Term Project Report

Computational Physics - Theory

Coupling Of Heat And Water Movement In Soil

Submitted by,

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Contents

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Abstract

In this project, the coupled transfer of water and heat in soil [3] is studied using a finite difference method. The project explores the intricate relationship between water movement and heat transfer in soil, where the transport of water influences the thermal properties of the soil. Firstly, the numerical solution is compared with trends observed in experimental results, ensuring the accuracy of our simulation in capturing real-world phenomena. Secondly, the model is validated by comparing it with an analytical solution. Our results demonstrate the successful reproduction of experimental outcomes, showcasing the effectiveness of our coupled water and heat transfer model in capturing the complex dynamics within soil systems.

1 Introduction

The coupling of heat and moisture dynamics within soil, crucial for understanding the ecological conditions supporting vegetation and microorganisms. Utilizing a one-dimensional soil column, numerical methods are employed to compute the coupled heat transfer with water, leveraging fundamental principles such as the heat balance equation (Fourier law) and the mass balance equation (Buckingham-Darcy equation).

Fourier's law of heat conduction describes the flow of heat through a material. In subsurface conditions, heat balance is primarily maintained by conduction and convection.The Buckingham-Darcy equation governs water movement in unsaturated soil, providing insights into moisture distribution.

The motion of water is dictated by soil water potentials, which represent the driving forces for water movement. These potentials, including matric and gravitational potentials, collectively define the soil water potential.

Variably saturated soil, which is the main focus here, is the soil in which the water content is not uniform throughout the soil profile.

1.1 Heat transfer in soil

Heat transfer in soil plays a crucial role in various environmental and engineering applications, including agriculture, geotechnical engineering, and thermal energy storage. Soil acts as a medium for the transfer of heat due to its thermal conductivity properties.
Fourier's law of heat conduction governs this process, stating that the heat flux (q) through a material is proportional to the negative gradient of temperature (∇T), i.e,

$$q = -k\nabla T \tag{1}$$

where:

q : Heat flux (W/m^2)
k : Thermal conductivity of the material (W/m·K)
∇T : 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.

1.2 Water movement in soil

Water movement in soil is a dynamic process governed by complex interactions between soil properties, environmental conditions, and plant physiology. As water percolates through the soil profile, it encounters various physical and chemical barriers, such as soil texture, structure, and organic matter content, which influence its movement and distribution. In unsaturated soil, the water is attracted to and held by the surfaces of the soil solids by capilliary potential, i.e, matric potential.
Buckingham saw that spatial gradients in this potential would act as a force to drive soil water flow and that resulting flow would be proportional to and in opposite direction of that gradient. In the Buckingham–Darcy's equation, the driving gradient includes the matric potential. The pressure potential is taken as zero in unsaturated conditions, and hydraulic conductivity is a function of water content. The textural properties of the soil dictating characteristics like water conductivity are described by the Mualem–van Genuchten model.

Matric potential as a function of water content is given by:

$$\psi(\theta_w) = \frac{(S_e^{-1/m} - 1)^{1/n}}{\alpha} \tag{2}$$

where $S_e = \frac{\theta_w - \theta_{res}}{\theta_{sat} - \theta_{res}}$.

The hydraulic conductivity as a function of water content is given by:

$$k(\theta_w) = K_s \cdot (S_e)^{0.5} \cdot \left[1 - \left(1 - (S_e)^{\frac{1}{m}}\right)^m\right]^2 \quad (3)$$

The water flux is calculated using:

$$q = -K(\theta)\frac{\partial \psi}{\partial z} \quad (4)$$

where:

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

1.3 Coupling of heat and water movement in soil

The coupling between heat and water in soil is a critical aspect of understanding various environmental processes, including plant growth, hydrology, and climate dynamics. As water moves through the soil matrix, it carries thermal energy with it, affecting the temperature distribution within the soil profile. Conversely, temperature gradients in the soil influence the movement and distribution of water, as they impact the soil's hydraulic properties and water retention capacity. This intricate coupling is further influenced by factors such as soil texture, organic matter content, and vegetation cover.
In Stallman,1965 [4], the coupled equation is derived to get:

$$k\frac{\partial^2 T}{\partial z^2} - vc_0\rho_0\frac{\partial T}{\partial z} = c\rho\frac{\partial T}{\partial t} \quad (5)$$

The analytical solution to this equation is the plot required in my project.

1.4 Finite difference method

The finite difference method is a numerical technique used to approximate solutions to differential equations. It is particularly useful for solving partial differential equations (PDEs) in which analytical solutions are difficult or impossible to obtain. The method works by discretizing the spatial domain into a grid of points as shown in fig.1 and approximating derivatives with finite difference approximations.

Consider a one-dimensional boundary value problem described by the differential equation

$$\frac{d^2u}{dx^2} = f(x) \quad (6)$$

subject to boundary conditions $u(a) = \alpha$ and $u(b) = \beta$, where a and b are the endpoints of the domain.

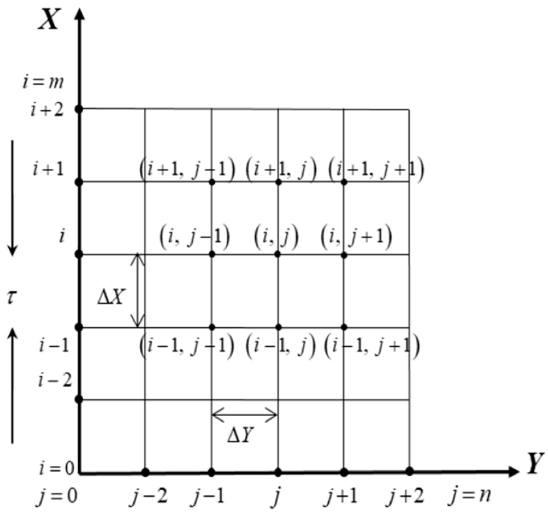

Figure 1: Finite difference grid space. Image source: [1]

To apply the finite difference method, we discretize the domain by dividing it into N equally spaced points x_i, with $i = 0, 1, 2, \ldots, N$ and $x_0 = a$ and $x_N = b$. Let u_i denote the approximate solution at the point x_i. We approximate the second derivative using a finite difference scheme, such as the central difference formula:

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} \quad (7)$$

where Δx is the spacing between grid points.

Substituting this approximation into the original differential equation, we obtain a system of algebraic equations representing the discretized problem. This system can then be solved using various numerical techniques, such as Gaussian elimination or iterative methods.

Finally, the solution u_i at each grid point x_i can be obtained, and the approximate solution to the original differential equation can be constructed by interpolating between these grid points.

In my experiment I used finite difference method to solve heat and water flow equations.

2 Simulations: Procedure

2.1 Discretization

Discretization is a process used in numerical methods to approximate continuous mathematical models or equations by dividing them into

discrete elements or intervals. In discretization, the continuous domain of the problem (such as space or time) is divided into a finite number of discrete elements or intervals.
Here, the soil column and time are discretised into cells where each component is computed for the cell. The model finds the dependent variable for each cell at discretised time intervals.

2.2 Heat transfer by conduction and convection

2.2.1 Heat conduction formulae

The heat balance equation is given as

$$q_h = \sum_{j=1-1}^{i+1} \frac{\lambda_{ij}\,(T_j - T_i)}{l_{ij}} \tag{8}$$

where,

- q_h is the net flux in the i^{th} cell(heat flux)
- λ_{ij} is the average effective thermal conductivity between the i^{th} and j^{th} cells
- T_j is the cell temperature
- T_i is the temperature of the cell neighboring the i^{th} cell at $j-1$ position
- l_{ij} is the length between the centers of the active and neighboring cell

The subscript i refers to the active cell, and j refers to the neighboring cell. l_{ij} represents the distance between the centers of the active and neighboring cells.

This equation expresses the net heat flux (q_h) into the i^{th} cell as the product of the average effective thermal conductivity (λ_{ij}) between the i^{th} and j^{th} cells, the temperature difference ($T_i - T_j$) between the active cell and its neighbor, and the reciprocal of the distance (l_{ij}^{-1}) between their centers.
Also,

$$\frac{q_h \Delta t}{l_i} = C_i \Delta T \tag{9}$$

where, C_i is the effective volumetric heat capacity

2.2.2 Water flow formulae

$$q_w = \sum_{j=i-1}^{i+1} \frac{k_{ij} \cdot (\psi + z)_j - (\psi + z)_i}{l_{ij}} \tag{10}$$

where,

- qw: Water flux at grid point i represents the amount of water flowing into or out of the grid point.
- kij: Hydraulic conductivity between grid points i and j represents the ability of water to flow through the soil between these points.
- psi: Matric potential represents the soil water potential, indicating the water's energy state and its ability to move within the soil.
- z: Vertical position represents the depth or height of the grid point within the soil profile.
- l_ij: Distance between grid points i and j represents the spacing between adjacent grid points, influencing the rate of water flow between them.

2.2.3 Coupling

Thermal conductivity (λ) and specific heat capacity (C) of the soil are functions of both temperature (T) and water content (θ). The coupling between hydraulic and thermal processes in a system is done by:

1. **Change in Pressure Head ($\Delta\psi_i$) Calculation**:
   - The flux of water ($q_{w,i}$) at a particular location i within the soil contributes to a change in the total water content, which, in turn, affects the pressure head (ψ).
   - The change in pressure head ($\Delta\psi_i$) from time t to time $t+1$ is calculated as the difference between the pressure head at time $t+1$ (ψ_{t+1}^i) and the pressure head at time t (ψ_t^i).
2. **Updating Total Water Content (θ_w)**:
   - The updated value of the total water content (θ_w) is determined based on the change in pressure head and the relationship between pressure head and water content ($\psi(\theta_w)$).
   - This relationship is the van Genuchten-Mualem model given in 1.2.
3. **Updating Volumetric Heat Capacity (C_i)**:
   - With the updated value of total water content (θ_w), the volumetric heat capacity (C_i) of the soil at location i is updated.
   - The volumetric heat capacity represents the amount of heat required to raise the temperature of a unit volume of soil by one unit.

4. **Energy Balance Module**:
   - The updated value of C_i is then used as input to the energy balance module, along with the computed heat flux ($q_{h,i}$) at location i.

2.2.4 Parameters

The parameters I used for the experiment are given in the table 2.

2.2.5 Expected plot

The plot of heat and moisture content coupled, as given in the paper [3] is shown below.

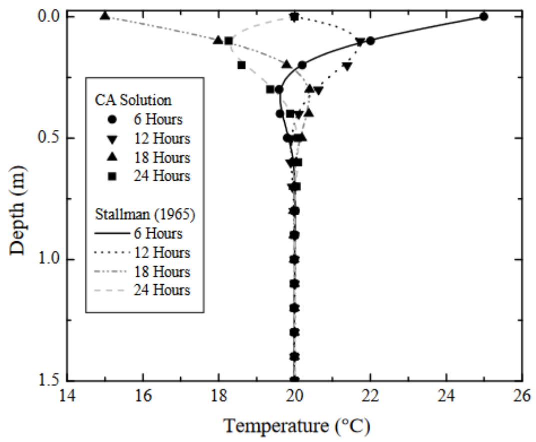

Figure 3: Comparison between the analytical (Stallman, 1965) and coupled CA model steady state solutions for conductive and convective heat transfer. The soil column in this example is infinitely long, initially at 20 ∘C, and the upper surface is subjected to a sinusoidal temperature with amplitude of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

2.3 Comparison with experiment: heat flow

The study conducted by Hua Jin et al. (2018)[2] involved coupling heat transfer with moisture content in a one-dimensional soil column. In their experimental setup, both the initial temperature and moisture content were assumed to be uniform throughout the soil column. The temperature at the starting point of the column served as the reference heat source temperature. Because the soil column was considered to be of considerable length, the temperature and moisture content at the outer boundaries remained constant and were not influenced by external factors.
I simulated the same, using the parameters, given in the fig.4.

2.3.1 Parameters

Parameters	Experiment 1
Soil thermal conductivity (J/(min·m·°C))	48
Soil particle density (kg/m^3)	2650
Heat capacity of soil(J/(kg·°C))	1739
Length of soil column (m)	1
Number of distance element	100
Time step (min)	1
Total time (h)	24
Initial soil temperature (°C)	20.6
Temperature of heat source (°C)	33.5
Porosity	0.4403
Water thermal conductivity (J/(min·m·°C))	35.94
Water density (kg/m^3)	1000
Heat capacity of moisture (J/(kg·°C))	4180
Initial moisture content (m^3/m^3)	0.08

Figure 4: Parameters for the comparison from [2]

2.3.2 Expected plot

The plot that was simulated along with experimental plot that is given in the paper, is shown below.

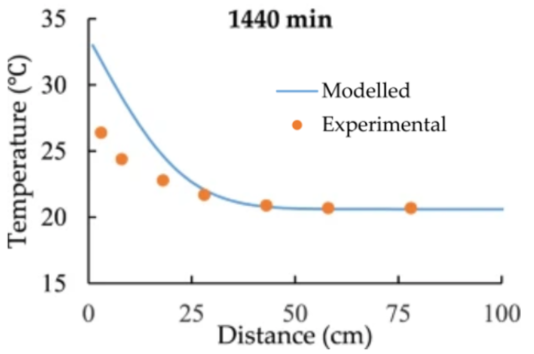

Figure 5: Hua Jin et.al(2018) [2] temperature profile for 1m soil column after 24 hours. Boundary condition 33.5°C

3 Observations and plots

Stallman's analytical solution[4] to the subsurface temperature profile in a semi-infinite porous medium in response to a sinusoidal surface temperature provides a test of the model The temperature variation is given by:

$$T(z_0, t) = T_{surf} + Asin(2\pi t/\tau) \qquad (11)$$

The soil column is infinitely long, initially at 20 degC, and the upper surface is subjected to a

Symbol	Parameter	Value
η	porosity	0.40
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	$2630\,\mathrm{kg\,m^{-3}}$
l	length of cell	0.01 m
t	length of time step in CA solution	1 s
q_f	specific flux	$4 \times 10^{-7}\,\mathrm{m\,s^{-1}}$ 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

Figure 2: Parameters used for heat and water coupling

sinusoidal temperature with amplitude of 5 ◦C and period of 24 h.

I simulated the coupled heat and water flow for different time periods, i.e, 6 hrs, 12 hrs and 24 hrs. Their respective plots are given in 6,7 and 8.
Also the plot obtained for the comparison with the experimental data from [2], is given in 9.

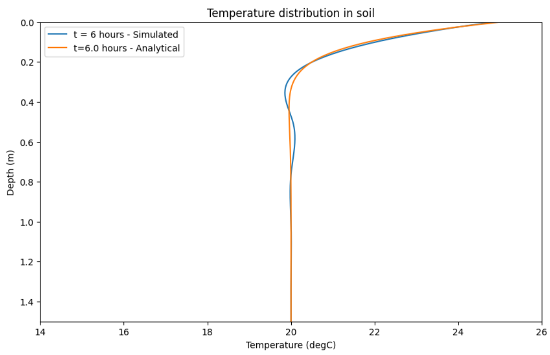

Figure 6: Plot for coupled heat and water flow for 6 hours

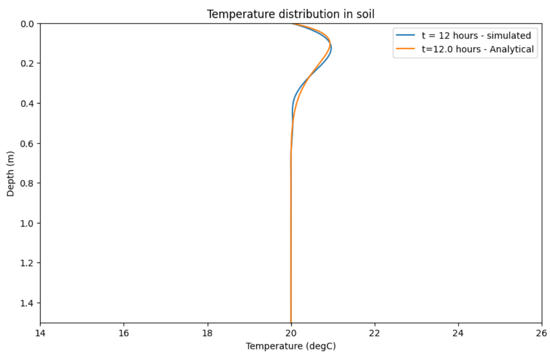

Figure 7: Plot for coupled heat and water flow for 12 hours

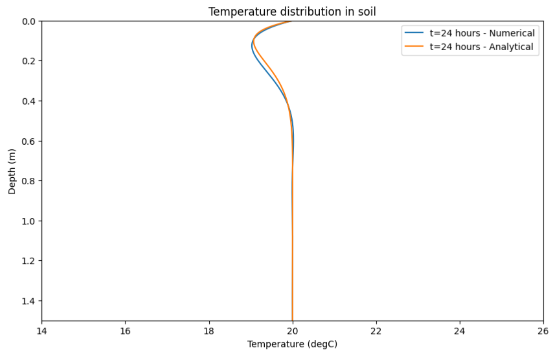

Figure 8: Plot for coupled heat and water flow for 24 hours

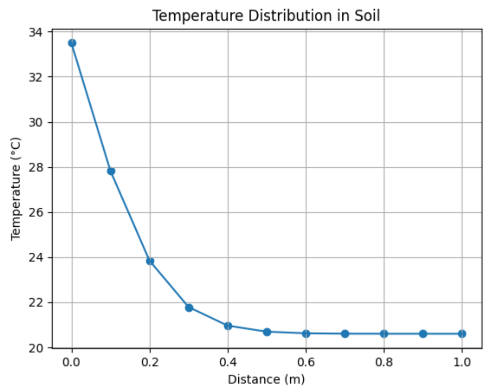

Figure 9: Numerically solved temperature profile for 1m soil column after 24 hours. Boundary condition 33.5 degree Celsius

4 Conclusions

In this project, I simulated the coupled transfer of water and heat in soil using a finite difference method. The outcomes of simulations showed the intricate relationship between water movement and heat transfer in soil, recognizing that the transport of water significantly influences the thermal properties of the soil.

Initially, I compared the numerical solution with trends observed in experimental results. Furthermore, I validated the model by comparing it with an analytical solution. Also, the model was compared to two results one with variable boundary condition and other fixed boundary condition.

The results demonstrate the successful reproduction of experimental outcomes. The consistency between the simulation results and the expected trends further supports the robustness of the model.

Overall, this project gave a deeper understanding of the interplay between water movement and heat transfer in soil, and could explore the application of finite difference method in real life examples.

References

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