Identification of Thermophysical Properties of the Soil in 3D-axisymmetric Coordinate System Using Inverse Problem
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Abstract
This paper is motivated by the studies of agricultural and archaeological soils. We introduce a numerical strategy in 3D axisymmetric coordinate system to estimate the thermophysical properties of a saturated porous medium (volumetric heat capacity \(\rho C_p\), thermal conductivity \(\lambda_s\) and porosity \(\phi\)) where a phase change problem (liquid/vapor) appears due to strong heating. The estimation of these thermophysical properties is done by inverse problem knowing the heating curves at selected points of the porous medium. In order to solve the inverse problem, we use the least square criterion in which sensitivity coefficients appear and which leads to a system of ordinary differential equations (ODE). At the stage of numerical computations, we propose a global approach based on the method of lines, where time and space discretizations are considered separately. The space discretization is done using a vertex-centered finite volume method; the discretization in time is done via an ODE solver combined with a modified Newton’s method to deal with the nonlinearity of the system of coupled equations.

Keywords: Inverse Problem, Saturated Porous Medium, Phase Change, Agricultural and Archaeological Soils, Gauss–Newton Method.

1. Introduction

The work presented in this paper is motivated by the studies of agricultural and archaeological soils. A systematic application of numerical modeling in a particular field of agriculture and archaeology which is the study of seed germination and archaeological hearths is presented. The authors introduce a numerical strategy in 3D axisymmetric coordinate system to estimate the thermophysical properties of the soil (volumetric heat capacity \(\rho C_p\), thermal conductivity \(\lambda_s\) and porosity \(\phi\)) of a saturated porous medium where a phase change problem (liquid/vapor) appears due to intense heating from above. The advantage of our 3D-axisymmetry configuration is that it is well adapted to the heating of a semi-infinite medium by a circular heating plate, which is a very simple device. Usually \(\phi\) is the porosity, however when the soil is not saturated (which should concern most cases), \(\phi\) may be taken equal to the part of water in the pores. This is of course an approximation which is correct for the energy balance but which neglects the capillary forces and the migration flow of the liquid inside the porous media; a complete model of such an unsaturated model is out of the scope of this paper.

The investigation of the thermal properties of the soil can have significant practical consequences such as evaluation of optimum conditions for plant growth and development and can be utilized for the control of thermal-moisture regime of soil in the field [2]. These properties influence how energy is partitioned in the soil profile so the ability to monitor them is a tool to manage the soil temperature regime that affects seed germination and growth. It can also provide information about the use of fire by ancient civilizations whether for cooking or heating ... [3].

The inverse problem, presented in this paper, consists of the estimation of thermophysical properties of the soil knowing the heating curves at selected points of the altered soil [4]. In general, the mathematical formulation of inverse problems leads to models that are typically ill-posed. According to Hadamard, a mathematical problem is ill-posed if one of the following properties is violated:

- For all admissible data, a solution exists.
- For all admissible data, the solution is unique and depends continuously on the data [6].

In such ill-posed inverse problems, we usually minimize a discrepancy between some experimental data and some model data [7]. In our problem, we use the least square criterion in which the sensitivity coefficients appear and where we try to minimize the discrepancy function which
is expressed as the norm of the difference between the experimental temperature and the synthetic ones [1]. The system composed of the energy equation together with three boundary initial problems resulting from differentiating the basic energy equation with respect to the soil properties must be solved [5].

At the stage of numerical computations, the Gauss Newton method is used to minimize the least square criterion; that requires the solution of a system of four highly nonlinear ordinary differential equations. We propose a global approach similar to that presented by [4]. Basically, our paper generalizes the 1D inverse problem presented by [4] to the 3D-axisymmetry configuration. It is important to note that in this new configuration, the solution was reached after taking into consideration the temperature history at different time steps which was not the case in [4] where the authors reached the solution by taking the temperature history at the final time only. This approach is based on the method of lines, where time and space discretizations are considered separately. The space discretization is done using a vertex-centered finite volume method; the discretization in time is done via an ODE solver that uses a BDF method and a modified Newton method to deal with the high nonlinearity. The code validation stage is based on the comparison between the numerical results and the synthetic data.

2. Mathematical formulation

Consider a porous medium in 3D axisymmetric coordinate system as shown in Fig. 1. \( \Omega \) is the bounded domain with boundary \( d\Omega = \Gamma^D \cup \Gamma^N \). The medium is heated from above with \( T_c \) (temperature of the fire) greater than the \( T_v \) (evaporation temperature which is normally 100°C).


In order to model the heat conduction transfer in the soil, we use the energy equation. We neglect the convection term of the heat equation so that the energy conservation equation for the unknown temperature \( T \) is expressed as:

\[
\frac{\partial T(x,t)}{\partial t} = \text{div}(\lambda(T)\nabla T(x,t)) \quad \text{in} \quad \Omega \times (0,t_{\text{end}}] \\
T(x,0) = T_0(x) \quad \text{in} \quad \Omega \\
T(x,t) = T^D(x,t) \quad \text{on} \quad \Gamma^D \times (0,t_{\text{end}}] \\
\nabla T(x,t).\nu = 0 \quad \text{on} \quad \Gamma^N \times (0,t_{\text{end}}] \quad (1)
\]

where \( T \) represents the temperature, \( T_0 \) is the initial temperature at \( t_0 = 0 \), \( T^D \) is \( T_c \) at the fire and \( T_0 \) elsewhere, \( \rho \) is the density, \( C \) is the specific heat capacity, \( \lambda \) is the conductivity, \( \phi \) is the porosity, the subscripts \( e \), \( f \) and \( s \) indicate the equivalent parameters of the medium, the properties of the fluid and the porous matrix properties respectively.

The effective volumetric heat capacity and the effective conductivity are defined by:

\[
(\rho C)_e = \phi (\rho C)_f + (1 - \phi)(\rho C)_s, \quad (2)
\]

and

\[
\frac{1}{\lambda_e} = \frac{\phi}{\lambda_f} + \frac{1 - \phi}{\lambda_s} \quad (3)
\]

The effective conductivity in equation (3) is calculated using the harmonic mean to test the algorithm. In real situation, the harmonic mean should be replaced by some approximated model, such as this of Kunii & Smith [10].

To avoid the tracking of the interface of the phase change problem (liquid/vapor) which appears when the water existing in the soil turns into gas, the apparent heat capacity (AHC) method is used because it allows a continuous treatment of a system involving phase transfer. In this method [8, 9], the latent heat is taken into account by integrating the heat capacity over the temperature, and the domain is considered to be treated as one region. The singularity in the AHC method which is presented in the formulation of thermo-physical properties defined by [8] is treated in [9]. The Dirac delta function, representing the equivalent heat capacity, (see Fig. 2 continuous lines) can be approximated by the normal distribution:

\[
\frac{d\sigma}{dT} = (\varepsilon \pi \Delta T^2) \exp\left[-\varepsilon^2(T - T_v)^2\right] \quad (4)
\]

where \( \varepsilon = \sqrt{\frac{2}{\Delta T}} \), \( \Delta T \) is the phase change interval and \( T_v \) is the phase change temperature. The integration of equation (4) yields the error functions approximations for the initial phase fraction:
\[ \sigma(T) = \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\varepsilon(T - T_p)}{\sqrt{2}} \right) \right) \] (5)

\[ \Delta T \]

**Fig.2.** Equivalent thermo-physical properties in the AHC method.

The smoothed coefficients (see Fig. 2 dashed lines) could be written as:

\[ C_f = C_i + (C_v - C_i) \sigma + \frac{1}{T} \frac{d\sigma}{dT} \] (6)

\[ \lambda_f = \lambda_i + (\lambda_v - \lambda_i) \sigma \] (7)

\[ \rho_f = \rho_i + (\rho_v - \rho_i) \sigma \] (8)

where \( L \) is the latent heat of phase change and the subscripts \( f \) and \( v \) indicate respectively the properties of the liquid phase (water) and that of the vapor. It is important to mention that the thermophysical properties of the fluid are temperature dependent and that is why the problem is highly nonlinear.

### 2.2. Inverse Problem

In order to solve the parametric inverse problem consisting of finding the volumetric heat capacity \((\rho C)_s\), the conductivity \(\lambda_s\) and the porosity \(\phi\) of the saturated soil, it is necessary to know the values of temperatures \(T_{bi}\) at selected points \(x_i\) of the porous medium domain for times \(t^f\): \(T^f_{gi} = T_g(x_i, t^f)\) where \(i = 1, 2, ..., M\) and \(f = 1, 2, ..., F\).

We use the least squares criterion to solve this inverse problem so we try to find the soil parameters that minimize the error function \(S\) which is defined by:

\[ S((\rho C)_s, \phi, \lambda_s) = \frac{1}{2} \sum_{i=1}^{M} \sum_{f=1}^{F} (T_{gi}^f - T_{gi})^2 \] (9)

where \(T_{gi}^f = T(x_i, t^f)\) are the temperatures being the solution of the direct problem for the assumed set of parameters at the points \(x_i\), \(i = 1, 2, ..., M\) for the time \(t^f, f = 1, 2, ..., F\) and \(T_{gi}\) are the measured temperatures at the same points \(x_i\) for time \(t^f\).

#### 2.2.1 Method of resolution

To illustrate the method of resolution, we define the following vectors:

\[ p^{(k)} = \begin{pmatrix} (\rho C)_s^{(k)} \\ \phi^{(k)} \\ \lambda_s^{(k)} \end{pmatrix} \]

\[ T_g = \begin{pmatrix} T_{g1}^1 \\ T_{g1}^2 \\ \vdots \\ T_{gM}^1 \\ T_{gM}^2 \\ \vdots \end{pmatrix} \]

\[ g(p^{(k)}) = \begin{pmatrix} T_{g1}^{1(k)} \\ T_{g1}^{2(k)} \\ \vdots \\ T_{gM}^{1(k)} \\ T_{gM}^{2(k)} \\ \vdots \end{pmatrix} \]

and the \( N \times 1 \) residual vector is defined by:

\[ r(p^{(k)}) = g(p^{(k)}) - T_g \] where \( N = M \times F \) and \( k \) is the iteration number. The Jacobian of the residual vector \( r(p^{(k)}) \) is defined by \( \frac{\partial r(p^{(k)})}{\partial p_{ij}} \) where \( i = 1, 2, ..., N \) and \( j = 1, 2, 3 \). The error function \( S \) defined by equation (9) can be written as \( S(p^{(k)}) = \frac{1}{2} r(p^{(k)})^T r(p^{(k)}) \) and its first derivative is given by: \( \nabla S(p^{(k)}) = J(p^{(k)})^T r(p^{(k)}) \). A necessary condition for \( p^* \) to be a local minimum of \( S(p^{(k)}) \) is that \( \nabla S(p^*) = 0 \) but it is not sufficient. It is required to show that the second derivative of \( S(p^{(k)}) \) is positive. For this reason, we choose to solve our non-linear least square problem by Gauss-Newton method because it doesn’t require the computation of the second derivative and has advantage to solve equation (8) by a small number of iterations and to converge quickly toward the local minimum of the error function \( S \). It proceeds by the iterations:

\[ p^{(k+1)} = p^{(k)} - J(p^{(k)})^{-1} J(p^{(k)})^T r(p^{(k)}) \] (10)

\[ J(p^{(k)}) \] is given by:

\[
J(p^{(k)}) = 
\begin{pmatrix}
W_1^{1(k)} & Z_1^{1(k)} & R_1^{1(k)} \\
W_1^{F(k)} & Z_1^{F(k)} & R_1^{F(k)} \\
W_2^{1(k)} & Z_2^{1(k)} & R_2^{1(k)} \\
W_2^{F(k)} & Z_2^{F(k)} & R_2^{F(k)} \\
\vdots & \vdots & \vdots \\
W_M^{1(k)} & Z_M^{1(k)} & R_M^{1(k)} \\
W_M^{F(k)} & Z_M^{F(k)} & R_M^{F(k)}
\end{pmatrix}
\]
where \( W_i^{f(k)} \) = \( \frac{\partial f_i}{\partial (pc)_{i(k)}} \rangle_{(pc)_{i(k)}} \), \( Z_i^{f(k)} \) = \( \frac{\partial f_i}{\partial \phi} \rangle_{\phi=\phi(k)} \)

and \( R_i^{f(k)} = \frac{\partial f_i}{\partial x_i} \rangle_{x_i=x_i(k)} \) are the sensitivity coefficients and \( k \) is the number of iterations.

### 2.2.2 Governed Equations

In the following, we present the heat equation (1) in 3D-axisymmetric coordinate system (see figure 3) together with 3 sensitivity equations resulting from the differentiation of the heat equation (11) with respect to the soil parameters.

![Fig.3. Discretization in 3D-axisymmetric coordinate system](image)

The heat diffusion equation in the 3D-axisymmetric coordinate system is given by:

\[
\frac{\partial (pc) \frac{\partial T}{\partial t}}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left( \lambda_e \frac{\partial T}{\partial r} \right) + \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial T}{\partial z} = \frac{\partial}{\partial z} \left( \lambda_e \frac{\partial T}{\partial z} \right) + \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial T}{\partial z} \]

(11)

with the following initial and boundary conditions:

\[
T(x, 0) = T_0(x) \quad \text{in } \Omega
\]

\[
T(x, t) = T^D(x, t) \quad \text{on } \Gamma^D \times (0, t_{\text{end}}) \quad \text{(Dirichlet)}
\]

\[
\nabla T(x, t), \nu = 0 \quad \text{on } \Gamma^N \times (0, t_{\text{end}}) \quad \text{(Neumann)}
\]

The three sensitivity equations are obtained by differentiating the heat diffusion equation with respect to the unknown parameters \( (pc) \), \( \phi \) and \( \lambda_e \) respectively. In order to determine the sensitivity coefficients \( (W, Z \text{ and } R) \) appearing in the Jacobian, we should solve the three sensitivity equations (12), (15) and (18):

**Differentiating with respect to \( (pc)_\nu \):**

\[
\frac{\partial W}{\partial t} + \frac{1}{(pc)_\nu} \frac{\partial (pc)_\nu}{\partial t} \frac{\partial W}{\partial z} + \frac{1}{(pc)_\nu} \frac{\partial}{\partial z} \left( \lambda_e \frac{\partial W}{\partial z} \right) + \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial W}{\partial z} = \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial W}{\partial z} \]

(12)

**Differentiating with respect to \( \phi \):**

\[
\frac{\partial (\rho C) \frac{\partial W}{\partial \phi}}{\partial (pc)_\nu} + \frac{\partial (pc)_\nu}{\partial \phi} \frac{\partial W}{\partial (pc)_\nu} = \frac{\partial (\rho C)_\nu}{\partial \phi} \frac{\partial W}{\partial (pc)_\nu} - \frac{1}{(pc)_\nu} \frac{\partial}{\partial z} \left( \lambda_e \frac{\partial W}{\partial z} \right) - \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial W}{\partial z} = \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial z} \frac{\partial W}{\partial z} \]

(15)

**Differentiating with respect to \( \lambda_e \):**

\[
\frac{\partial W}{\partial \phi} + \frac{1}{(pc)_\nu} \frac{\partial (pc)_\nu}{\partial \phi} \frac{\partial W}{\partial x} + \frac{1}{(pc)_\nu} \frac{\partial}{\partial x} \left( \lambda_e \frac{\partial W}{\partial x} \right) - \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial x} \frac{\partial W}{\partial x} = \frac{1}{\lambda_e} \frac{\partial \lambda_e}{\partial x} \frac{\partial W}{\partial x} \]

(17)

These 3 sensitivity equations (12), (15) and (18) are completed with adequate initial and boundary conditions analogous to those in equation (11) but in homogenous form. \( W, Z \text{ and } R \) are the unknowns of the
sensitivity equations and $T$ is the solution of equation (11).

2.3 Numerical Strategy

The obtained system of coupled equations (sensitivity equations + heat diffusion equation) is a nonlinear system of ordinary partial differential equations. To solve this system, we propose a global approach similar to that presented by [4]. This approach is based on the method of lines, where time and space discretizations are considered separately. The space discretization is done using a vertex-centered finite volume method; the discretization in time is done by an Euler implicit scheme. The system of coupled equations (11), (12), (15) and (18) is discretized in space using the vertex-centered finite volume method in 3D axisymmetric coordinate system. The computational domain is divided into a grid or mesh of dimensions $\Delta r$ and $\Delta z$ as shown in Fig.3. After spatial discretization, the system of coupled equations can be written as a linear system:

\[
\begin{pmatrix}
M(T) & 0 & 0 & 0 \\
A_w(T) & 1 & 0 & 0 \\
A_z(T) & 0 & 1 & 0 \\
A_r(T) & 0 & 0 & 1 \\
\end{pmatrix}
\begin{pmatrix}
dT \\
dw \\
dz \\
dr \\
\end{pmatrix}
+ 
\begin{pmatrix}
N(T) & 0 & 0 & 0 \\
0 & B_w(T) & 0 & 0 \\
0 & 0 & B_z(T) & 0 \\
0 & 0 & 0 & B_r(T) \\
\end{pmatrix}
\begin{pmatrix}
T \\
w \\
z \\
r \\
\end{pmatrix}
= b \quad (21)
\]

which is an ordinary differential equation. By classical transformations and by letting $Y = \begin{pmatrix} T \\ W \\ Z \\ R \end{pmatrix}$, the system (21) can be written in the general form:

\[
\begin{cases}
Y' = F(T, Y) \\
Y(t_0) = Y_0
\end{cases}
\quad (22)
\]

We use an ODE solver to solve this system, this solver applies a time discretization scheme using Backward Differentiation Formula (BDF) because at each time step a system of nonlinear equations using a modified Newton method must be solved.

2.4 Algorithm

The aim of the inverse problem is the calculation of the parameters’ vector $p$ which makes the values of the temperature $T(t)$, calculated by the forward problem, approach the experimental temperature $T_{exp}(t)$. The algorithm is as follows:

1. Choose an initial value $p^{(0)}$ of $p$ at iteration $k=0$.
2. Solve the system (21) formed of the coupled equations using $p^{(k)}$ to define the properties of the soil.
3. Deduce the values of $T_i^{f,(k)}, W_i^{f,(k)}, Z_i^{f,(k)}$, and $R_i^{f,(k)}$ for $i = 1, 2, \ldots, M$ and $f = 1, 2, \ldots, F$.
4. Calculate the value of $r(p^{(k)})$ and that of the Jacobian $J(p^{(k)})$.
5. Solve the linear system $p^{(k+1)} = p^{(k)} - J(p^{(k)})^{-1} J(p^{(k)}) r(p^{(k)})$ for $p^{(k+1)}$.
6. Calculate $S(p^{(k)})$. If $S(p^{(k)}) < \varepsilon$, end (the criterion of convergence must be determined). If not, iterate: $p^{(k)} \leftarrow p^{(k+1)}$ and go to 2.

2.5 Some validation examples

The code validation stage is based on the comparison between the numerical results and synthetic data. First, we choose a plausible example where the soil properties (volumetric heat capacity, thermal conductivity and porosity) are given constant values. These values are used by the forward problem to calculate the temperatures at different points of the domain which in return plays the role of the experimental data in the inverse problem. Table 1 shows that the numerical results are in good agreement with the exact experimental ones. From table 2, we can notice that if the initial guess of $(\rho C)_s$ is equal to its exact value then $\phi$ converge to their exact values. The final results of $\phi$ and $\lambda_s$ are shown in figures 4 and 5.

To study the influence of the initial guess of $(\rho C)_s$ on the convergence, we consider table 3. The computations show that we have relatively a good convergence for $\phi$ and $\lambda_s$. However, the convergence of $(\rho C)_s$ is far from the exact solution. This is might be due to the fact that the heat equation is not sensitive to $(\rho C)_s$ in comparison to the other parameters ($\phi$ and $\lambda_s$). In most of the cases, $(\rho C)_s$ stays equal to its initial guess.

<table>
<thead>
<tr>
<th>Table 1. Properties of the soil obtained by inverse problem</th>
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<tr>
<td>$(\rho C)_s$</td>
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3. Conclusion

The idea of this paper is the inverse problem which consists of the estimation of thermophysical properties of the soil knowing the temperature at selected points of the domain. In order to solve this inverse problem, we used the least square criterion where we try to minimize the error function between real measures and synthetic ones. The coupled system composed of the energy equation together with the three sensitivity boundary initial problems resulting from differentiating the basic energy equation with respect to the soil properties must be solved. To overcome the high nonlinearity of the coupled system, we used Gauss–Newton’s method. According to Gauss Newton’s method, the convergence rate should be linear [11] but we obtained poor convergence (see tables 1 and 3) except when we removed $(\rho C)_s$ (see table 2). The code validation stage is based on the comparison between the numerical results and the synthetic data which shows good agreement and convergence is obtained after about 10 iterations. The rate of convergence of our inverse problem is linear which agrees with the order of convergence of Gauss Newton method.

Our problem of interest is very difficult to be applied to real data because convergence cannot be obtained for relatively small $\Delta T$. In this case, the numerical solution will be far from the physical one. It appears that it is necessary to reduce both the temperature interval $\Delta T$ and the mesh size in order to get accurate results but this will lead to a high numerical cost.

4. References