Simulating heat transport with a standard solute transport code

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1. Overview

In general, the transport of heat in groundwater systems is a coupled process. Changes in temperature affect the density of water, and the changes in water density perturb the groundwater flow field that moves heat by convection. Although the coupling is relatively weak, the solution of coupled problems is significantly more challenging that simulating uncoupled groundwater flow or solute transport. For example, coupled processes generally cannot be simulated with screening-level analytical approaches. If we de-couple the heat transport problem by assuming that groundwater flow is not affected by temperature, we can simulate the movement of heat in flowing groundwater (more particularly the distribution of temperature) using a standard analytical solution for solute transport code such as ATRANS, or a standard numerical solution such as MT3DMS.

For uncoupled analyses, we can apply standard solute transport codes with the following substitutions:

$$\rho_b K_d \rightarrow \frac{(1-\theta)\,c_s \rho_s}{c_w \rho_w}$$

$$D^* \rightarrow \frac{\lambda}{\theta c_w \rho_w}$$

⇒ **Regardless of the significance of coupling in a particular application, we recommend that a preliminary analysis be conducted in which coupling is neglected. The results from the first-cut analysis with a simplified approach will provide a good approximation and can be used to check the results of more comprehensive approaches.**

In the remainder of this note we explain where the variable substitutions come from, and provide the results from an illustrative example analysis.

2. Governing equation for the transport of heat in the subsurface

If we neglect internal sources and sinks and assume full saturation, the statement of conservation of heat in the subsurface can be written as:

$$\frac{\partial}{\partial t}(H) = -\frac{\partial}{\partial x_i}\left[q_i c_w \rho_w (T - T_0)\right] + \frac{\partial}{\partial x_i}\left[\lambda \delta_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right] + \frac{\partial}{\partial x_i}\left[\theta c_w \rho_w D_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right]$$

<u>Terms</u>:

H	heat content;
T	temperature;
T_0	reference temperature;
q_i	Darcy flux;
c_w	specific heat of water;
ρ_w	density of water;
λ	conductivity;
D_{ij}	dispersion coefficient tensor; and
θ	saturated water content (porosity).

Several references denote the product $c_w\rho_w$ as C_w, the heat capacity of water.

The left-hand side of the conservation statement represents the rate of change of heat content per unit volume of porous medium. The terms on the right-hand side represent the divergence of the convective, conductive and dispersive heat fluxes, respectively.

The heat content can be expanded as:

$$H = \left[\theta c_w \rho_w + (1-\theta) c_s \rho_s\right](T - T_0)$$

Substituting into the statement of heat conservation yields:

$$\frac{\partial}{\partial t}\left(\left[\theta c_w \rho_w + (1-\theta) c_s \rho_s\right](T - T_0)\right) = -\frac{\partial}{\partial x_i}\left[q_i c_w \rho_w (T - T_0)\right] + \frac{\partial}{\partial x_i}\left[\lambda \delta_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right] + \frac{\partial}{\partial x_i}\left[\theta c_w \rho_w D_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right]$$

This is the governing equation for heat transport.

The form of the governing equation for heat transport appears relatively complex, but the interpretation and specification of the parameters is straightforward. The governing equation can be simplified if we define a thermal retardation factor:

$$R = \frac{\theta c_w \rho_w + (1-\theta) c_s \rho_s}{\theta c_w \rho_w} = 1 + \frac{(1-\theta) c_s \rho_s}{\theta c_w \rho_w}$$

If we divide the governing equation through by $\theta c_w \rho_w$ we obtain:

$$R \frac{\partial}{\partial t}(T - T_0) = -\frac{\partial}{\partial x_i}\left[v_i (T - T_0)\right] + \frac{\partial}{\partial x_i}\left[\frac{\lambda}{\theta c_w \rho_w} \delta_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right] + \frac{\partial}{\partial x_i}\left[D_{ij} \frac{\partial}{\partial x_j}(T - T_0)\right]$$

Finally, let us write the governing equation in terms of the relative temperature *U*, defined as T-T_0:

$$R \frac{\partial U}{\partial t} = -\frac{\partial}{\partial x_i}\left[v_i U\right] + \frac{\partial}{\partial x_i}\left[\frac{\lambda}{\theta c_w \rho_w} \delta_{ij} \frac{\partial U}{\partial x_j}\right] + \frac{\partial}{\partial x_i}\left[D_{ij} \frac{\partial U}{\partial x_j}\right]$$

This form is very similar to the governing equation for solute transport:

$$R \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x_i}\left[v_i C\right] + \frac{\partial}{\partial x_i}\left[D^* \delta_{ij} \frac{\partial C}{\partial x_j}\right] + \frac{\partial}{\partial x_i}\left[D_{ij} \frac{\partial C}{\partial x_j}\right]$$

The following processes are analogous for the transport of heat and solutes in the subsurface:

- Thermal retardation ↔ Retardation
- Thermal convection ↔ Advection
- Thermal conduction ↔ Diffusion
- Thermal dispersion ↔ Dispersion

3. Example uncoupled calculations

We examine the solution of Coats and Smith (1964) that Ward et al. (1984) use as a benchmark solution for the coupled numerical heat transport code SWIFT.

The governing equation for the uncoupled one-dimensional transport of heat in a steady, uniform flow field is:

$$\left(1+\frac{(1-\theta)\,\rho_r c_r}{\theta \rho_w c_w}\right)\frac{\partial T}{\partial t}=-\frac{q}{\theta}\frac{\partial T}{\partial x}+\left(\alpha_L\frac{|q|}{\theta}+\frac{\lambda}{\theta\rho_w c_w}\right)\frac{\partial^2 T}{\partial x^2}$$

Subject to:

$$T(x,0)=T_0$$
$$T(0,t)=T_1$$
$$T(\infty,t)=T_0$$

Ward et al. (1984) confirm that the results of the Coats and Smith (1964) solution can be matched with the SWIFT code. In this example we show that the results can also be matched using an analogous analytical solution for solute transport.

If we define the following transport parameters can be written as:

$$R=1+\frac{(1-\theta)\,\rho_r c_r}{\theta\rho_w c_w}$$

$$D_{eff}^{*}=\frac{\lambda}{\theta\rho_w c_w}$$

and define the relative concentration as:

$$c=\frac{T-T_0}{T_1-T_0}$$

the governing equation for heat transport becomes:

$$R\frac{\partial c}{\partial t}=-\frac{q}{\theta}\frac{\partial c}{\partial x}+D\frac{\partial^2 c}{\partial x^2}$$

Dividing through by R and designating $v' = q/R$ and $D' = D/R$, the governing equation becomes:

$$\frac{\partial c}{\partial t} = -v' \frac{\partial c}{\partial x} + D' \frac{\partial^2 c}{\partial x^2}$$

In terms of the relative concentration, the boundary and initial conditions become:

$$c(x,0) = c_0$$
$$c(0,t) = 0$$
$$c(\infty,t) = 0$$

Ogata and Banks (1961) presented the solution for this solute transport problem.

Input parameters

Ward et al. (1984) assume the following parameter values for their calculations.

Parameter	**Value**
Darcy flux, q	3.53×10^{-7} m/s
Saturated water content (Porosity), θ	0.10
Specific heat of water, c_w	4185 J/kg-°C
Density of water, ρ_w	1000 kg/m^3
Specific heat of rock, c_r	1254.7 J/kg-°C
Density of rock, ρ_r	1602 kg/m^3
Longitudinal dispersivity, α_L	14.4 m
Thermal conductivity, λ	2.16 J/s-m-°C
Initial temperature, T_0	37.78°C
Influent temperature, T_1	93.33°C

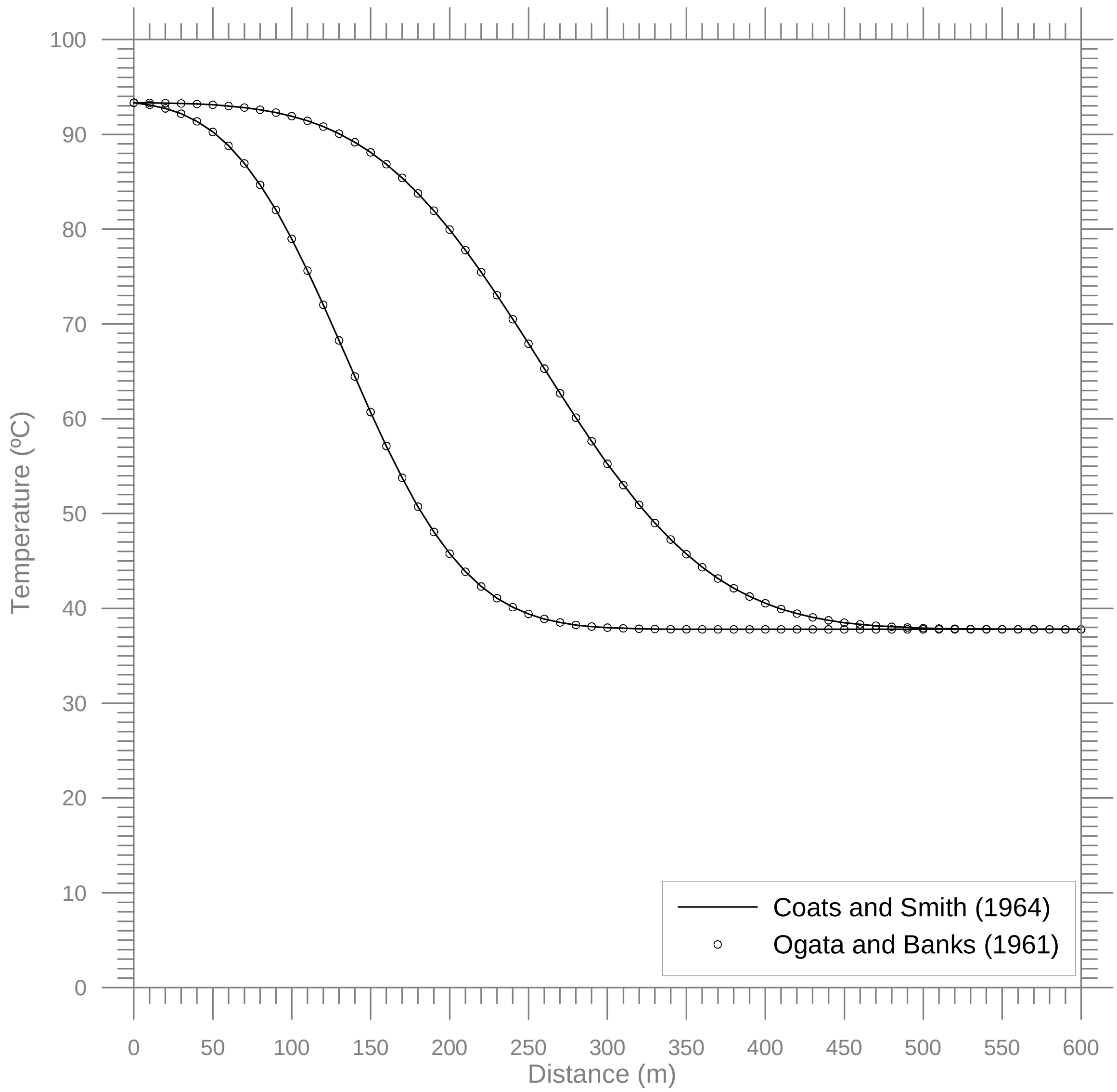
Intermediate calculations

$$R = 1 + \frac{(1-\theta)\rho_r c_r}{\theta \rho_w c_w} = 5.323$$

$$D_{eff}^* = \frac{\lambda}{\theta \rho_w c_w} = 5.161\times10^{-6}\ m^2/s$$

Results

The results for the heat transport solution (solid line: Coats and Smith, 1964) and the solute transport solution (points: Ogata and Banks, 1961) are plotted below. The results are identical, confirming that the interpretation of the change of variables for heat transport is correct.



4. References

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