

1 **Coupled cellular automata for frozen soil processes**

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9

10 **Abstract**

11 Heat and water movement in variably saturated freezing soils is a strongly coupled  
12 phenomenon. The coupling is a result of the effects of sub-zero temperature on soil water  
13 potential, heat carried by water moving under pressure gradients, and dependency of soil  
14 thermal and hydraulic properties on soil water content. This makes water and heat movement  
15 in variably saturated soils a highly non-linear coupled process. This study presents a one-  
16 dimensional cellular automata (direct solving) model to simulate coupled heat and water  
17 transport with phase change in variably saturated soils. The model is based on first order mass  
18 and energy conservation principles. The water and energy fluxes are calculated using first  
19 order empirical forms of Buckingham-Darcy's law and Fourier's heat law respectively. The  
20 water-ice phase change is handled by integrating along experimentally determined soil  
21 freezing curve (unfrozen water content and temperature relationship) obviating the use of  
22 apparent heat capacity term. This approach highlights a further subtle form of coupling one in  
23 which heat carried by water perturbs the water content – temperature equilibrium and  
24 exchange energy flux is used to maintain the equilibrium rather than affect temperature  
25 change. The model is successfully tested against analytical and experimental solutions.  
26 Setting up a highly non-linear coupled soil physics problem with a physically based approach  
27 provides intuitive insights into an otherwise complex phenomenon.

## 1 1 Introduction

2 Variably saturated soils in northern latitudes undergo repeated freeze-thaw cycles. Freezing  
3 reduces soil water potential considerably because soil retains unfrozen water (Dash et al.,  
4 1995). Resulting steep hydraulic gradients move considerable amounts of water upward from  
5 deeper warmer soil layers that accumulates behind the freezing front. The resulting  
6 redistribution of water alters soil thermal and hydraulic properties, and transports heat from  
7 one soil zone to another. As water freezes to ice, the latent heat maintains soil temperatures  
8 close to 0°C for long periods of time. The water and energy redistribution has significant  
9 implications for regional hydrology, infrastructure and agriculture. Understanding the physics  
10 behind this complex coupling remains an active area of research. Field studies have been  
11 widely used to better understand the mechanism of these thermo-hydraulic cycles (e.g.,  
12 Hayashi et al., 2007). Innovative column studies under controlled laboratory settings have  
13 allowed further insights by isolating the effects of factors that drive soil freezing and thawing,  
14 a separation impossible to achieve in the field (e.g., Nagare et al., 2012). Mathematical  
15 models, describing the mechanism of water and heat movement in variably saturated freezing  
16 soils, have been developed to complement these observational studies. Analytical solutions of  
17 freezing and thawing front movement have been developed and applied (e.g. Stefan, 1889;  
18 Hayashi et al., 2007) and numerical models have replicated the freezing induced water  
19 redistribution with reasonable success (e.g., Hansson et al., 2004). Optimization of existing  
20 numerical modelling approaches also remains an active area of research. For example,  
21 improvements to numerical solving techniques to address sharp changes in soil properties,  
22 especially behind freezing and thawing fronts, and during special conditions such as  
23 infiltration into frozen soils have been reported recently (e.g. Dall'Amico et al., 2011).

24 Although the coupling of heat and water movement in variably saturated freezing soils is  
25 complex, fundamental laws of heat and water movement coupled with principles of energy  
26 and mass conservation are able to explain the physics to a larger extent. There is a paradigm  
27 shift in modelling of water movement in variably saturated soils using physically based  
28 approaches. For example, HydroGeoSphere and Parflow (Brunner and Simmons, 2012; Kollet  
29 and Maxwell, 2006) are examples of codes that explicitly use Richard's equation to model  
30 subsurface flow. Thus, use of derived terms such as specific yield is not required. Mendicino  
31 et al. (2006) reported a three dimensional CA (direct solving) model to simulate moisture  
32 transfer in unsaturated zone. Cervarolo et al. (2010) extended the application of this CA

1 model by coupling it with a surface-vegetation-atmosphere-transfer scheme to simulate water  
2 and energy flow dynamics. Direct solving allows for unstructured grids while describing the  
3 coupled processes based on first order equations. Use of discrete first order formulations  
4 allow one to relax the smoothness requirements for the numerical solutions being sought. This  
5 has advantages, particularly in large scale models, wherein use of relatively coarse spatial  
6 discretization maybe feasible. Therefore, it is important to expand application of direct  
7 solving to further complicated unsaturated soil processes.

8 This study presents a coupled CA model to simulate heat and water transfer in variably  
9 saturated freezing soils. The system is modelled in terms of the empirically observed heat and  
10 mass balance equations (Fourier's heat law and Buckingham-Darcy equation) and using  
11 energy and mass conservation principles. The water-ice phase change is handled with a total  
12 energy balance including sensible and latent heat components. In a two-step approach similar  
13 to that of Engelmark and Svensson (1993), the phase change is brought about by the residual  
14 energy after sensible heat removal has dropped the temperature of the system below freezing  
15 point. Knowing the amount of water that can freeze, the change in soil temperature is then  
16 modelled by integrating along the soil freezing curve. To our knowledge, coupled cellular  
17 automata have not yet been used to explore simultaneous heat and water transport in frozen  
18 variably saturated porous media. The model was validated against the analytical solutions of  
19 (1) heat conduction problem (Churchill, 1972), (2) steady state convective and conductive  
20 heat transport in unfrozen soils (Stallman, 1965), (3) unilateral freezing of a semi-infinite  
21 region (Lunardini, 1985), and (4) the experimental results of freezing induced water  
22 redistribution in soils (Mizoguchi, 1990).

23

## 24 **2 Cellular Automata**

25 Cellular automata were first described by von Neumann (1948) (see von Neumann and Burks,  
26 1966). The CA describe the global evolution of a system in space and time based on a  
27 predefined set of local rules (transition rules). Cellular automata are able to capture the  
28 essential features of complex self-organizing cooperative behaviour observed in real systems  
29 (Ilachinski, 2001). The basic premise involved in CA modelling of natural systems is the  
30 assumption that any heterogeneity in the material properties of a physical system is scale  
31 dependent and there exists a length scale for any system at which material properties become  
32 homogeneous (Hutt and Neff, 2001). This length scale characterizes the construction of the

1 spatial grid cells (elementary cells) or units of the system. There is no restriction on the shape  
2 or size of the cell with the only requirement being internal homogeneity in material properties  
3 in each cell. One can then recreate the spatial description of the entire system by simple  
4 repetitions of the elementary cells. The local transition rules are results of empirical  
5 observations and are not dependant on the scale of homogeneity in space and time. The basic  
6 assumption in traditional differential equation solutions is of continuity in space and time. The basic  
7 discretization in models based on traditional numerical methods needs to be over grid spacing  
8 much smaller than the smallest length scale of the heterogeneous properties making solutions  
9 computationally very expensive. The CA approach is not limited by this requirement and is  
10 better suited to simulate spatially large systems at any resolution, if the homogeneity criteria  
11 at elementary cell level are satisfied (Ilachinski, 2001; Parsons and Fonstad, 2007). In fact, in  
12 many highly non-linear physical systems such as those describing critical phase transitions in  
13 thermodynamics and statistical mechanical theory of ferromagnetism, discrete schemes such  
14 as cellular automata are the only simulation procedures (Hoekstra et al., 2010).

15 On the flip side, explicit schemes like CA are not unconditionally convergent and hence given  
16 a fixed space discretization, the time discretization cannot be arbitrarily chosen. Another  
17 limitation of the CA approach was thought to be the need for synchronous updating of all  
18 cells for accurate simulations. However, CA models can be made asynchronous and can be  
19 more robust and error resistant than a synchronous equivalent (Hoekstra et al., 2010).

20 The following section (2.1) describes a 1D CA in simplified, but precise mathematical terms.  
21 It is then explained with an example of heat flow (without phase change) in a hypothetical soil  
22 column subjected to a time varying temperature boundary condition.

## 23 **2.1 Mathematical Description**

24 Let  $S_i^t$  be a discrete state variable which describes the state of the  $i^{\text{th}}$  cell at time step  $t$ . If one  
25 assumes that an order of  $N$  elementary repetitions of the unit cell describe the system  
26 spatially, then the complete macroscopic state of the system is described by the ordered  
27 Cartesian product  $S_1^t \otimes S_2^t \otimes \dots \otimes S_i^t \otimes \dots \otimes S_N^t$  at time  $t$ . Let a local transition rule  $\phi$  be  
28 defined on a neighbourhood of spatial indicial radius  $r$ ,  $\phi : S_{i-r}^t \otimes S_{i-r+1}^t \otimes \dots \otimes S_{i+r}^t \rightarrow S_i^{t+1}$   
29 where  $i \in [1+r, N-r]$ . The global state of the system is defined by some global mapping,  $\chi$ :  
30  $S_1^t \otimes S_2^t \otimes \dots \otimes S_i^t \otimes \dots \otimes S_N^t \rightarrow \mathbf{G}^t$  where  $\mathbf{G}^t$  is the global state variable of the system defining  
31 the physical state of the system at time  $t$ . Given this algebra of the system,  $\mathbf{G}^{t+1}$  is given by

1 
$$\mathbf{G}^{t+1} = \chi(\phi(\omega_1^t) \otimes \phi(\omega_2^t) \otimes \dots \otimes \phi(\omega_i^t) \otimes \dots \otimes \phi(\omega_N^t)) \quad (1)$$

2 where  $\omega_i^t = S_{1-r}^t \otimes S_{i-r+1}^t \otimes \dots \otimes S_{i+r}^t$ . The quantity  $r$  is generally called the radius of interaction  
 3 and defines the spatial extent on which interactions occur on the local scale. In the case of the  
 4 1D CA, the only choice of neighbourhood which is physically viable is the standard von  
 5 Neumann neighbourhood (Fig. 1).

6 **2.2 Physical description based on heat flow problem in a hypothetical soil  
 7 column**

8 Let us consider the CA simulation of heat flow in a soil column of length  $L_c$  and a constant  
 9 cross sectional area. The temperature change in the column is driven by a time varying  
 10 temperature boundary condition applied at the top. It is assumed that no physical variation in  
 11 the soil properties exist in the column at length intervals smaller than  $\Delta x$ . Each cell in the 1D  
 12 CA model can therefore be assumed to be of length  $\Delta x$ . Therefore, the column can be  
 13 discretized using  $L_c/\Delta x$  elementary cells. To simulate the spatio-temporal evolution of soil  
 14 temperature in the column, an initial temperature for each elementary cell has to be set. To  
 15 study the behaviour of the soil column under external driving (time varying temperature), a  
 16 fictitious cell is introduced at the top and/or the bottom of the soil column and subjected to  
 17 time varying temperatures. The transition rules need to be defined now. Once the transition  
 18 rules of heat exchange between neighbours are defined, the fictitious boundary cells interact  
 19 with the top and/or bottom cells of the soil column as any other internal cell based on the  
 20 prescribed rules and the predefined temperature time series. Although the same set of rules  
 21 govern interaction among all cells of the column, heat exchange cannot affect the temperature  
 22 of the fictitious cells as that would corrupt the boundary conditions. This is handled by  
 23 assigning infinite specific heats to the fictitious cells. This allows evolution of the internal  
 24 cells and the boundary cells according to the same mathematical rules / empirical equations.  
 25 The preceding mathematical description of the CA algebra is based on the assumption that the  
 26 state variable defining each cell is discrete in space and time. But soil temperatures are  
 27 considered to be continuous in space and time. The continuous description of the soil  
 28 temperature can be adapted to the CA scheme by considering small time intervals over which  
 29 the temperature variations are not of interest and hence for all practical purposes can be  
 30 assumed constant. Conditions for convergence of the numerical temperature profile set an  
 31 upper limit on the size of this time interval for a given value of  $\Delta x$ . Therefore, once the length

1 scale of homogeneity  $\Delta x$  in the system and the local update rules have been ascertained, the  
 2 CA is ready for simulation under the given initial and boundary conditions. Eq. (2) and Eq.  
 3 (3) [section 3], applied sequentially, would be the local update rules for this simple case of  
 4 heat flow in a soil column (without phase change) driven by time varying temperatures at the  
 5 top.

6 The meaning of the terms used in the mathematical description of CA can now be explained  
 7 with respect to the heat flow simulation for the hypothetical soil column:  $S_i^t$  is the temperature  
 8 of the  $i^{\text{th}}$  cell at time  $t$ ,  $r=1$ ,  $\phi$  is a sequential application of Eq. (2) and Eq. (3) describing heat  
 9 loss/gain by a cell due to temperature gradients with its two nearest neighbours and  
 10 temperature change due to the heat loss/gain, respectively, and  $\chi$  is the identity mapping.

11

### 12 3 Coupled heat and water transport in variably saturated soils

13 The algorithm developed for this study simultaneously solves the heat and water mass  
 14 conservation in the same time step. The implementation is based on the assumption of nearest  
 15 neighbour interactions, i.e.  $r=1$ . The one-dimensional conductive heat transport in variably  
 16 saturated soils can be given by the heat balance equation

$$17 \quad q_h = \sum_{\zeta=i-1}^{i+1} \lambda_{i,\zeta} \cdot \frac{T_\zeta - T_i}{l_{i,\zeta}}, \quad \zeta \neq i, \quad (2)$$

18 where subscripts  $i$  and  $\zeta$  refer to the cell and its active neighbours,  $q_h$  is the net heat flux  
 19 ( $\text{Js}^{-1}\text{m}^{-2}$ ) for the  $i^{\text{th}}$  cell,  $T$  is cell temperature ( $^{\circ}\text{C}$ ),  $\lambda_{i,\zeta}$  is average effective thermal conductivity  
 20 of the region between the  $i^{\text{th}}$  and the  $\zeta^{\text{th}}$  cells ( $\text{Js}^{-1}\text{m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ ), and  $l_{i,\zeta}$  is the distance between the  
 21 centres of the  $i^{\text{th}}$  and the  $\zeta^{\text{th}}$  cells (m). Effective thermal conductivity can be calculated using  
 22 one of the popular mixing models (e.g., Johansen, 1975; Campbell, 1985). The empirical  
 23 relationship between heat flux from Eq. (2) and resulting change in cell temperature  
 24 ( $\Delta T_i = T_i^{t+\Delta t} - T_i^t$ ) is given as

$$25 \quad Q_{h,i} = \frac{q_h \cdot \Delta t}{l_i} = C_i \cdot \Delta T_i, \quad (3)$$

26 where  $l_i$  is the length of the cell (m) and  $C_i$  ( $\text{Jm}^{-3} \text{ }^{\circ}\text{C}^{-1}$ ) is the effective volumetric heat capacity  
 27 of the cell such that

$$28 \quad C_i = C_w \theta_w + C_{ice} \theta_{ice} + C_s \theta_s + C_a \theta_a, \quad (4)$$

1 where  $\theta$  is volumetric fraction ( $\text{m}^3\text{m}^{-3}$ ) and subscripts  $w$ ,  $ice$ ,  $s$ , and  $a$  represent water, ice, soil  
2 solids and air fractions.

3 The mass conservation equation in 1D can be written as

4 
$$\rho_w \cdot \frac{\Delta\Theta}{\Delta t} + \rho_w \cdot \frac{q_w}{l_i} + \rho_w \cdot S_s = 0, \quad (5)$$

5 
$$\Theta = \theta_w + \frac{\rho_{ice}}{\rho_w} \theta_{ice}, \quad (6)$$

6  $\rho$  is density ( $\text{kgm}^{-3}$ ),  $\Theta$  is the total volumetric water content ( $\text{m}^3\text{m}^{-3}$ ),  $q_w$  is the Buckingham-  
7 Darcy flux ( $\text{ms}^{-1}$ ), and  $S_s$  is sink/source term. In unfrozen soils,  $\theta_{ice} = 0$  and  $\Theta = \theta_w$ .

8 Buckingham-Darcy's equation is used to describe the flow of water under hydraulic head  
9 gradients wherein it is recognized that the soil matric potential ( $\psi$ ) and hydraulic conductivity  
10 ( $k$ ) are functions of liquid water content ( $\theta_w$ ). The dependency of  $\psi$  and  $k$  on  $\theta_w$  can be  
11 expressed as a constitutive relationship. The constitutive relationships proposed by Mualem-  
12 van Genuchten (van Genuchten, 1980) defining  $\psi(\theta_w)$  and  $k(\theta_w)$  are used in this study

13 
$$\psi(\theta_w) = \frac{\left[ (S_e)^{-\frac{1}{m}} - 1 \right]^{\frac{1}{n}}}{\alpha}, \quad (7)$$

14 
$$k(\theta_w) = K_s \cdot (S_e)^{0.5} \cdot \left[ 1 - \left( 1 - (S_e)^{\frac{1}{m}} \right)^m \right]^2, \quad (8)$$

15 
$$S_e = \frac{\theta_w - \theta_{res}}{\eta - \theta_{res}}, \quad (9)$$

16 where  $\theta_{res}$  ( $\text{m}^3\text{m}^{-3}$ ) is the residual liquid water content,  $\eta$  ( $\text{m}^3\text{m}^{-3}$ ) is total porosity,  $K_s$  ( $\text{ms}^{-1}$ ) is  
17 the saturated hydraulic conductivity, and  $\alpha$  ( $\text{m}^{-1}$ ),  $n$  and  $m$  are equation constants such that  
18  $m = 1 - 1/n$ . For an elementary cell in a 1D CA model, the Buckingham-Darcy flux in its  
19 simplest form can be written as

20 
$$q_w = \sum_{\zeta=i-1}^{i+1} k_{i,\zeta} \cdot \frac{(\psi + z)_{\zeta} - (\psi + z)_i}{l_{i,\zeta}}, \quad \zeta \neq i, \quad (10)$$

21 where all subscripts have the same meaning as introduced so far,  $z$  is the cell elevation and  $k$   
22 represents the average hydraulic conductivity of the region between the  $i^{th}$  and the  $\zeta^{th}$  cells. In

1 this study, phase change and associated temperature change is brought about by integrating  
2 along a soil freezing curve (SFC). SFCs can be defined because the liquid water content in  
3 frozen soils must have a fixed value for each temperature at which the liquid and ice phases  
4 are in equilibrium, regardless of the amount of ice present (Low et al., 1968). Soil freezing  
5 curves for different types of soils developed from field and laboratory observations between  
6 liquid water content and soil temperature have been widely reported (e.g., Anderson and  
7 Morgenstern, 1973; Shahli and Stadler, 1996). Van Genuchten's model can be used to define  
8 a SFC (Eq. 7), wherein  $\psi(\theta_w)$  is replaced with  $T(\theta_w)$ , and  $n$ ,  $m$  and  $\alpha$  ( $^{\circ}\text{C}^{-1}$ ) are equation  
9 constants.

10

## 11 4 The coupled CA model

12 Fig. 2 shows a flow chart describing the algorithm driving the coupled CA code. The code  
13 was written in MATLAB<sup>®</sup>. Let the superscript  $t$  denote the present time step and subscript  $i$   
14 be the spatial index across the grid where each node represents centres of the cell. The thermal  
15 conduction and hydraulic conduction modules represent two different algorithms that  
16 calculate the net heat ( $q_{h,i}$ ) and water ( $q_{w,i}$ ) fluxes respectively across the  $i^{th}$  cell. In essence,  
17 the thermal conduction and hydraulic conduction codes run simultaneously and are not  
18 affected by each other in the same time step. However, the processes are not independent and  
19 are coupled through updating of model parameters and state variables at end of each time  
20 step. Hydraulic conduction is achieved by applying Eq. (10) to each elementary cell using the  
21 hydraulic gradients between it and its immediate neighbours ( $r=1$ ). Similarly, Eq. (2) is used  
22 to calculate the heat flux between each elementary cell and its immediate neighbours using  
23 the corresponding thermal gradients. The change in mass due to the flux  $q_{w,i}$  is used to obtain  
24 change in pressure head ( $\Delta\psi_i = \psi_i^{t+\Delta t} - \psi_i^t$ ) from  $\psi(\theta_w)$  relationship. The updated value of total  
25 water content is then used to update the volumetric heat capacity  $C_i$  (Eq. 4). The updated value of  $C_i$   
26 is used as an input to the energy balance module along with computed heat flux  
27  $q_{h,i}$ . This represents the first stage of coupling between hydraulic and thermal processes. The  
28 energy balance module computes the total change in ice and water content due to phase  
29 change, and the total temperature change ( $\Delta T_i$ ) due to a combination of thermal conduction  
30 and phase change.

31 The energy balance module is explained using an example of a system wherein the soil  
32 temperature is dropping and phase change may take place if cell temperature drops below

1 freezing point of pure water ( $T_{fw} = 0$  °C). Inside the energy balance module, the change in  
 2 temperature ( $\Delta T_i$ ) is calculated using Eq. (3) and values of  $C_i$  and  $Q_{h,i}$  assuming that only  
 3 thermal conduction takes place. If the computed  $\Delta T_i$  for a given cell is such that  $T_i^{t+\Delta t} \geq T_{fw}$ ,  
 4 then water cannot freeze; cell temperatures are updated without phase change and the code  
 5 moves into the next time step. In the approach of this study, phase change and associated  
 6 temperature change can occur if and only if the present cell temperature ( $T_i$ ) and water content  
 7 ( $\theta_{w,i}$ ) represent a point on the SFC. This point along the SFC (Fig. 3) is defined here as the  
 8 critical state point ( $T_{crit}$ ,  $\theta_{wcrit}$ ). If  $\Delta T_i$  gives  $T_i^{t+\Delta t} < T_{fw}$  for any cell, then freezing point  
 9 depression along the SFC accounts for change in temperature due to freeze-thaw. The  
 10 freezing point depression or  $T_{crit}$  is defined for the cell by comparing the cell  $\theta_{w,i}$  with the  
 11 SFC. However, the coupled nature of heat and water transport in soils perturbs the critical  
 12 state from time to time, e.g., when freezing induces water movement towards the freezing  
 13 front or infiltration into frozen soil leads to accumulation or removal of extra water from any  
 14 cell. In such a case,  $Q_{h,i}$  needs to be used to bring the cell to the critical state. This may require  
 15 thermal conduction without phase change ( $T_{crit} > T_i$ ) or freezing of water without temperature  
 16 change ( $T_{crit} < T_i$ ). This process gives us an additional change in temperature or water content  
 17 which is purely due to the fact that the additional water accumulation disturbs the critical  
 18 state. This is another and a subtle form of coupling between heat and water flow. Because of  
 19 the above consideration to perturbation of critical state caused by additional water  
 20 added/removed from a cell, infiltration into frozen soils during the over-winter or spring melt  
 21 events need no further modifications to the process of water and heat balance.

22 If  $Q_{h,i}$  is such that a cell can reach critical state and still additional heat needs to be removed,  
 23 then this additional heat ( $Q_{res,i}$ ) removal leads to freezing of water. Freezing of water leads to  
 24 change in the temperature of the cell such that

$$25 \quad \min\left(\theta_{w,i}, \frac{Q_{res,i}}{L_f}\right) = \int_{T_{crit}}^{T_{new,i}} d\theta_{w,i}, \quad (11)$$

26 where  $L_f$  is the latent heat of fusion (334000 J kg<sup>-1</sup>) and  $T_{new,i}$  is the new temperature of the cell  
 27 (Fig. 3). If the change in water content due to freezing is such that  $\theta_{w,i} = \theta_{res}$ , then no further  
 28 freezing of water can take place and  $Q_{res,i}$  is used to decrease the temperature of the cell using  
 29 Eq. (3) and the updated value of  $C_i$  (i.e., after accounting for change in  $C_i$  due to phase  
 30 change). The soil thawing case is exactly similar as described above; the only dissimilarity is  
 31 that a different SFC may be used if hysteretic effects are observed in SFC paths as observed in

1 studies by Quinton and Hayashi (2008), and Smerdon and Mendoza (2010). If the cell  
2 temperature is above freezing, then the matric potential is calculated using Eq. (7). For cell  
3 temperatures below freezing point, the water pressure (matric potential) can be determined by  
4 the generalized Clausis-Clapeyron equation by assuming zero ice gauge pressure

$$5 \quad L_f \cdot \frac{\Delta T_i}{T_i + 273.15} = g \cdot \Delta \Psi_i, \quad (12)$$

6 where  $g$  is acceleration due to gravity ( $9.81 \text{ ms}^{-2}$ ). At the end of the energy balance  
7 calculations, temperatures of all the cells are updated using the  $\Delta T_i$  computed in energy  
8 balance module. Water content for each cell is updated by considering the change due to  
9 freeze/thaw inside the energy balance module and  $q_{w,i}$ . Hydraulic conductivity of each cell is  
10 updated (Eq. 8) using the final updated values of water content. Pressure and total heads in  
11 each cell are updated considering water movement (Eq. 7) and freezing/thawing (Eq. 12). The  
12 volumetric heat capacity of each cell is updated one more time (Eq. 4) to incorporate the  
13 changes due to freeze/thaw inside the energy balance module. Thermal conductivity of each  
14 cell is updated using a mixing model (e.g., Johansen, 1975). This completes all the necessary  
15 updates and the model is ready for computations of the next time step.

16 The CA scheme described here is not unconditionally convergent. Hence, the size of the time  
17 step cannot be arbitrarily chosen. In our implementation of the CA model, adaptive time  
18 stepping has been achieved following the convergence analysis reported in Appendix A.

19

20 **5 Comparison with analytical solutions**

21 **5.1 Heat transfer by pure conduction**

22 The ability of the CA model to simulate pure conduction under hydrostatic conditions was  
23 tested by comparison to the analytical solution of one-dimensional heat conduction in a finite  
24 domain given by Churchill (1972). A soil column with total length ( $L_c$ ) of 4 m was assumed to  
25 have different initial temperatures in its upper ( $T_u = 10 \text{ }^\circ\text{C}$ ) and lower ( $T_l = 20 \text{ }^\circ\text{C}$ ) halves  
26 (Fig. 4). The system is hydrostatic at all times and there is no flow. At the interface, heat  
27 conduction due to the temperature gradient will occur until the entire domain reaches an  
28 average steady state temperature of  $15^\circ\text{C}$ . The analytical solution given by Churchill (1972)  
29 can be expressed as

$$1 \quad T(z, t) = T_u \cdot \left[ 0.5 + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2n-1} \cdot \cos\left(\frac{(2n-1) \cdot \pi \cdot z}{L_c}\right) \cdot \exp\left(-\left[\frac{(2n-1) \cdot \pi}{L_c}\right]^2 \cdot \left(\frac{\lambda}{C}\right) \cdot t\right) \right], \quad (13)$$

$$2 \quad + T_l \cdot \left[ 0.5 - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2n-1} \cdot \cos\left(\frac{(2n-1) \cdot \pi \cdot z}{L_c}\right) \cdot \exp\left(-\left[\frac{(2n-1) \cdot \pi}{L_c}\right]^2 \cdot \left(\frac{\lambda}{C}\right) \cdot t\right) \right]$$

3  
4 The parameters used in analytical examples for Churchill (1972), and CA code are given in  
5 Table 1. There is excellent agreement between the analytical solution and the CA simulation  
6 (Fig. 4).

7 **5.2 Heat transfer by conduction and convection**

8 Stallman's analytical solution (1965) to the subsurface temperature profile in a semi-infinite  
9 porous medium in response to a sinusoidal surface temperature provides a test of the CA  
10 model's ability to simulate one dimensional heat convection and conduction in response to a  
11 time varying Dirichlet boundary.

12 Given the temperature variation at the ground surface described by

$$13 \quad T(z_0, t) = T_{surf} + A \cdot \sin\left(\frac{2 \cdot \pi \cdot t}{\tau}\right), \quad (14)$$

14 the temperature variation with depth is given by

$$15 \quad T(z, t) = A e^{-\alpha z} \cdot \sin\left(\frac{2 \cdot \pi \cdot t}{\tau} - b \cdot z\right) + T_{\infty}, \quad (15)$$

$$16 \quad \alpha = \left\{ \left[ \left( \frac{\pi C \rho}{\lambda \tau} \right)^2 + \frac{1}{4} \left( \frac{q_f C_w \rho_w}{2\lambda} \right)^4 \right]^{0.5} + \frac{1}{2} \left( \frac{q_f C_w \rho_w}{2\lambda} \right)^2 \right\}^{0.5} - \left( \frac{q_f C_w \rho_w}{2\lambda} \right), \quad (16)$$

$$17 \quad \beta = \left\{ \left[ \left( \frac{\pi C \rho}{\lambda \tau} \right)^2 + \frac{1}{4} \left( \frac{q_w C_w \rho_w}{2\lambda} \right)^4 \right]^{0.5} + \frac{1}{2} \left( \frac{q_w C_w \rho_w}{2\lambda} \right)^2 \right\}^{0.5}, \quad (17)$$

1 where  $A$  is the amplitude of temperature variation ( $^{\circ}\text{C}$ ),  $T_{\text{surf}}$  is the average surface  
 2 temperature over a period of  $\tau$  (s),  $T_{\infty}$  is the initial temperature of soil column and temperature  
 3 at infinite depth, and  $q_f$  is the specific flux through the column top.

4 The parameters used in analytical examples for Stallman (1965), and CA code are given in  
 5 Table 2. The coupled CA code is able to simulate the temperature evolution due to conductive  
 6 and convective heat transfer as seen from the excellent agreement with the analytical solution  
 7 (Fig. 5).

8 **5.3 Heat transfer with phase change**

9 Lunardini (1985) presented an exact analytical solution for propagation of subfreezing  
 10 temperatures in a semi-infinite, initially unfrozen soil column with time  $t$ . The soil column is  
 11 divided into three zones (Fig. 6a) where zone 1 is fully frozen with no unfrozen water; zone 2  
 12 is ‘mushy’ with both ice and water; and zone 3 is fully thawed. The Lunardini (1985) solution  
 13 as described by McKenzie et al. (2007) and is given by following set of equations:

$$14 \quad T_1 = (T_m - T_s) \cdot \frac{\text{erf}\left(\frac{x}{2\sqrt{D_1 t}}\right)}{\text{erf}(\vartheta)} + T_s, \quad (18)$$

$$15 \quad T_2 = (T_f - T_m) \cdot \frac{\text{erf}\left(\frac{x}{2\sqrt{D_4 t}}\right) - \text{erf}(\gamma)}{\text{erf}(\gamma) - \text{erf}\left(\vartheta \sqrt{\frac{D_1}{D_4}}\right)} + T_f, \quad (19)$$

$$16 \quad T_3 = (T_0 - T_f) \cdot \frac{-\text{erfc}\left(\frac{x}{2\sqrt{D_3 t}}\right)}{\text{erf}\left(\gamma \sqrt{\frac{D_4}{D_3}}\right)} + T_0, \quad (20)$$

17 where  $T_1$ ,  $T_2$ , and  $T_3$  are the temperatures at distance  $x$  from the temperature boundary for  
 18 zones 1, 2, and 3 respectively;  $T_0$ ,  $T_m$ ,  $T_f$ , and  $T_s$  are the temperatures of the initial conditions,  
 19 the solidus, the liquidus, and the boundary respectively;  $D_1$  and  $D_3$  are the thermal  
 20 diffusivities for zones 1 and 3, defined as  $\lambda_1/C_1$  and  $\lambda_3/C_3$  where  $C_1$  and  $C_3$ , and  $\lambda_1$  and  $\lambda_4$  are  
 21 the volumetric bulk-heat capacities ( $\text{Jm}^{-3} \text{ }^{\circ}\text{C}^{-1}$ ) and bulk thermal conductivities ( $\text{Js}^{-1}\text{m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ )

1 respectively of the two zones. The thermal diffusivity of zone 2 is assumed to be constant  
 2 across the transition region, and the thermal diffusivity with latent heat,  $D_4$ , is defined as:

$$3 \quad D_4 = \frac{\lambda_2}{C_2 + \left( \frac{\gamma_d L_f \Delta \xi}{T_f - T_m} \right)}, \quad (21)$$

4 where  $\gamma_d$  is the dry unit density of soil solids, and  $\Delta \xi = \xi_1 - \xi_3$  where  $\xi_1$  and  $\xi_3$  are the ratio of  
 5 unfrozen water to soil solids in zones 1 and 3 respectively. For a time  $t$  in the region from  $0 \leq$   
 6  $x \leq X_1(t)$  the temperature is  $T_1$  and  $X_1(t)$  is given by:

$$7 \quad X_1(t) = 2\vartheta \sqrt{D_1 t}, \quad (22)$$

8 and from  $X_1(t) \leq x \leq X(t)$  the temperature is  $T_2$  where  $X(t)$  is given by:

$$9 \quad X(t) = 2\gamma \sqrt{D_4 t}, \quad (23)$$

10 and for  $x \geq X(t)$  the temperature is  $T_3$ . The unknowns,  $\vartheta$  and  $\gamma$ , are obtained from solution of  
 11 the following two simultaneous equations

$$12 \quad \frac{(T_m - T_s)}{(T_m - T_f)} \cdot e^{-\vartheta^2 \left( 1 - \frac{D_1}{D_4} \right)} = \frac{\frac{\lambda_2}{\lambda_1} \operatorname{erf}(\vartheta) \sqrt{\frac{D_1}{D_4}}}{\operatorname{erf}(\gamma) - \operatorname{erf} \left( \vartheta \sqrt{\frac{D_1}{D_4}} \right)}, \quad (24)$$

$$13 \quad \frac{(T_m - T_f) \frac{\lambda_2}{\lambda_1}}{(T_0 - T_f)} \cdot \sqrt{\frac{D_3}{D_4}} \cdot e^{-\gamma^2 \left( 1 - \frac{D_4}{D_3} \right)} = \frac{\operatorname{erf}(\gamma) - \operatorname{erf} \left( \vartheta \sqrt{\frac{D_1}{D_4}} \right)}{\operatorname{erfc} \left( \gamma \sqrt{\frac{D_4}{D_3}} \right)}, \quad (25)$$

14 The verification example based on Lunardini (1985) analytical solution used in this study is  
 15 the same as used by McKenzie et al. (2007). Lunardini (1985) assumed the bulk-volumetric  
 16 heat capacities of the three zones, and thermal conductivities in each zone to be constant. It  
 17 was also assumed for the sake of the analytical solution that the unfrozen water varies linearly  
 18 with temperature. As stated by Lunardini (1985), if unfrozen water varies linearly with  
 19 temperature then an exact solution may be found for a three zone problem. Although this will  
 20 be a poor representation of a real soil system, it will constitute a valuable check for

1 approximate solution methods. The linear freezing function used in this study is shown in Fig.  
2 6b and the parameters used in Lunardini's analytical solution are given in Table 3. The  
3 excellent agreement between the analytical solution and coupled CA model simulations (Fig.  
4 7a and Fig. 7b) for two different cases of  $T_m$  shows that the model is able to perfectly simulate  
5 the process of heat conduction with phase change.

6

7 **6 Comparison with experimental data**

8 Hansson et al. (2004) describe laboratory experiments of Mizoguchi (1990) in which freezing  
9 induced water redistribution in 20 cm long Kanagawa sandy loam columns was observed. The  
10 coupled CA code was used to model the experiment as a validation test for simulation of frost  
11 induced water redistribution in unsaturated soils. Four identical cylinders, 8 cm in diameter  
12 and 20 cm long, were packed to a bulk density of  $1300 \text{ kgm}^{-3}$  resulting into total porosity of  
13  $0.535 \text{ m}^3 \text{ m}^{-3}$ . The columns were thermally insulated from all sides except the tops and brought  
14 to uniform temperature ( $6.7^\circ\text{C}$ ) and volumetric water content ( $0.33 \text{ m}^3 \text{ m}^{-3}$ ). The tops of three  
15 cylinders were exposed to a circulating fluid at  $-6^\circ\text{C}$ . One cylinder at a time was removed  
16 from the freezing apparatus and sliced into 1 cm thick slices after 12, 24, and 50 hours. Each  
17 slice was oven dried to obtain total water content (liquid water + ice). The fourth cylinder was  
18 used to precisely determine the initial condition. The freezing induced water redistribution  
19 observed in these experiments was simulated using the coupled CA code. Parameters used  
20 were: saturated hydraulic conductivity of  $3.2 \times 10^{-6} \text{ ms}^{-1}$  and van Genuchten parameters  $\alpha =$   
21  $1.11 \text{ m}^{-1}$ ,  $n = 1.48$ . The hydraulic conductivity of the cells with ice was reduced using an  
22 impedance factor of 2. Thermal conductivity formulation of Campbell (1985) as modified and  
23 applied by Hansson et al. (2004) was used. In their simulations of the Mizoguchi (1990)  
24 experiments, Hansson et al. (2004) calibrated the model using a heat flux boundary at the top  
25 and bottom of the columns. The heat flux at the surface and bottom was controlled by heat  
26 conductance terms multiplied by the difference between the surface and ambient, and bottom  
27 and ambient temperatures, respectively. Similar boundary conditions were used in the CA  
28 simulations. The value of heat conductance at the surface was allowed to decrease nonlinearly  
29 as a function of the surface temperature squared using the values reported by Hansson et al.  
30 (2004). The heat conductance coefficient of  $1.5 \text{ Js}^{-1} \text{ m}^{-2} \text{ }^\circ\text{C}^{-1}$  was used to simulate heat loss  
31 through the bottom. Hansson and Lundin (2006) observed that the four soil cores used in the  
32 experiment performed by Mizoguchi (1990) were quite similar in terms of saturated hydraulic

1 conductivity, but probably less so in terms of the water holding properties where more  
2 significant differences were to be expected. Such differences in water holding capacity would  
3 result in significant differences in unsaturated hydraulic conductivities of the columns at  
4 different times during the freezing experiments. The simulated values of total water content  
5 agree very well with the experimental values (Fig. 8). The region with sharp drop in the water  
6 content indicates the position of the freezing front. There is clear freezing induced water  
7 redistribution, which is one of the principal phenomena for freezing porous media and is well  
8 represented in the coupled CA simulations. Mizoguchi's experiments have been used by  
9 number of researcher for validation of numerical codes (e.g., Hansson et al., 2004; Painter,  
10 2011; Daanen et al., 2007). The CA simulation shows comparable or improved simulation for  
11 total water content as well as for the sharp transition at the freezing front.

12

## 13 **7 Conclusions**

14 The study provides an example of application of direct solving to simulate highly non-linear  
15 processes in variably saturated soils. The modelling used a one dimensional cellular automata  
16 (CA) structure wherein two cellular automata models simulate water and heat flow separately  
17 and are coupled through an energy balance module. First order empirical laws in conjunction  
18 with energy and mass conservation principles are shown to be succesful in describing the  
19 tightly coupled nature of the heat and water transfer. In addition, use of an observed soil  
20 freezing curve (SFC) is shown to obviate use of non-physical terms such as apparent heat  
21 capacity and provide insights into a further subtle mode of coupling. This approach of  
22 coupling and use of SFC is easy to understand and follow from physical point of view and  
23 straight forward to implement in a code. The results were successfully verified against  
24 analytical solutions of heat flow due to pure conduction, conduction with convection, and  
25 conduction with phase change using analytical solutions. In addition, freezing induced water  
26 redistribution was successfully verified with experimental data.

27

## 28 **Appendix A: Convergence analysis**

29 The CA scheme described in this paper is not unconditionally convergent. Hence, the size of  
30 the time step cannot be arbitrarily chosen. In this section we present a detailed evaluation of  
31 the convergence criteria of our code to address the choice of the time step.

1 The heat and flow convergence criteria are derived one after another. We start with the heat  
 2 balance portion. The local energy balance is the basic principle used in our approach. This is  
 3 imposed by ensuring flux continuity of heat. The local heat balance is described by Eq. (1)  
 4 and (2) and freeze-thaw effect. For a 1D CA application, assuming  $r=1$ , this can be written as

$$5 C_i l_i \frac{\tilde{T}_i^{t+\Delta t} - \tilde{T}_i^t}{\Delta t} + \rho_w L_f l_i \frac{\tilde{\theta}_{wi}^{t+\Delta t} - \tilde{\theta}_{wi}^t}{\Delta t} = \lambda_{i,i+1} \frac{\tilde{T}_{i+1}^t - \tilde{T}_i^t}{l_i} + \lambda_{i,i-1} \frac{\tilde{T}_{i-1}^t - \tilde{T}_i^t}{l_i} \quad (\text{A1})$$

6 where  $l_i$  is the uniform cell size and  $\lambda_{i,i+1}$  and  $\lambda_{i,i-1}$  are average effective thermal conductivity  
 7 of the region between the  $i^{th}$ , and the  $i+1^{th}$  and  $i-1^{th}$  cells respectively. The second term on the  
 8 left hand side of equation is the contribution of freeze-thaw to the thermal energy  
 9 conservation.  $\tilde{T}_i^t = T_i^t + e_i^t$  is some approximation of the exact solution for temperature  $T_i^t$  at  
 10 time  $t$  and cell index  $i$  given an approximation error  $e_i^t$ . Similarly,  $\tilde{\theta}_{wi}^t = \theta_{wi}^t + e_i^t$  is an  
 11 approximation, subject to the discretization error  $e_i^t$ , of the exact solution for the volumetric  
 12 fraction of water  $\theta_{wi}^t$ . It is useful to rewrite equation in the following simpler form in order to  
 13 decouple the thermal and hydraulic processes in terms of known parameters

$$14 C_i l_i \frac{\tilde{T}_i^{t+\Delta t} - \tilde{T}_i^t}{\Delta t} + \left( \rho_w L_f \frac{\tilde{\theta}_{wi}^{t+\Delta t} - \tilde{\theta}_{wi}^t}{\tilde{T}_i^{t+\Delta t} - \tilde{T}_i^t} \right) \cdot l_i \frac{\tilde{T}_i^{t+\Delta t} - \tilde{T}_i^t}{\Delta t} = \lambda_{i,i+1} \frac{\tilde{T}_{i+1}^t - \tilde{T}_i^t}{l_i} + \lambda_{i,i-1} \frac{\tilde{T}_{i-1}^t - \tilde{T}_i^t}{l_i} \quad (\text{A2})$$

15 The quantity in parentheses in the second term in equation can be approximated as  
 16  $\rho_w L_f d\theta_w/dT|_{T=T_i^t}$  where  $d\theta_w/dT|_{T=T_i^t}$  is the slope of the soil freezing curve at  $T = T_i^t$ , a known  
 17 quantity. Finally, we introduce the term,  $C_i' = C_i + \rho_w L_f d\theta_w/dT|_{T=T_i^t}$  as apparent heat capacity,  
 18 and rewrite eq. (A1) as

$$19 C_i' l_i \frac{\tilde{T}_i^{t+\Delta t} - \tilde{T}_i^t}{\Delta t} = \lambda_{i,i+1} \frac{\tilde{T}_{i+1}^t - \tilde{T}_i^t}{l_i} + \lambda_{i,i-1} \frac{\tilde{T}_{i-1}^t - \tilde{T}_i^t}{l_i} \quad (\text{A3})$$

20 Rearranging the terms, we obtain

$$21 e_i^{t+\Delta t} = e_i^t \left( 1 - \frac{\bar{\lambda}_i \Delta t}{l_i^2 C_i'} \right) + \frac{\lambda_{i,i+1} \Delta t}{l_i^2 C_i'} e_{i+1}^t + \frac{\lambda_{i,i-1} \Delta t}{l_i^2 C_i'} e_{i-1}^t + \\ \left[ \frac{\lambda_{i,i+1} \Delta t}{l_i^2 C_i'} T_{i+1}^t + \frac{\lambda_{i,i-1} \Delta t}{l_i^2 C_i'} T_{i-1}^t + T_i \left( 1 - \frac{\bar{\lambda}_i \Delta t}{l_i^2 C_i'} \right) - T_i^{t+\Delta t} \right] \quad (\text{A4})$$

22 where  $\bar{\lambda}_i = \lambda_{i,i-1} + \lambda_{i,i+1}$ . Replacing all the error terms by maximum absolute error term,  
 23 defined as  $E_t = \max\{|e_i^t|\}$ , we obtain

1 
$$\Delta t \leq \frac{l_i^2 C'_i}{\bar{\lambda}_i} \quad (\text{A5})$$

2 All coefficients of error terms on the right hand side of equation (A4) are either positive or  
 3 zero. Given this, the upper bound on the error at time  $t+\Delta t$ , defined as  $E_t^{t+\Delta t} = \max\{|e_i^{t+\Delta t}|\}$ ,  
 4 must be

5 
$$E^{t+\Delta t} \leq E^t + \max\{f(T, \lambda)\} = E^t + F \quad (\text{A6})$$

6 where  $f(T, \lambda)$  is the term in squared brackets in Eq. (A4) and  $F = \max\{f(T, \lambda)\}$ . Therefore as long  
 7 as Eq. (A5) is satisfied, the error always has an upper bound controlled solely by the  
 8 discretization error. This is the condition for stability. But, because  $C'_i$  is a function of time, an  
 9 adaptive time stepping scheme would be well suited to solve the problem. The adaptive time  
 10 stepper would need to satisfy Eq. (A5) at each time step.

11 As long as the thermal energy balance component of our CA algorithm obeys the time  
 12 stepping-spatial discretization relationship in Eq. (A5) it remains stable. For such time-step  
 13 control, using the Lax-Richtmeyer equivalence theorem, one only needs to show that the  
 14 thermal module represents a consistent numerical approximation to the full diffusion equation  
 15 (including  $C'_i$  to account for the freeze-thaw effect) in order to prove convergence of our  
 16 method. To do this we note the following recurrence relations

17 
$$E^{t+\Delta t} \leq E^t + F \leq E^{t-\Delta t} + 2F \leq E^0 + (n+1)F, \quad t = n\Delta t \quad (\text{A7})$$

18 It is worthwhile to note that here we have assumed a constant value of  $F$  through all time  
 19 steps. We argue below that this does not affect the generality of the convergence analysis that  
 20 follows next.

21 Clearly, if the only source of error in our approximate solution is discretization of a  
 22 continuous process, then our initial values must be error free i.e.  $E^0 = 0$ . Therefore,

23 
$$E^{t+\Delta t} \leq (n+1)F \quad (\text{A8})$$

24 Now from definition of  $f(T, \lambda)$  we have

25 
$$f(T, \lambda) = \left[ \frac{1}{l_i} \left( \lambda_{i,i+1} \frac{T_{i+1}^t - T_i^t}{l_i} - \lambda_{i,i-1} \frac{T_{i-1}^t - T_i^t}{l_i} \right) - C'_i \frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} \right] \frac{\Delta t}{C'_i} \quad (\text{A9})$$

26 For  $\lim \Delta t, l_i \rightarrow 0$ , we have the cluster of terms within the square brackets converge to the  
 27 expression

1 
$$\frac{\partial}{\partial z} \left( \lambda(z) \frac{\partial H}{\partial z} \right) - C \cdot \frac{\partial T}{\partial t} \quad (\text{A10})$$

2 As  $T$  is an exact solution of the above diffusion equation form, we must have the terms within  
 3 square bracket converge to 0 as  $\lim \Delta t, l_i \rightarrow 0$ . This argument for the boundedness of  $F$  as  
 4  $\Delta t, l_i \rightarrow 0$  holds at each time step and, hence, would have led to the same conclusion if we  
 5 would have used a time variable maximum value of  $f(T, \lambda)$  in equation (A8). Therefore, in  
 6 general, at any time  $t$

7 
$$\lim_{\Delta t, l_i \rightarrow 0} E^t \rightarrow 0 \quad (\text{A11})$$

8 This formally shows that our numerical algorithm, with time stepping satisfying Eq. (A5), is  
 9 consistent and hence follows the convergence of the thermal module.

10 We can construct a similar convergence analysis for the hydraulic module. But we will  
 11 approach this problem from the continuum version of the modified Richard's equation for  
 12 variably saturated flow for the sake of brevity. The modified Richard's equation for variably  
 13 saturated flow can be written as (in the absence of a source term)

14 
$$\frac{\partial \theta_w}{\partial t} + \frac{\rho_{ice}}{\rho_w} \frac{\partial \theta_{ice}}{\partial t} = \frac{\partial}{\partial z} \left( k(z) \frac{\partial H}{\partial z} \right) \quad (\text{A12})$$

15 The left hand side of Eq. (A12) follows from the continuum version of the first term on the  
 16 left hand side of Eq. (5) where Eq. (6) has been used to eliminate  $\theta$ . The term on the right  
 17 hand side is the Darcy flux, introduced as the continuum version of Eq. (10) where the total  
 18 head  $H = \psi + z$ . The effect of freeze-thaw on the total head can be accounted for as a Clausis-  
 19 Clapeyron process as given in Eq. (12). To make this clear, we rewrite Eq. (A12) as follows

20 
$$\left( \frac{\partial \theta_w}{\partial H} + \frac{\rho_{ice}}{\rho_w} \frac{\partial \theta_{ice}}{\partial T} \frac{\partial T}{\partial H} \right) \frac{\partial H}{\partial t} = \frac{\partial}{\partial z} \left( k \left( \frac{\partial H}{\partial z} \right) \right) \quad (\text{A13})$$

21 We can make use of the following relations to eliminate the gradients within the parentheses  
 22 on the left hand side of Eq. (A13)

23 
$$\frac{\partial \theta_{ice}}{\partial T} = - \frac{L_f}{gT} \frac{\partial \theta_w}{\partial H} \quad (\text{A14})$$

24 
$$\frac{\partial T}{\partial H} = \frac{gT}{L_f} \quad (\text{A15})$$

1 Therefore, we can rewrite Eq. (A12) finally as

2

$$\left(1 - \frac{\rho_{ice}}{\rho_w}\right) C_w \frac{\partial H}{\partial t} = \frac{\partial}{\partial z} \left( k(z) \frac{\partial H}{\partial z} \right) \quad (\text{A16})$$

3 where  $C_w = \partial \theta_w / \partial H|_{H=H(t)}$  is the local slope of the soil retention curve which can be derived  
4 from Eq. (7). Eq. (A16) now has the same form as the expression in Eq. (A10). It is  
5 immediately clear that, if one would have followed the full formal arguments as outlined for  
6 the thermal module, the condition for stability of the variably saturated flow dynamics part of  
7 our algorithm is of the form

8

$$\Delta t \leq \frac{l_i^2 C'_w}{\bar{k}_i} \quad (\text{A17})$$

9 where  $C'_w = C_w (1 - \rho_{ice} / \rho_w)$  and  $\bar{k}_i = k_{i,i-1} + k_{i,i+1}$ . We refer the reader to Mendicino et al.  
10 (2006) for a rigorous proof that, as long as this stability condition is satisfied, guarantees a  
11 consistent solution to the water flow. The formal argument is exactly equivalent to that  
12 presented by us for the heat flow problem. Combining Eq. (A5) Eq. (A17), the following  
13 condition gives stability and convergence conditions for the overall CA problem

14

$$\Delta t \leq \min \left( \frac{l_i^2 C'_w}{\bar{k}_i}, \frac{l_i^2 C'_i}{\bar{\lambda}_i} \right) \quad (\text{A18})$$

15

## 16 Authorship Statement

17 Ranjeet M. Nagare, Pathikrit Bhattacharya and Jaya Khanna are equal authors on this paper.

18

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26

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1 Table 1 Simulation parameters for heat conduction problem. Analytical solution for this  
 2 example is given by Eq. (13) as per Churchill (1972).

Symbol	Parameter	Value
$\eta$	Porosity	0.35
$\lambda$	bulk thermal conductivity	2.0 $\text{Js}^{-1}\text{m}^{-1}\text{^oC}^{-1}$
$C_w$	volumetric heat capacity of water	4174000 $\text{Jm}^{-3}\text{^oC}^{-1}$
$C_s$	volumetric heat capacity of soil solids	2104000 $\text{Jm}^{-3}\text{^oC}^{-1}$
$\rho_w$	density of water	1000 $\text{kgm}^{-3}$
$\rho_s$	density of soil solids	2630 $\text{kgm}^{-3}$
$l$	length of cell	0.01 m
$t$	length of time step in CA solution	1 second

3

1 Table 2 Simulation parameters for predicting subsurface temperature profile in a semi-infinite  
 2 porous medium in response to a sinusoidal surface temperature. The analytical solution to this  
 3 one dimensional heat convection and conduction problem in response to a time varying  
 4 Dirichlet boundary is given by Eq. (14)-(17) as per Stallman (1965).

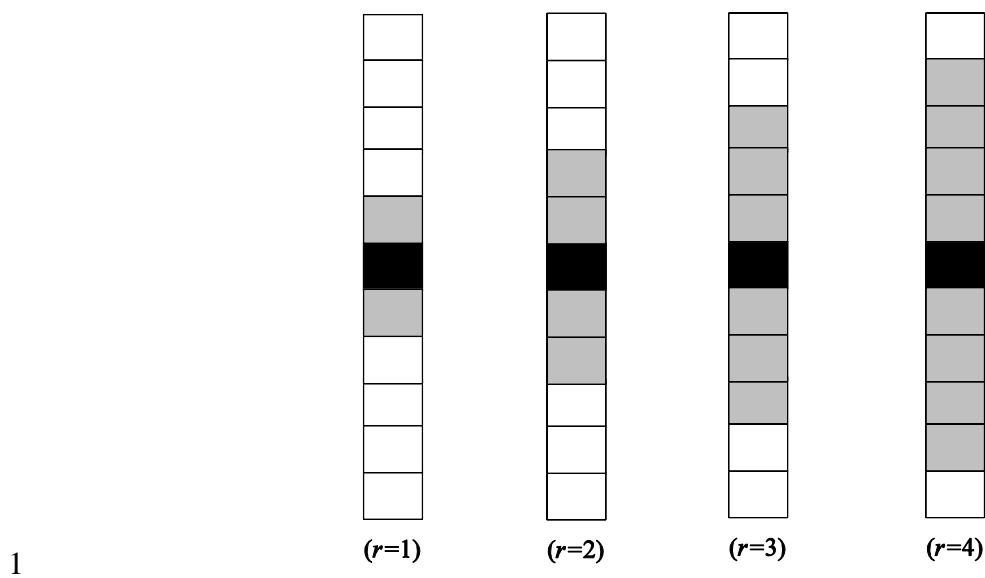
Symbol	Parameter	Value
$\eta$	Porosity	0.40
$\lambda$	bulk thermal conductivity	$2.0 \text{ Js}^{-1}\text{m}^{-1}\text{ }^{\circ}\text{C}^{-1}$
$C_w$	volumetric heat capacity of water	$4174000 \text{ Jm}^{-3}\text{ }^{\circ}\text{C}^{-1}$
$C_s$	volumetric heat capacity of soil solids	$2104000 \text{ Jm}^{-3}\text{ }^{\circ}\text{C}^{-1}$
$\rho_w$	density of water	$1000 \text{ kgm}^{-3}$
$\rho_s$	density of soil solids	$2630 \text{ kgm}^{-3}$
$l$	length of cell	0.01 m
$t$	length of time step in CA solution	1 second
$q_f$	specific flux	$4 \times 10^{-7} \text{ ms}^{-1}$ downward
$\tau$	period of oscillation of temperature at the ground surface	24 hours
$A$	amplitude of the temperature variation at the ground surface	5 $^{\circ}\text{C}$
$T_{surf}$	average ambient temperature at the ground surface	20 $^{\circ}\text{C}$
$T_{\infty}$	ambient temperature at depth	20 $^{\circ}\text{C}$

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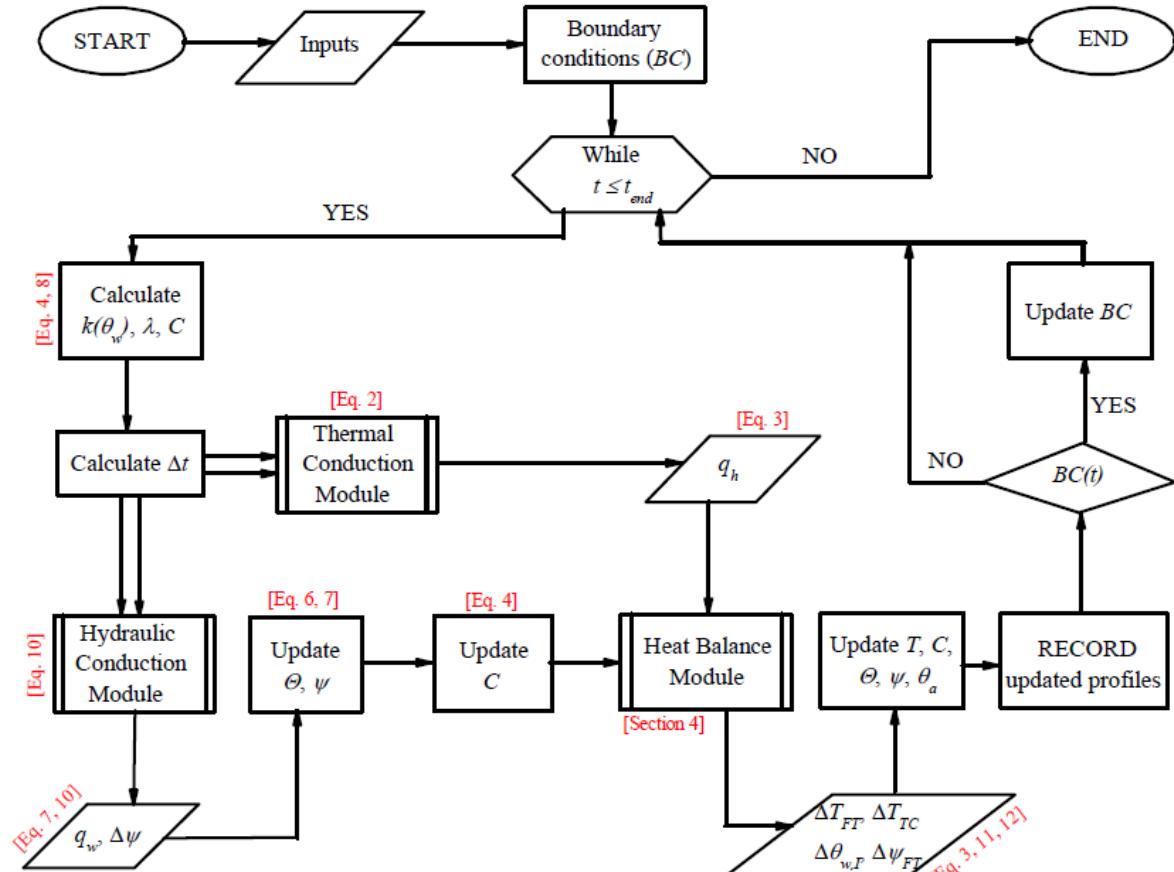
1 Table 3 Simulation parameters for predicting subsurface temperature profile with phase  
 2 change in a three zone semi-infinite porous medium. The analytical solution to this one  
 3 dimensional problem with sensible and latent heat zones is given by Eq. (18)-(25) as per  
 4 Lundardini (1985).

Symbol	Parameter	Value
$\eta$	Porosity	0.20
$\lambda_1$	bulk thermal conductivity of frozen zone	$3.464352 \text{ Js}^{-1}\text{m}^{-1}\text{C}^{-1}$
$\lambda_2$	bulk thermal conductivity of mushy zone	$2.941352 \text{ Js}^{-1}\text{m}^{-1}\text{C}^{-1}$
$\lambda_3$	bulk thermal conductivity of unfrozen zone	$2.418352 \text{ Js}^{-1}\text{m}^{-1}\text{C}^{-1}$
$C_1$	bulk-volumetric heat capacity of frozen zone	$690360 \text{ Jm}^{-3}\text{C}^{-1}$
$C_2$	bulk-volumetric heat capacity of mushy zone	$690360 \text{ Jm}^{-3}\text{C}^{-1}$
$C_3$	bulk-volumetric heat capacity of unfrozen zone	$690360 \text{ Jm}^{-3}\text{C}^{-1}$
$\xi_1$	fraction of liquid water to soil solids in frozen zone	0.0782
$\xi_3$	fraction of liquid water to soil solids in unfrozen zone	0.2
$l$	length of cell	0.01 m
$t$	length of time step in CA solution	1 second
$L_f$	Latent heat of fusion	$334720 \text{ Jkg}^{-1}$
$\gamma_d$	dry unit density of soil solids	$1680 \text{ kgm}^{-3}$
$T_s$	surface temperature at the cold end	-6 °C
$T_m$	temperature at the boundary of frozen and mushy zones	-1 °C, -4 °C
$\gamma^*$	equation parameter estimated using Eq. (24) and (25)	1.395, 2.062
$\vartheta^*$	equation parameter estimated using Eq. (24) and (25)	0.0617, 0.1375
$T_0$	initial temperature of the soil column	4 °C

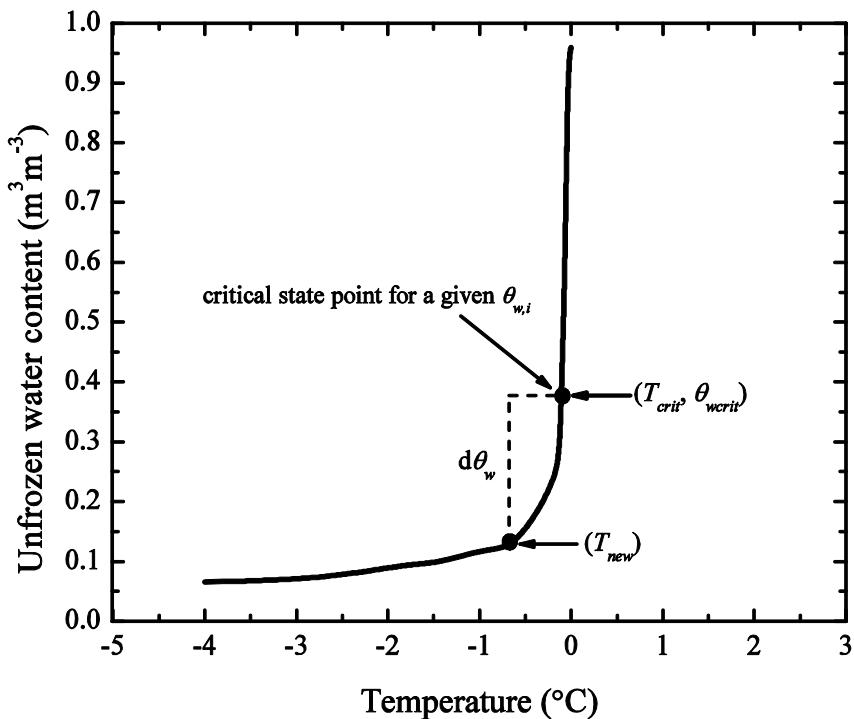
5 \* values taken from McKenzie et al. (2007).



2 **Figure 1** One dimensional cellular automata grids based on von Neumann neighbourhood  
3 concept. How many neighbours (grey cells) interact with an active cell (black) is controlled  
4 by indicial radius ( $r$ ).  
5



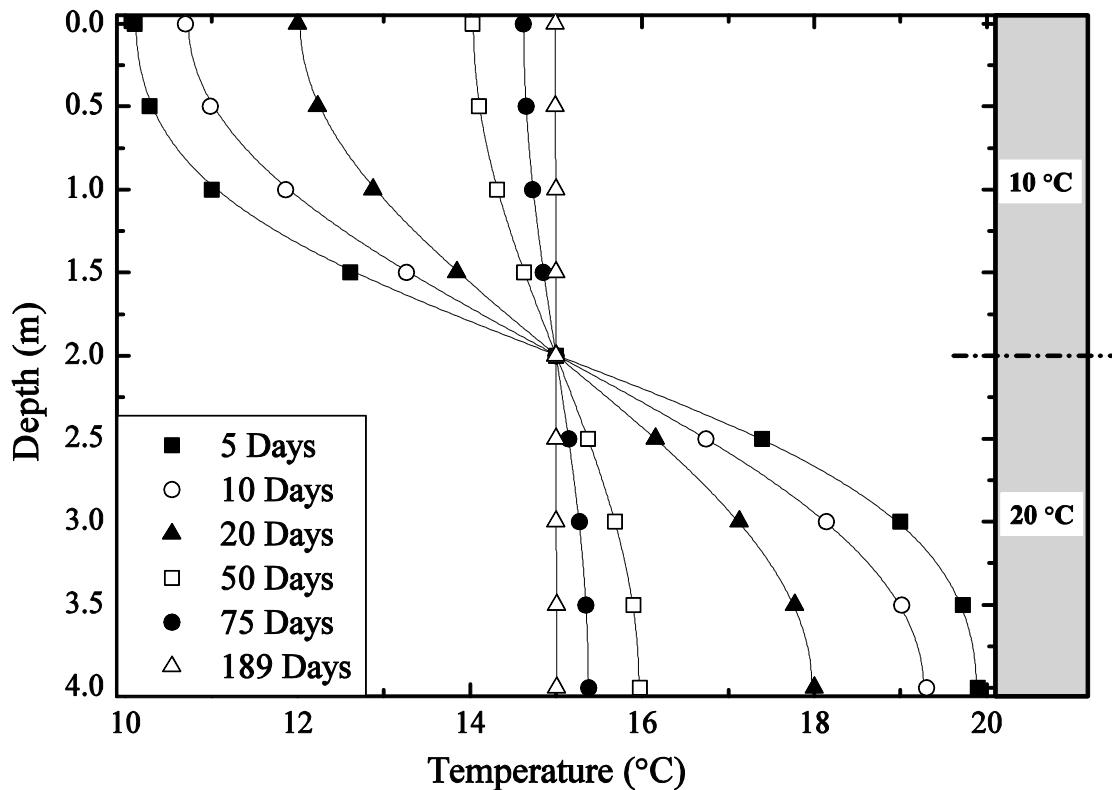
1 **Figure 2** Flow chart describing the algorithm driving the coupled CA code. Subscripts  $TC$ ,  
 2  $HC$  and  $FT$  refer to changes in physical quantities due to thermal conduction, hydraulic  
 3 conduction and freeze-thaw processes respectively. Hydraulic conduction and thermal  
 4 conduction are two different CA codes coupled through updating of volumetric heat capacity  
 5 and the freeze-thaw module to simulate the simultaneous heat and water movement in soils.  
 6 Corresponding equations or sections containing module description are shown in red text in  
 7 squared brackets.  
 8



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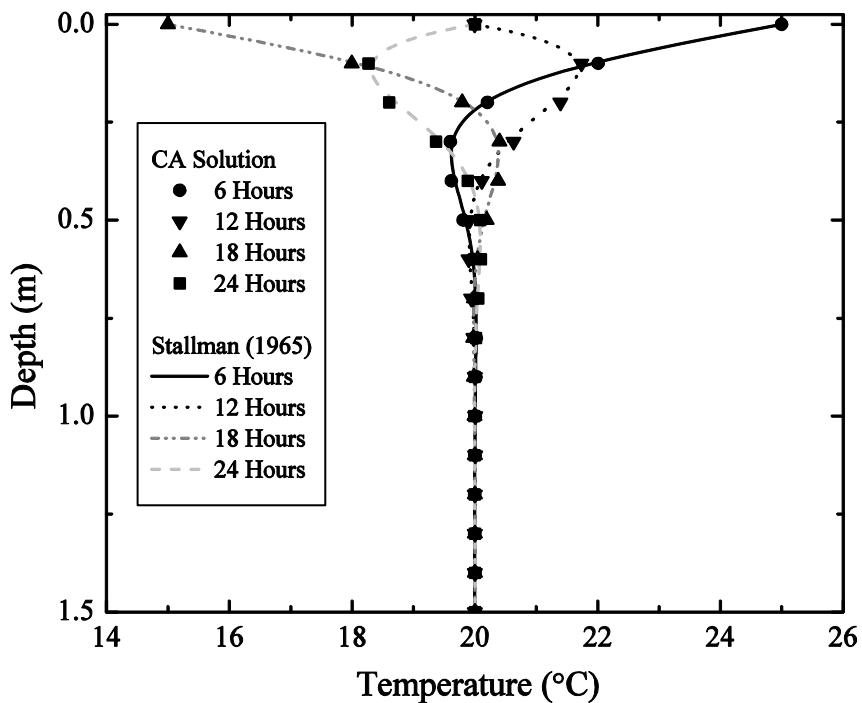
2 **Figure 3** Graphical description of the phase change approach used in this study. The curve is  
 3 a soil freezing curve for a hypothetical soil. The change in water content ( $d\theta_w$ ) due to  $Q_{res,i}$  is  
 4 used to determine  $T_{new}$  by integrating along the SFC (Equation 11).

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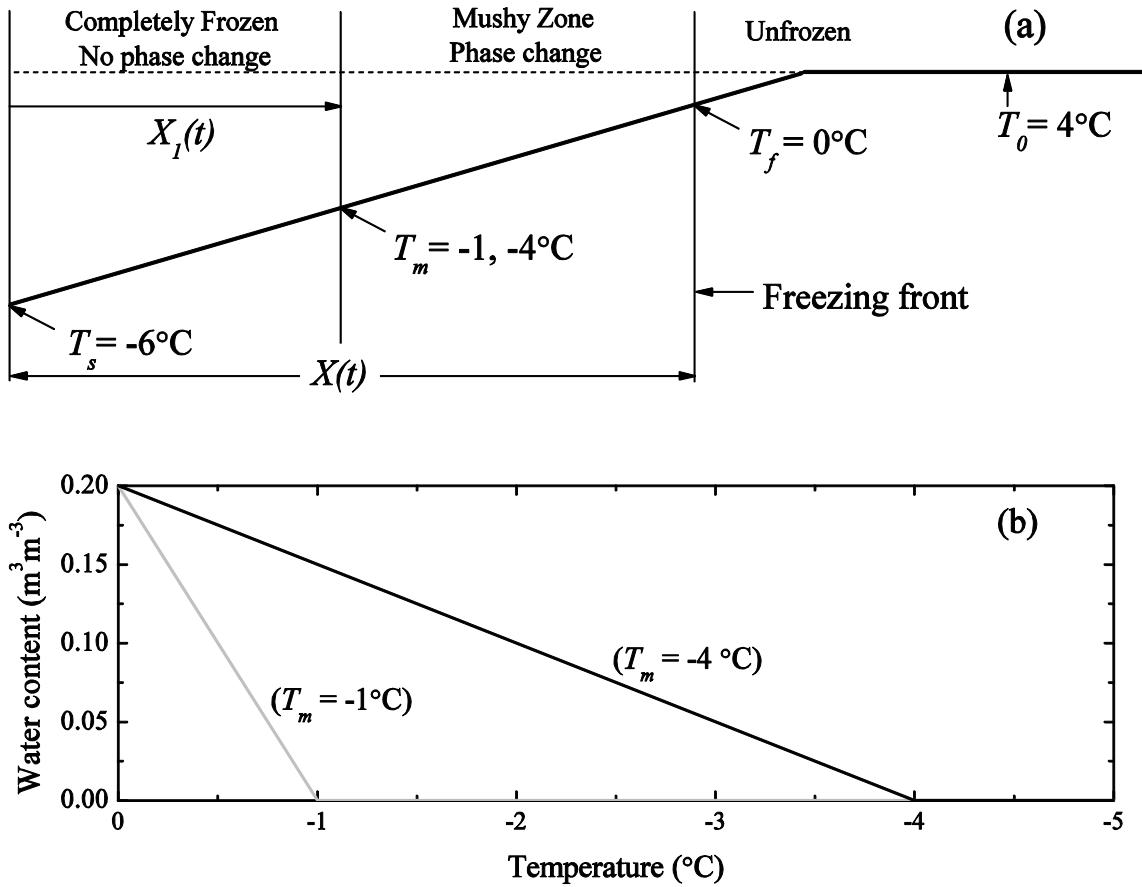


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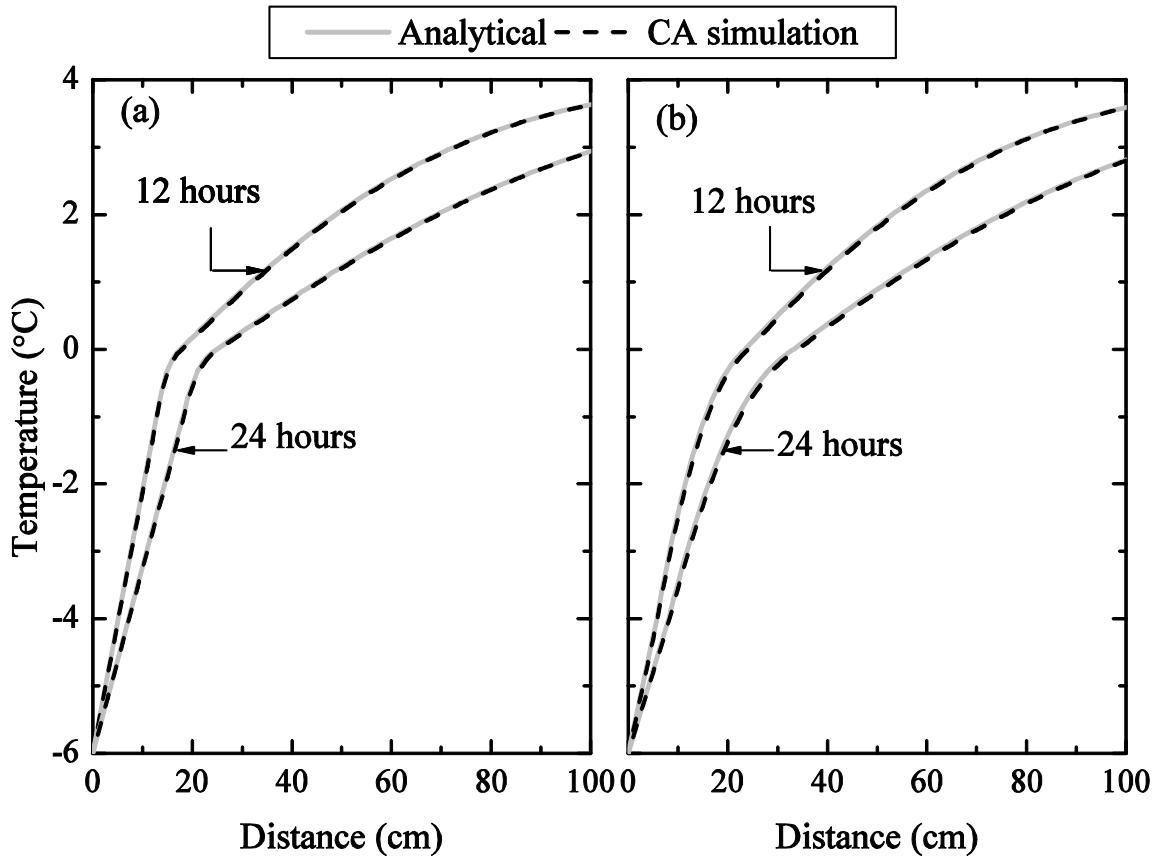
2 **Figure 4** Comparison between the analytical solution given by Churchill (1972) and coupled  
 3 cellular automata model simulation for a perfectly thermally insulated 4 m long soil column.  
 4 Lines represent the analytical solution and symbols represent the CA solution for time points  
 5 as shown in the legend. The initial temperature distribution is shown on the right.  
 6



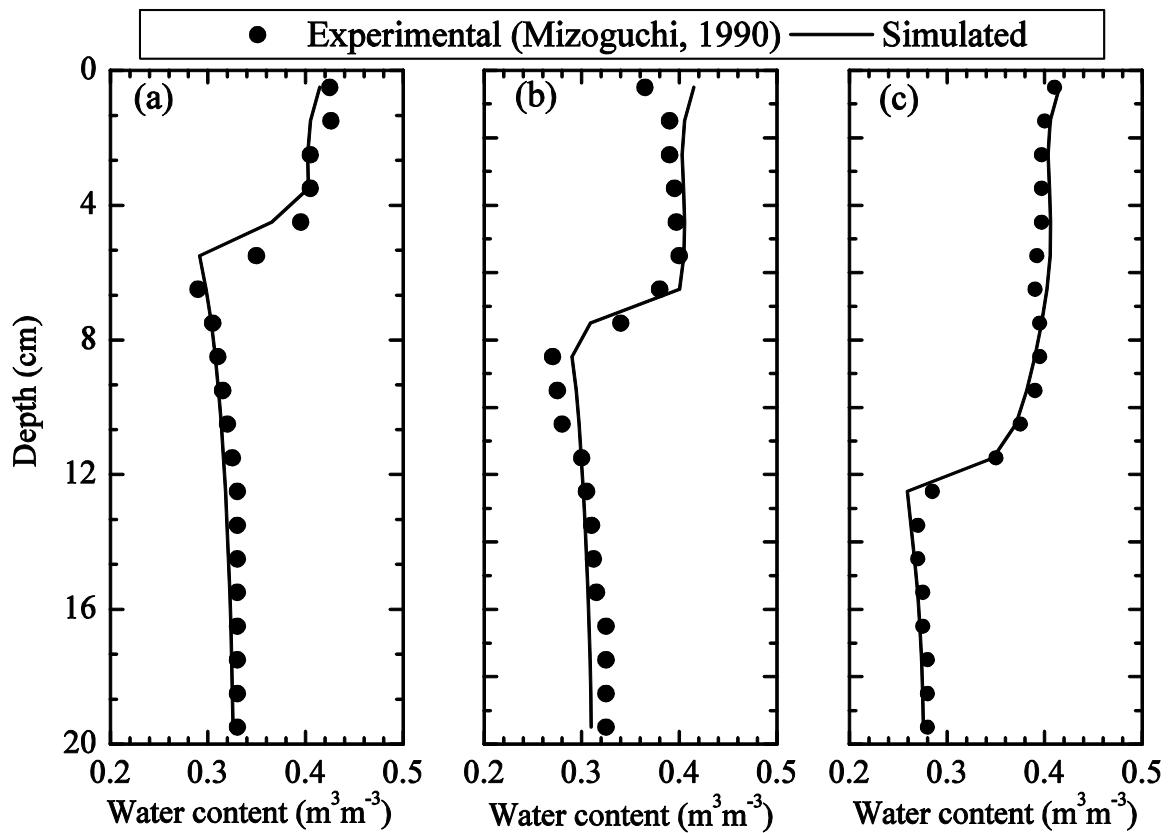
1  
2 **Figure 5** Comparison between analytical (Stallman, 1965) and coupled CA model steady  
3 state solutions for conductive and convective heat transfer. The soil column in this example is  
4 infinitely long, initially at 20 °C, and upper surface is subjected to a sinusoidal temperature  
5 with amplitude of 5 °C and period of 24 hours.  
6



1      **Figure 6** (a) Diagram showing the setting of Lunardini (1985) three zone problem. Equations  
2      18, 19, and 20 are used to predict temperatures in completely frozen zone (no phase change  
3      and sensible heat only), mushy zone (phase change and latent heat + sensible heat), and  
4      unfrozen zone (sensible heat only) respectively. (b) Linear freezing function used to predict  
5      unfrozen water contents for two cases used in this study ( $T_m = -1^\circ\text{C}$  and  $T_m = -4^\circ\text{C}$ ).  
6  
7



1  
2 **Figure 7** Comparison between analytical solution of heat flow with phase change (Lunardini,  
3 1985) and coupled CA model solutions for heat transfer with phase change. Lunardini (1985)  
4 solution is shown and compared with CA simulation for two cases (a)  $T_m = -1^\circ\text{C}$  and (b)  $T_m =$   
5  $-4^\circ\text{C}$  (Table 3, Figure 6).  
6



1

2 **Figure 8** Comparison of total water content (ice + water) between experimental (Mizoguchi,  
3 1990 as cited by Hansson, 2004) and coupled CA model results: (a) 12 hours, (b) 24 hours,  
4 and (c) 50 hours.