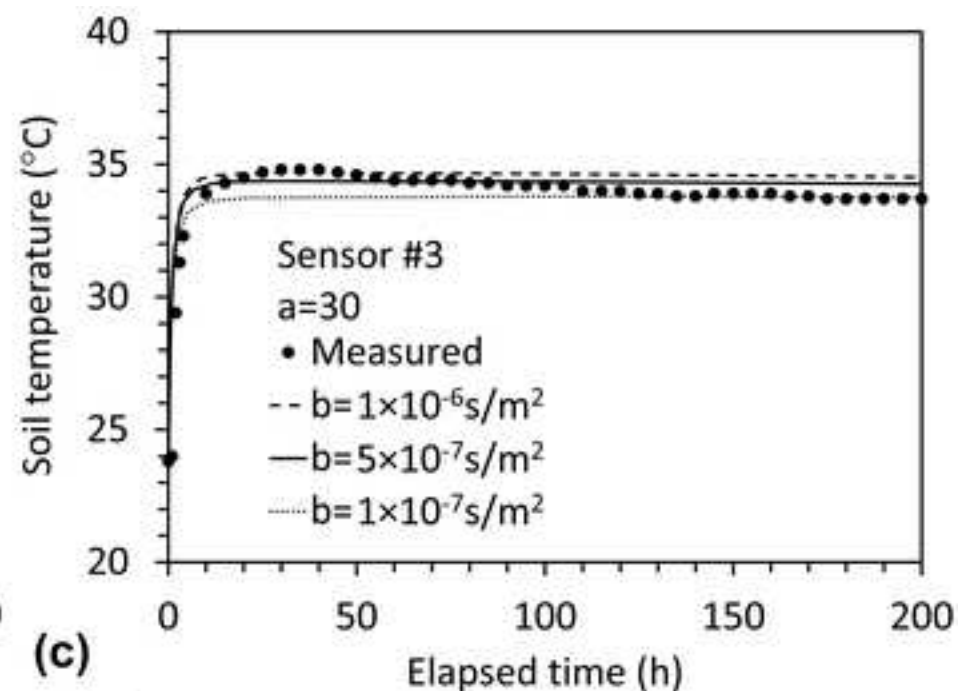
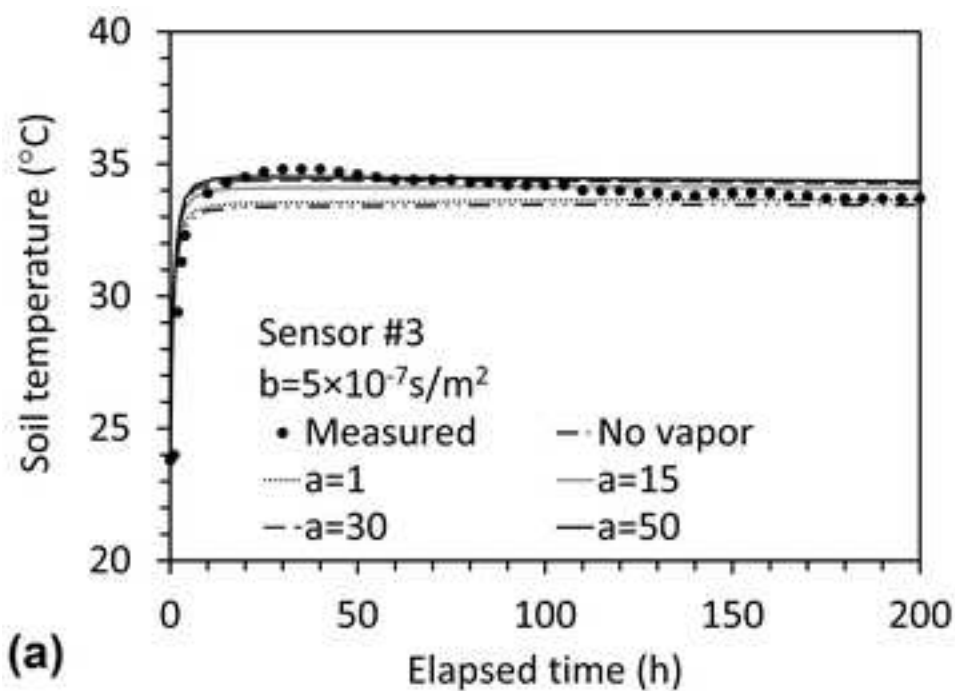


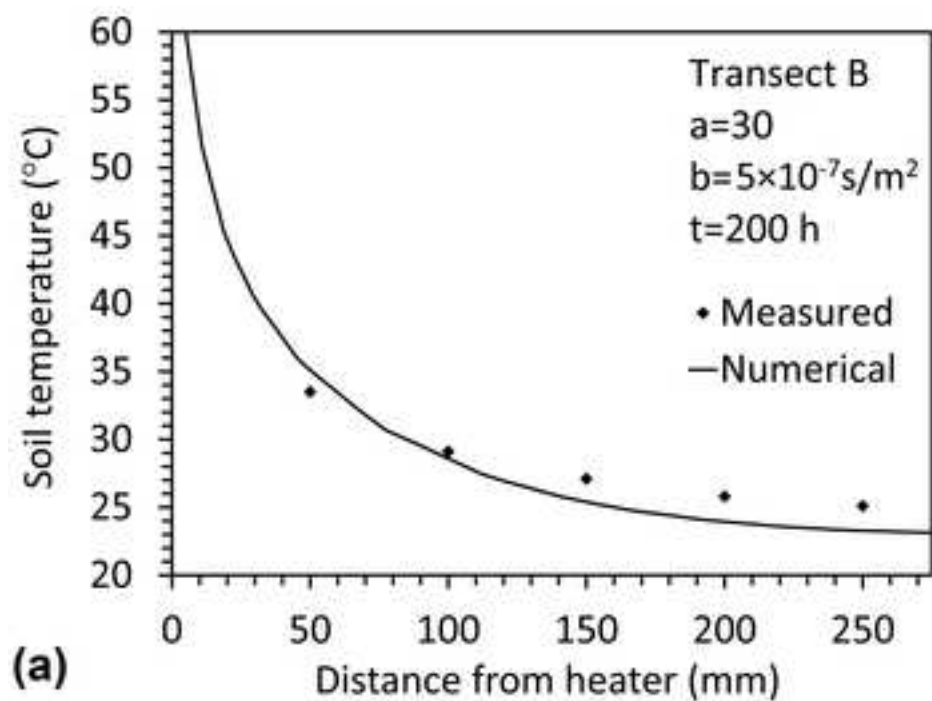
(a)



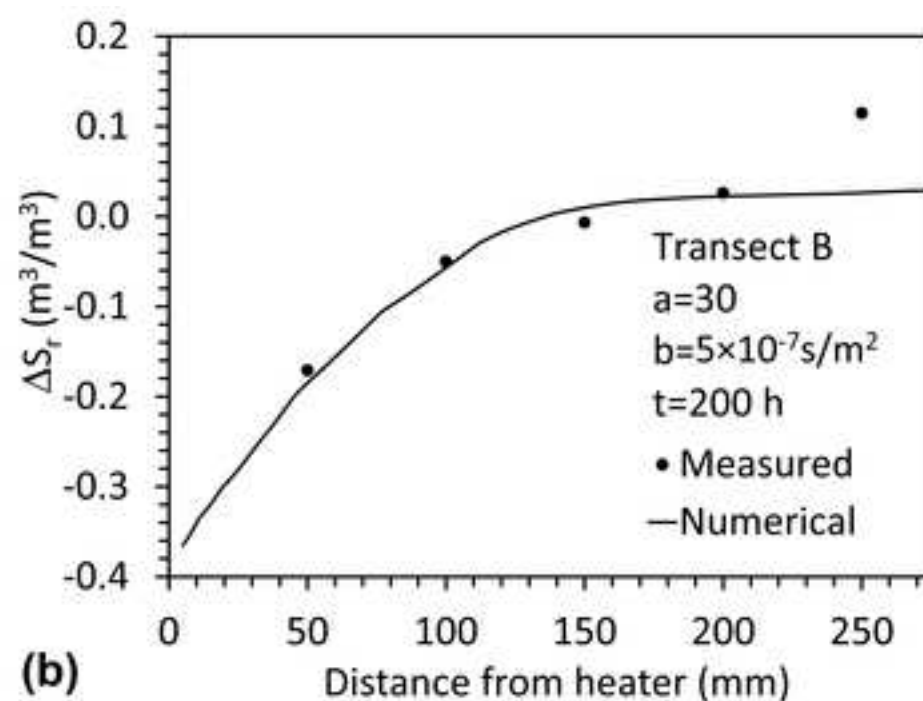
(b)





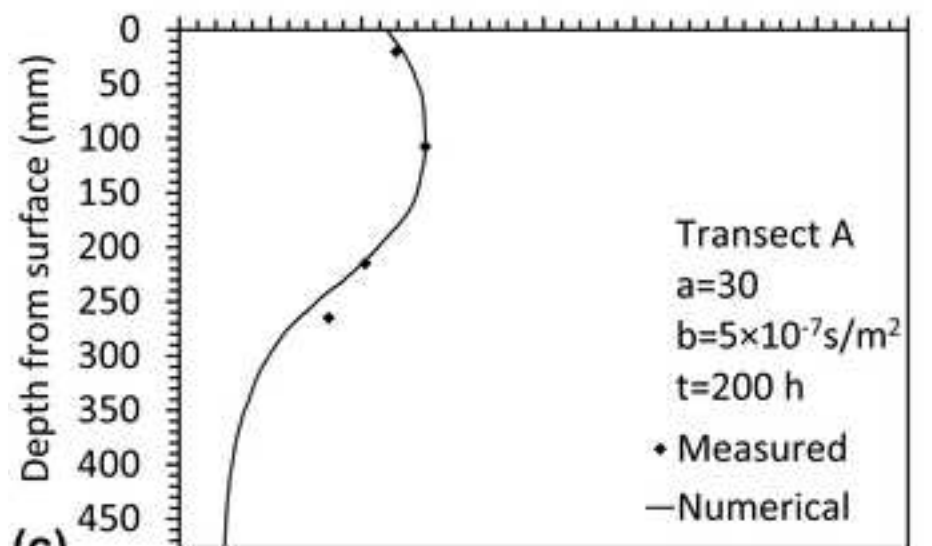


(a)



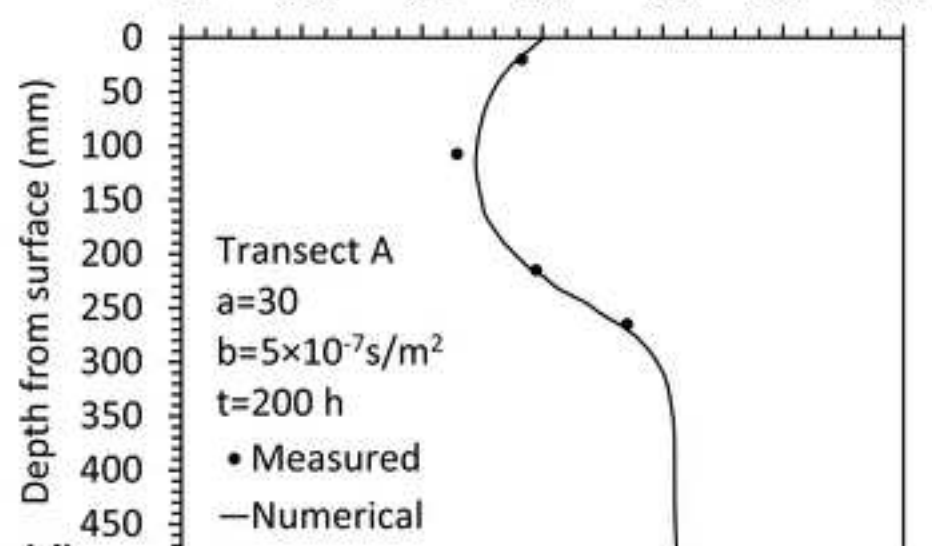
(b)

Soil temperature (°C)
 20 25 30 35 40 45 50 55 60

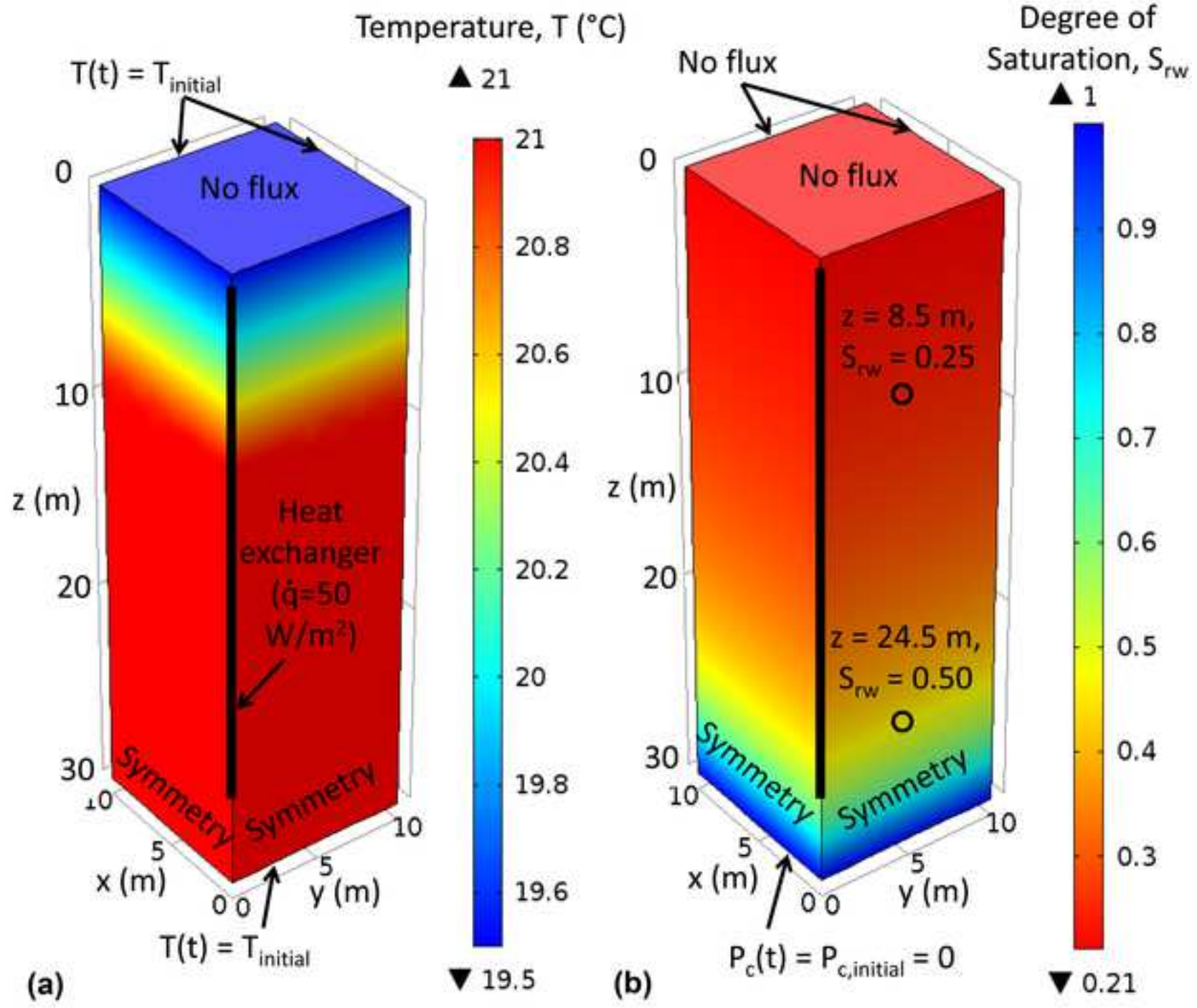


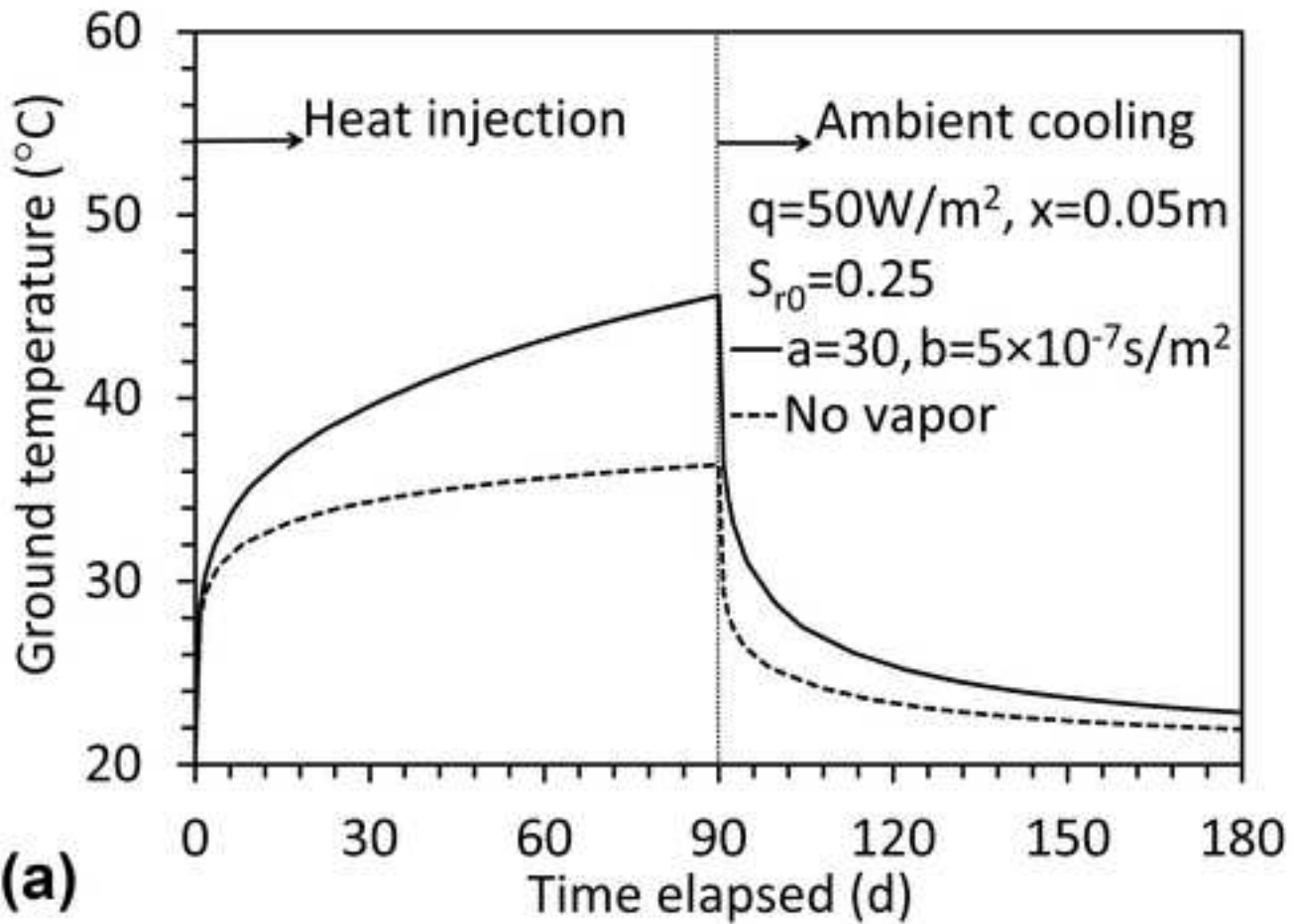
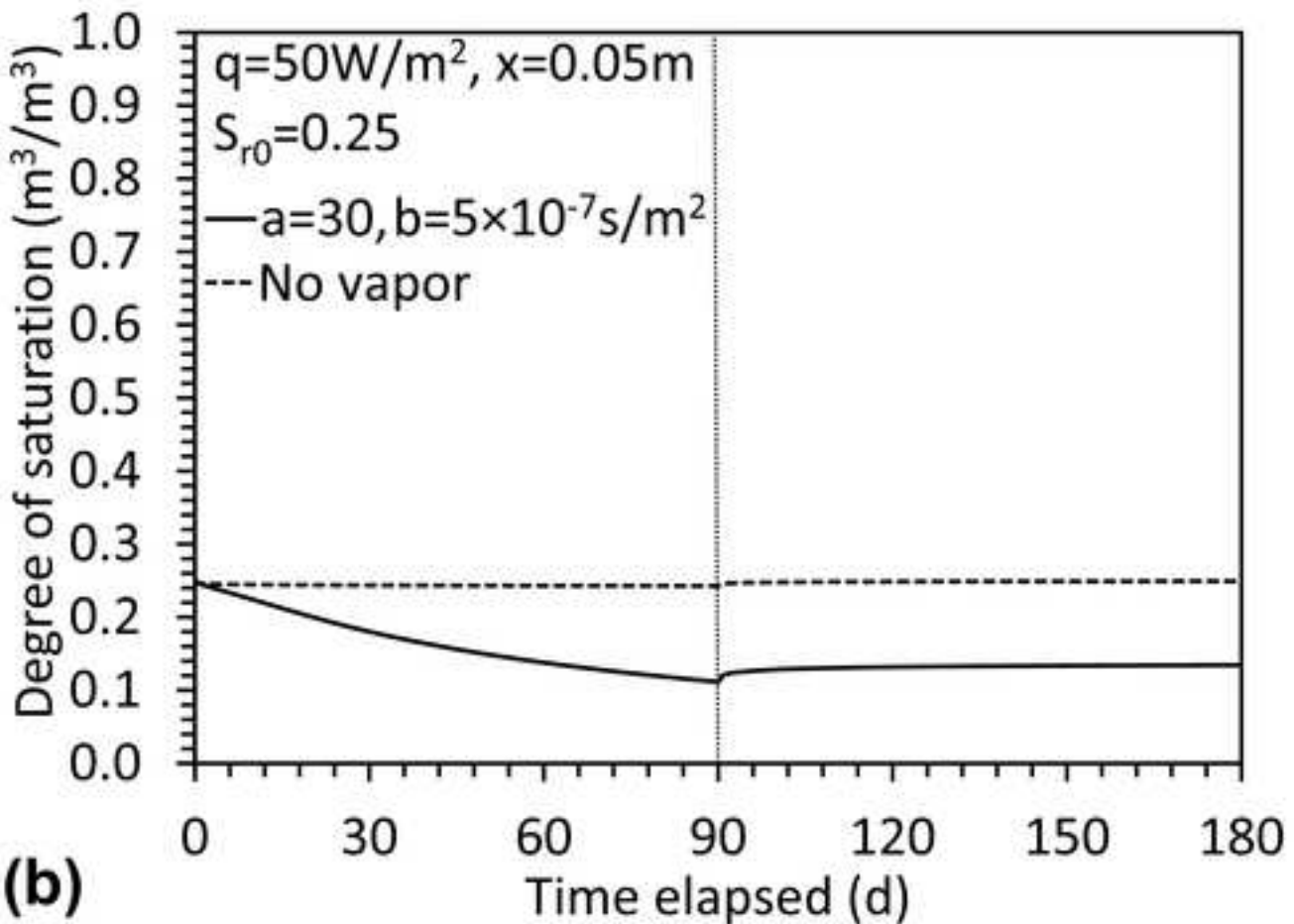
(c)

ΔS_r (m³/m³)
 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2



(d)



**(a)****(b)**

