Coupled water and heat flow in one dimensional soil column

Under the supervision of

Dr. Subhasish Basak and Dr. Jaya Khanna

Submitted by:Mohamed Junaid

2011087

4th year Integrated MSc

National Institute of Science Education and Research

Bhubaneswar

Abstract

The flow of heat and water is highly coupled and occurs very commonly in nature. In this work the coupling due to dependency of soil thermal and hydraulic properties on soil water content has been studied and simulated.Water moving through soil carries with it heat, and soil water content influences soil thermal properties. The coupled transfer is modelled here using finite difference method and Range Kutta time stepping method.We conduct two simulations: one focusing solely on heat transfer through conduction and another examining the combined effects of conduction and convection in heat transfer.

1 INTRODUCTION

The commonly used model of soil considers it to be quasi-homogeneous consisting of a matrix of individual solid grains between which are interconnected pore spaces that can contain varying amounts of water and air. The ratio of the volume of these pore spaces to the total volume of the soil is called porosity.

$$\phi = \frac{V_a + V_w}{V_s} \tag{1}$$

where V_a, V_w, and V_s are the volumes of air, water, and mineral grains respectively. The amount of water present in the soil is given simply as the ratio between the volume of water to the volume of soil.

$$\theta = \frac{V_w}{V_s} \tag{2}$$

From the definition, it can be seen that the water content θ can take any value between 0 to ϕ. When the water content in a soil is equal to the porosity, it cannot hold any more water and is called saturated soil. Variably saturated soil is the soil in which the water content is not uniform throughout the soil profile. Analysing interplay between heat transfer and water flow relies on fundamental principles, including the heat balance equation (Fourier's law) and the mass balance equation (Buckingham-Darcy equation). coupled process of transfer of heat and water is simulated using finite difference method and Range Kutta time stepping method

2 Theoretical background

2.1 heat flow

Soil serves as a conduit for heat transfer, driven by its inherent thermal conductivity characteristics. This phenomenon is regulated by Fourier's law of heat conduction, which asserts that the heat flux (q) across a substance is directly linked to the negative temperature gradient (∇T), expressed as:

$$q = -k\nabla T \tag{3}$$

where: q is Heat flux (W/m^2), k is Thermal conductivity of the material (W/m·K), ∇T is Temperature gradient (K/m). In the context of soil, this law implies that heat flows from regions of higher temperature to regions of lower temperature within the soil profile. The flow of heat can be described by Fourier's empirical heat law, given as

$$q_h = C \cdot \Delta T_c \tag{4}$$

where C is the effective volumetric heat capacity, expressed as

$$C = C_w\theta_w + C_i\theta_i + C_s\theta_s + C_a\theta_a \tag{5}$$

where θ represents volumetric fractions, and subscripts w, i, s, and a denote the fractions of water, ice, soil solids, and air, respectively.

Equation (3) is then used to balance heat flow with neighboring cells. The one-dimensional conductive heat transport in variably saturated soils is governed by the heat balance equation:

$$q_h = \sum_{\zeta=i-1}^{i+1} \lambda_{i,\zeta} \cdot \frac{T_\zeta - T_i}{l_{i,\zeta}}, \quad \zeta \neq i \tag{6}$$

where subscripts i and ζ refer to the cell and its active neighbors, q_h is the net heat flux for the ith cell, T is the cell temperature (°C), $\lambda_{i,\zeta}$ is the average effective thermal conductivity of the region between the ith and the ζth cells, and $l_{i,\zeta}$ is the distance between the centers of the ith and the ζth cells (m).

2.2 Water flow

The Buckingham–Darcy equation governs water flow in unsaturated soil, combining Darcy's law with the continuity equation in Richards' equation. It characterizes flow under a hydraulic head gradient, determining the matric potential and hydraulic conductivity as functions of water content. The flux is expressed as the product of saturated hydraulic conductivity and the driving gradient, accounting for gravitational, solute, and pressure potentials. The equation incorporates the matric potential into the driving gradient and assumes zero pressure potential under unsaturated conditions. Soil textural properties, influencing water conductivity, are described by the Mualem–van Genuchten model. Matric potential as a function of water content is given by:

$$\psi(\theta_w) = \frac{\left(S_e^{-1/m} - 1\right)^{1/n}}{\alpha}$$

where $S_e = \frac{\theta_w - \theta_{\text{res}}}{\theta_{\text{sat}} - \theta_{\text{res}}}$. The hydraulic conductivity as a function of water content is given by:

$$k(\theta_w) = K_s \cdot (S_e)^{0.5} \cdot \left(1 - (1 - (S_e)^{\frac{1}{m}})^m)\right)^2 \tag{7}$$

The water flux is calculated using:

$$q_z = -K(\theta) \cdot \frac{d[z + \psi(\theta)]}{dz}$$

where: q is the Water flux density (m/s) , $K(\theta)$ is the Unsaturated hydraulic conductivity (m/s) , ψ is the Pressure head (m), z is the Vertical position (m), $\theta$is the Soil moisture content

Adapting the equation for the discrete model, we get the following form of the equation as,

$$q_w = \sum_{\zeta=i-1}^{i+1} k_{i,\zeta} \cdot \frac{(\psi + z)_\zeta - (\psi + z)_i}{l_{i,\zeta}}, \quad \zeta \neq i \tag{9}$$

where z is the cell elevation and k here represents the average hydraulic conductivity of the region between the ith and the ζth cells.

2.3 finite difference method

deriving the 2nd order formula for centered derivatives.

$$f'_i = a_{-1} f_{i-1} + a_0 f_i + a_1 f_{i+1}. \tag{8}$$

where $f_i = f(x_i)$, $f'_i = f'(x_i)$, $f_{i-1} = f(x_i - \delta x)$, and $f_{i+1} = f(x_i + \delta x)$. Here δx is the distance between adjacent cells in the mesh (assume a uniform mesh, so $\delta x =$ const). The function f is known everywhere on the mesh, but but for f'_i we need the coefficients a_{-1}, a_0, and a_1. Similarly:

$$f"_i = b_{-1} f_{i-1} + b_0 f_i + b_1 f_{i+1} \tag{9}$$

for solving b_{-1}, b_0, and b_1. expand $f(x)$ up to 2nd order in x, and we get the matrix

$$\begin{pmatrix} f_{i-1} \\ f_i \\ f_{i+1} \end{pmatrix} = \begin{pmatrix} (-1)^0 & (-1)^1 & (-1)^2 \\ 0^0 & 0^1 & 0^2 \\ 1^0 & 1^1 & 1^2 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \delta x \\ c_2 \delta x^2 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \delta x \\ c_2 \delta x^2 \end{pmatrix}$$

Then, solving the resulting matrix equation by matrix inversion to obtain the expansion coefficients which, in turn, are used to get f'_i and $f"_i$. we Invert the 3×3 matrix in equation

(9) to obtain c_0, $c_1\delta x$, and $c_2\delta x^2$ in terms of f_{i-1}, f_i, and f_{i+1}. Then differentiate equation (7) and set $x = x_i$ to get $f'_i = c_1, \quad f"_i = 2c_2$. Then we get,

$$f'_i = \frac{-f_{i-1} + f_{i+1}}{2\delta x} \tag{10}$$

$$f"_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{\delta x^2} \tag{11}$$

The truncation error can be reduced by extending the method up to any order, but this increased accuracy comes at a cost as the computational time increases. For cells on the mesh boundary, one can only calculate the spatial derivatives using points on the mesh. Using methods analogous to those above, one can show that the 2nd order expressions are then given by

$$f'_i = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2\delta x}, \quad f"_i = \frac{2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}}{\delta x^2}, \tag{12}$$

and

$$f'_i = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2\delta x}, \quad f"_i = \frac{2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}}{\delta x^2}. \tag{13}$$

2.4 runge-kutta 4th order

The generalized form of the RK4 method is used for solving a set of coupled differential equations of the form:

$$\frac{d\vec{y}}{dx} = \vec{f}(x, \vec{y})$$

where $\frac{d\vec{y}}{dx}$ represents the set of equations $\{y_1(y_1, y_2, y_3, ..., x), y_2(y_1, y_2, y_3, ..., x), \ldots\}$, and $\vec{f}(x, \vec{y})$ represents the set of equations $\{f_1(\vec{y}, x), f_2(\vec{y}, x), f_3(\vec{y}, x), \ldots\}$. Here the RK4 equations are:

$$k1 = h\vec{f}(x_n, y_n)$$

$$k2 = h\vec{f}\left(x_n + \frac{h}{2}, y_n + \frac{k1}{2}\right)$$

$$k3 = h\vec{f}\left(x_n + \frac{h}{2}, y_n + \frac{k2}{2}\right)$$

$$k4 = h\vec{f}(x_n + h, y_n + k3)$$

$$y_{n+1} = y_n + \frac{k1 + 2k2 + 2k3 + k4}{6}$$

This is done in a loop for the required number of steps and convergence.

3 Comparison with analytical solutions

3.1 Heat transfer by pure conduction

The heat equation given by Churchill's (1972) for a perfectly thermally insulated coloumn of soil for pure conduction is

$$k\frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial t} \tag{14}$$

by a proper choice of the unit of time, we can write k=1 in the heat equation, where k is the diffusivity. The performance of the code in simulating pure conduction under hydrostatic conditions was assessed through comparison with Churchill's (1972) analytical solution for one-dimensional heat conduction in a finite domain. This evaluation involved analyzing a soil column with a total length L_c of 4 m. The upper half was assigned an initial temperature of $T_u = 10\,°C$, while the lower half was set to $T_l = 20\,°C$ (refer to Fig. 1). Throughout the simulation, the system maintained hydrostatic conditions without any flow. Heat conduction occurred at the interface due to the temperature gradient until the entire domain reached an average steady-state temperature of $15\,°C$. Churchill's (1972) analytical solution is formulated as follows:

$$T(z,t) = T_u \cdot \left(0.5 + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}\cdot\cos\left(\frac{(2n-1)\cdot\pi\cdot z}{L_c}\right)\cdot\exp\left(-\left(\frac{(2n-1)\cdot\pi}{L_c}\right)^2\cdot\left(\frac{\lambda}{C}\right)\cdot t\right)\right)$$
$$+ T_l \cdot \left(0.5 - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}\cdot\cos\left(\frac{(2n-1)\cdot\pi\cdot z}{L_c}\right)\cdot\exp\left(-\left(\frac{(2n-1)\cdot\pi}{L_c}\right)^2\cdot\left(\frac{\lambda}{C}\right)\cdot t\right)\right) \quad (15)$$

The expected plot from Nagare(2014) is given in FIG. 2

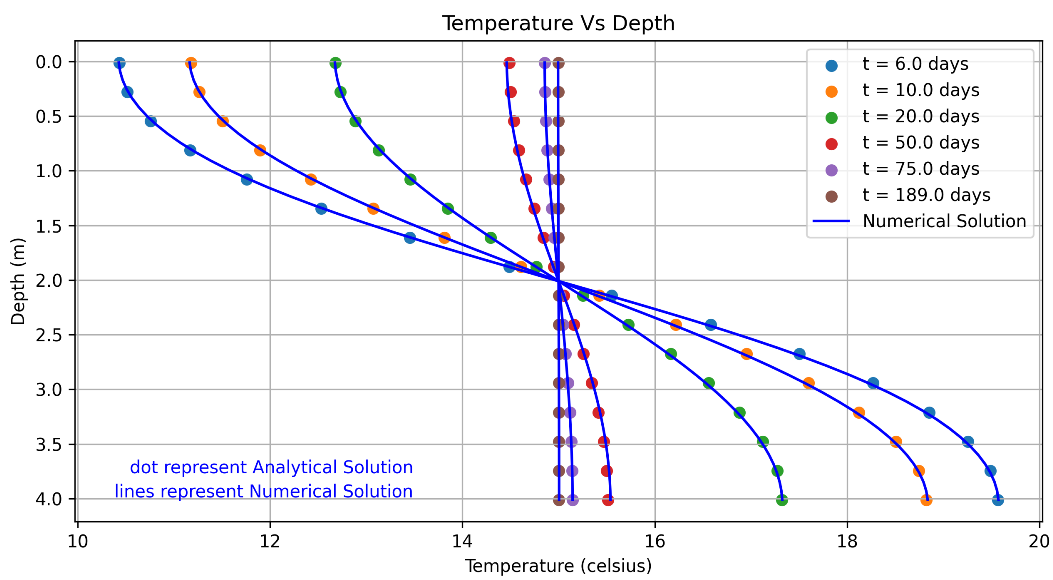

Figure 1: Comparison between the analytical solution given by Churchill (1972) and our simulation for a perfectly thermally insulated 4 m long soil column. Lines represent the numerical solution and dots represent analytical solution for time points as shown in the legend.

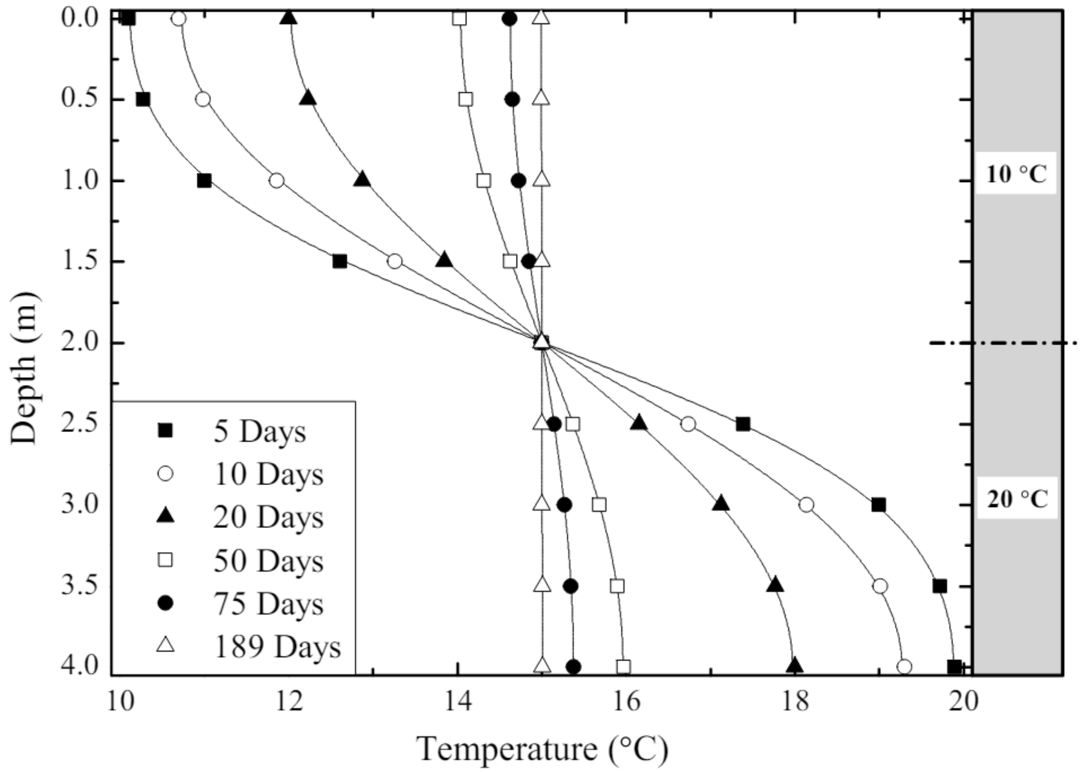

Figure 2: expected plot for pure conduction from Nagare(2014). Lines represent the analytical solution and symbols represent the CA solution for time points as shown in the legend.

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

Symbol	Parameter	Value
η	Porosity	0.35
λ	Bulk thermal conductivity	$2.0\,\mathrm{J\,s^{-1}\,m^{-1}\,{}^{\circ}C^{-1}}$
C_w	Volumetric heat capacity of water	$4,174,000\,\mathrm{J\,m^{-3}\,{}^{\circ}C^{-1}}$
C_s	Volumetric heat capacity of soil solids	$2,104,000\,\mathrm{J\,m^{-3}\,{}^{\circ}C^{-1}}$
ρ_w	Density of water	$1000\,\mathrm{kg\,m^{-3}}$
ρ_s	Density of soil solids	$2630\,\mathrm{kg\,m^{-3}}$

3.2 Heat transfer by conduction and convection

One-dimensional anisothermal flow of an incompressible fluid through homogeneous porous mediums can be described by (Stallman,1965)

$$k\frac{\partial^2 T}{\partial z^2} - vc_0\rho_0\frac{\partial T}{\partial z} = c\rho\frac{\partial T}{\partial t} \tag{16}$$

where T is temperature, z is distance along the direction of flow, t is time, v is the fluid velocity , c_0 and ρ_0 are the specific heat and density of the fluid, respectively, c and ρ are the specific heat and density of the fluid and medium in combination, respectively, and k is the heat conductivity of the fluid and medium in combination.

Stallman's analytical solution (1965) for the subsurface temperature profile in a semi-infinite porous medium, responding to a sinusoidal surface temperature, serves as a benchmark to evaluate the our code's capability to simulate one-dimensional heat convection and conduction in the presence of a time-varying Dirichlet boundary condition. Given the temperature variation at the ground surface described by

$$T\left(z_0, t\right) = T_{\text{surf}} + A \cdot \sin\left(\frac{2 \cdot \pi \cdot t}{\tau}\right) \tag{17}$$

the temperature variation with depth is given by

$$T\left(z, t\right) = A \cdot e^{-a \cdot z} \cdot \sin\left(\frac{2 \cdot \pi \cdot t}{\tau} - b \cdot z\right) + T_{\infty} \tag{18}$$

$$a = \left\{\left[\left(\frac{\pi C\rho}{\lambda\tau}\right)^2 + \frac{1}{4}\left(\frac{q_{\text{f}}C_{\text{w}}\rho_{\text{w}}}{2\lambda}\right)^4\right]^{0.5} + \frac{1}{2}\left(\frac{q_{\text{f}}C_{\text{w}}\rho_{\text{w}}}{2\lambda}\right)^2\right\}^{0.5} - \left(\frac{q_{\text{f}}C_{\text{w}}\rho_{\text{w}}}{2\lambda}\right),$$

$$b = \left\{\left[\left(\frac{\pi C\rho}{\lambda\tau}\right)^2 + \frac{1}{4}\left(\frac{q_{\text{f}}C_{\text{w}}\rho_{\text{w}}}{2\lambda}\right)^4\right]^{0.5} + \frac{1}{2}\left(\frac{q_{\text{f}}C_{\text{w}}\rho_{\text{w}}}{2\lambda}\right)^2\right\}^{0.5},$$

In the provided expression, A represents the amplitude of temperature variation (°C),

T_{surf} denotes the average surface temperature over a period of τ (s), T_∞ stands for the initial temperature of the soil column and the temperature at infinite depth, and q_f represents the specific flux through the column top.

The parameters utilized in the analytical examples for Stallman (1965) and the simulation code are detailed in Table 2. The coupled simulation code demonstrates its capability to replicate the temperature evolution resulting from conductive and convective heat transfer, as evidenced by its agreement with the analytical solution (Fig. **??**).

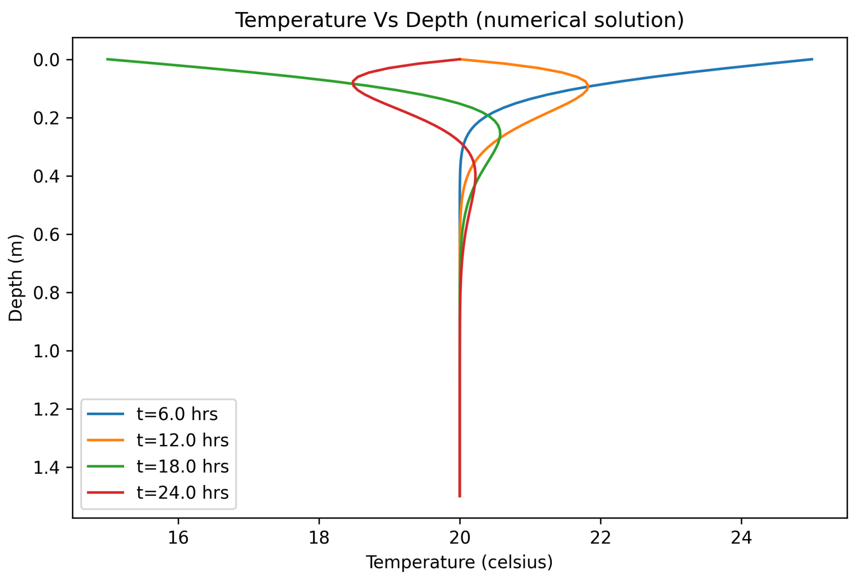

Figure 3: coupled simulation model steady state solutions for conductive and convective heat transfer. The soil column in this example is initially at 20 Celcius, and the upper surface is subjected to a sinusoidal temperature with amplitude of 5 celcius and period of 24 h

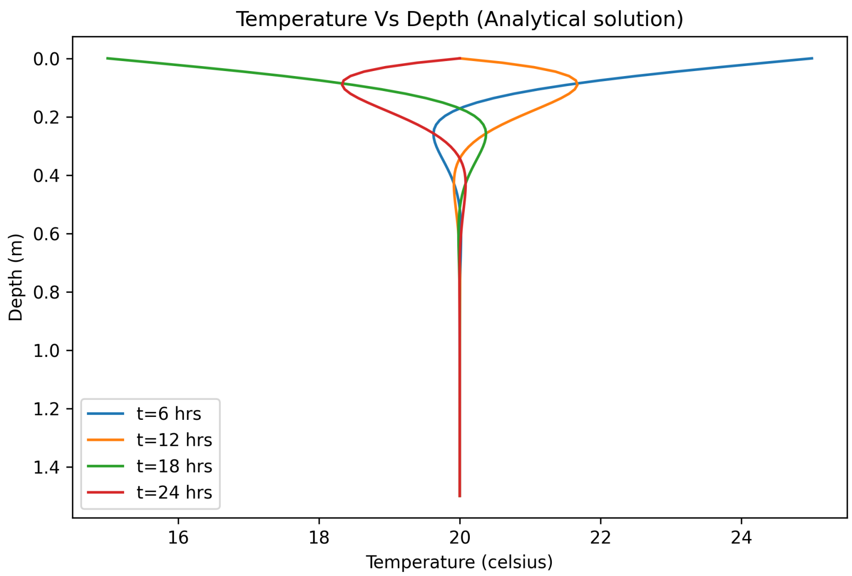

Figure 4: analytical (Stallman, 1965) steady state solutions for conductive and convective heat transfer. The soil column in this example is initially at 20 Celcius, and the upper surface is subjected to a sinusoidal temperature with amplitude of 5 celcius and period of 24 h

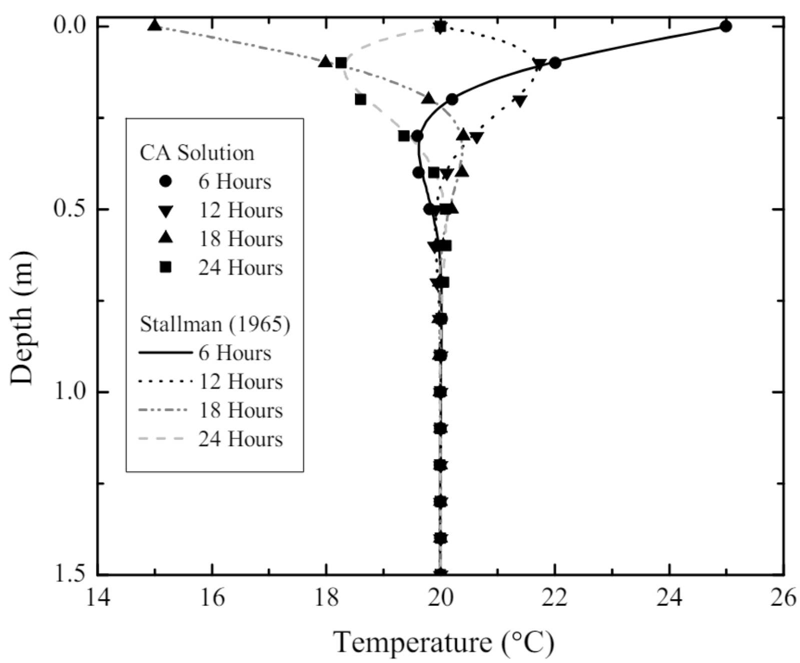

Figure 5: expected plot for coupled conductive and convective heat transfer from Nagare(2014). Lines represent the analytical solution and symbols represent the CA solution for time points as shown in the legend.

Table 2: Simulation parameters for predicting the subsurface temperature profile in a semi-infinite porous medium in response to a sinusoidal surface temperature.

Symbol	**Parameter**	**Value**
η	Porosity	0.40
λ	Bulk thermal conductivity	2.0 J s^{-1} m^{-1} $°C^{-1}$
C_w	Volumetric heat capacity of water	$4,174,000$ J m^{-3} $°C^{-1}$
C_s	Volumetric heat capacity of soil solids	$2,104,000$ J m^{-3} $°C^{-1}$
ρ_w	Density of water	1000 kg m^{-3}
ρ_s	Density of soil solids	2630 kg m^{-3}
l	Length of cell	0.01 m
t	Length of time step in simulation solution	1 s
q_f	Specific flux	4×10^{-7} m s^{-1} downward
τ	Period of oscillation of temperature at the ground surface	24 h
A	Amplitude of the temperature variation at the ground surface	5 °C
T_{surf}	Average ambient temperature at the ground surface	20 °C
T_∞	Ambient temperature at depth	20 °C

4 Conclusion

The coupled equations for water flow based on Buckingham Darcy's law and heat flow based on Fourier's heat low was solved numerically by using finite difference approach and Runge Kutte time advancing. The performance of the code in simulating pure conduction under hydrostatic conditions was assessed through comparison with Churchill's (1972) analytical solution for one-dimensional heat conduction in a finite domain and the model was able to simulate the temperature evolution due to pure conduction successfully. The performance of the code in simulating coupled heat transfer by conduction and convection was was assessed through comparison with analytical (Stallman, 1965) steady state solutions for conductive and convective heat transfer and model succesfully reproduced the result.The project provided a comprehensive insight into the relationship between water flow and heat transfer within soil.

REFERENCES

1. Ranjeet Nagare, Pathikrit Bhattacharya, Jaya Khanna, and R. Schincariol. Coupled cellular automata for frozen soil processes. SOIL Discussions, 1:119–150, 05 2014.

2. Churchill, R. V.: Operational mathematics, McGraw-Hill Companies, New York, 1972.

3. Stallman, R. W.: Steady 1-dimensional fluid flow in a semi-infinite porous medium with sinusoidal surface temperature, J. Geophys. Res., 70, 2821–2827, 1965.

4. Van Genuchten, M. T.: A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892–898, 1980.