PARAMETER IDENTIFICATION OF A NUMERICAL TRANSPORT CODE

G. Danko, and A. Jain, Mackay School of Mines
University of Nevada, Reno
Reno, NV 89557, (775) 784 4284

ABSTRACT

A parameter identification process is presented to obtain effective, resultant properties of a numerical transport code. The method is demonstrated using NUFT (Nonisothermal Unsaturated-Saturated Flow and Transportation model) [1], as a transport code, and the effective heat conductivity and thermal diffusivity as effective parameters. A numerical application example shows that effective transport code in a variety of boundary conditions.

INTRODUCTION

Numerical transport codes represent a family of engineering software used to simulate transport processes associated e.g., with heat, mass, or momentum. Computational software packages for transports involving macroscopic flows are referred to as Computational Fluid Dynamic (CFD) models. Computational software packages used to simulate conductive, diffusive, or advective transport in porous and/or fractured media, such as rock are the Porous Media Codes (PMC). NUFT [1] is an example of PMC. In complex technical calculations, such as a ventilation analysis of a subsurface opening surrounded with porous and wet rock, both CFD and PMC codes are needed. MULTIFLUX is an example of a code that couples the solutions of a PMC and a CFD, while keeping the original codes unchanged, without effectively merging the PMC and CFD codes into one software. Since coupling is made through data transfer and management, transport parameter identification plays a key role in the process.

PARAMETER IDENTIFICATION CONCEPT

The paper demonstrates a simple transport parameter identification technique. NUFT is used as a PMC, and the effective heat conductivity (k_{eff}) and thermal diffusivity (α_{eff}) are selected to represent two transport parameters. The definition of the effective properties is as follows:

$$\sum_{N}(T_{PMC} - T_{cond}(k_{eff}, \alpha_{eff}))^2 = \min \qquad \text{(Eq. 1)}$$

where:

- T_{PMC} is the temperature field calculated with the PMC software due to a well-defined perturbation
- T_{cond} is the temperature field calculated with a conduction-only model for the same geometry and perturbation
- N is the number of temperature values with respect to both time and location involved in the evaluation

Since $T_{cond}(k_{eff},a_{eff})$ is dependent on both parameters in the argument, a two-dimensional optimization can be used to determine their values. The minimization of the squared error-of-fit will be referred to as a least-square-fit (LSQ) method. This method, in principle, agrees with the evaluation of effective thermophysical properties from in situ measurements using the Rapid Evaluation of K and Alpha (REKA) method [2]. The analogy is flawless between evaluating transport parameters from in situ temperature measurements and from calculated temperatures obtained from the PMC. In principle, the arrangement used in the REKA method can be applied for parameter identification. An application regarding the use of the REKA arrangement for parameter identification is presented in another publication [3]. However, a much simpler one-dimensional geometrical arrangement can be used in the PMC parameter identification.

The k_{eff} and α_{eff} properties represent the complex set of hydrothermal properties and processes of the porous media at a given location. The T_{PMC} temperature field is determined from NUFT. This model is set up for a one-dimensional insulated rod with a length that can be considered infinite for practical, numerical considerations. The thermal perturbation is a step-change temperature pulse applied at time zero at the free end of the rod at $x = 0$. The arrangement is shown in Fig. 1. The change in the temperature field is inverse-evaluated against k_{eff} and α_{eff} using a known analytical solution for the conduction-only case according to Carslaw and Jaeger [4] as follows:

$$T_{cond}(x, t) = T_{wall} \cdot erfc\left(\frac{x}{2\sqrt{\alpha_{eff} t}}\right) \quad \text{(Eq. 2)}$$

where:

T_{wall} is the wall temperature
x is the distance across the porous media
α_{eff} is the effective thermal diffusivity
t is the time

Eq. (2) has only one unknown parameter, α_{eff}, allowing to use a one-dimensional optimization when solving Eq. (1). This unknown α_{eff} can be determined first. The other parameter, k_{eff}, can be evaluated from the temperature distribution calculated by NUFT. Alternatively, the heat flux density, q_{PMC} at $x = 0$ directly evaluated by NUFT can be used to back-calculate k_{eff}.

For the evaluation by comparison, the heat flux at the end of the rod is calculated using the derivative of the temperature field in Eq. (2) at $x = 0$, and multiplying by k_{eff} as follows:

$$q_{cond}(t)\big|_{x=0} = k_{eff} \frac{1}{\sqrt{\pi \alpha_{eff} t}} \quad \text{(Eq. 3)}$$

In order to achieve the best fit value for k_{eff}, a minimum condition is defined:

$$\sum_{M} \left(q_{PMC} - q_{cond}(k_{eff})\right)^2 = \min \quad \text{(Eq. 4)}$$

Where M is number of heat flux density values with respect to time divisions, involved in the evaluation.

The expression for the best k_{eff} can be obtained analytically from Eq. (5):

$$k_{eff} = \frac{\sum_{i=1}^{M} q_{PMC}(t_i)}{\sum_{i=1}^{M} \frac{1}{\sqrt{\pi \alpha_{eff} t_i}}} \qquad \text{(Eq. 5)}$$

NUMERICAL EXAMPLE

Evaluation was made for two different sets of spatial discretization. In case 1 the first thousand divisions are 1×10^{-4}m from 0 to 0.1m, then logarithmically increasing division from 0.1 to 40.099m. Incase 2 the first thousand divisions are 1×10^{-3}m from 0 to 1m, then logarithmically increasing division from 1 to 40.099m.

The one-dimensional rod is shown in Fig. 1.

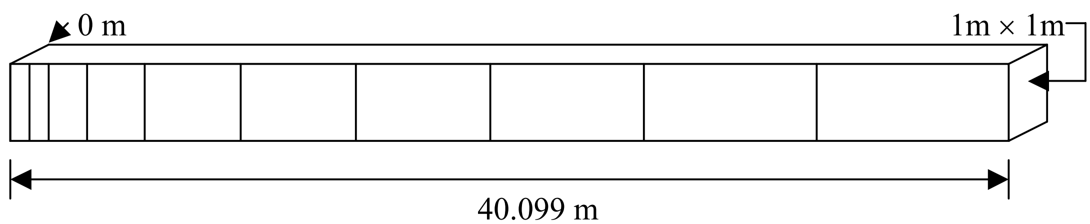

Fig. 1 Domain of Parameter identification model

The NUFT3.0s [5] input parameters included the temperature boundary condition and discretized time and space, in addition to the porous and fracture material properties shown in the Table I. NUFT3.0s was used for the temperature field and heat flow simultaneously, assuming dual-porosity, fractured, and partially saturated medium.

Table I. Input Parameters for NUFT

	Matrix Property		Fracture Property	
Porosity	1.31×10^{-1}		1.1×10^{-2}	
Solid Density	2.512×10^{3}		2.794×10^{-2}	
Specific Heat	900		900	
	Liquid Saturated	Gas Saturated	Liquid Saturated	Gas Saturated
Conductivity	1.998	1.187	2.222×10^{-2}	1.32×10^{-2}
Saturation	0.5	0.5	0.01	0.01

The temperature fields obtained for the matrix and the fracture elements are used in the calculation of the effective thermal diffusivity and heat conductivity according to Eqs. (1) and (5).
The output of the NUFT 3.0s provides the temperature and partial vapor pressure field, and the heat and moisture fluxes. The variation of the temperature field for the matrix rock element in the CASE 1 is shown in Fig. 2. The temperature field results for Case 2 are similar to those for Case 1and not shown for brevity.

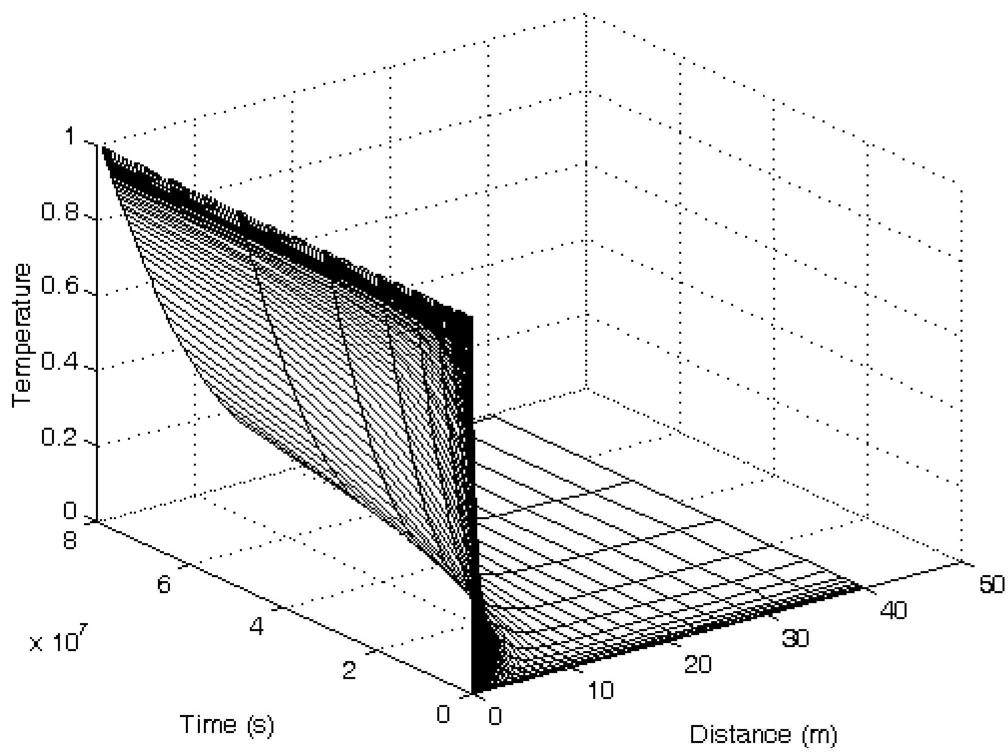

Fig. 2: Temperature Variation According to NUFT, Rock Matrix Domain CASE 1

IDENTIFICATION RESULTS

Case 1: The LSQ values of α were found to be 5.3968×10^{-7} and 5.3897×10^{-7} for the temperature field for the fracture and matrix domains, respectively. The LSQ values of thermal conductivity were 1.3653 and 1.3644 for fracture and matrix domains.
Case 2: The LSQ values of α for the CASE 2 were found to be 5.3160×10^{-7} and 5.3172×10^{-7} for the temperature field for the fracture and the matrix domains respectively. The values of thermal conductivity were 1.3569 and 1.3567 for the fracture and the matrix domains.
The effective conductivity value of 1.36 favorably agrees with the expected value of 1.37, the weighted average of 1.998 and 1.187 for the saturation of 0.2343. The effective diffusivity also falls in the expected regime. However, these effective properties are resultant values incorporating various material properties with weighted averages in addition to the convective effects. This perfect agreement found in the example indicates that the flow of heat is dominantly heat conduction.

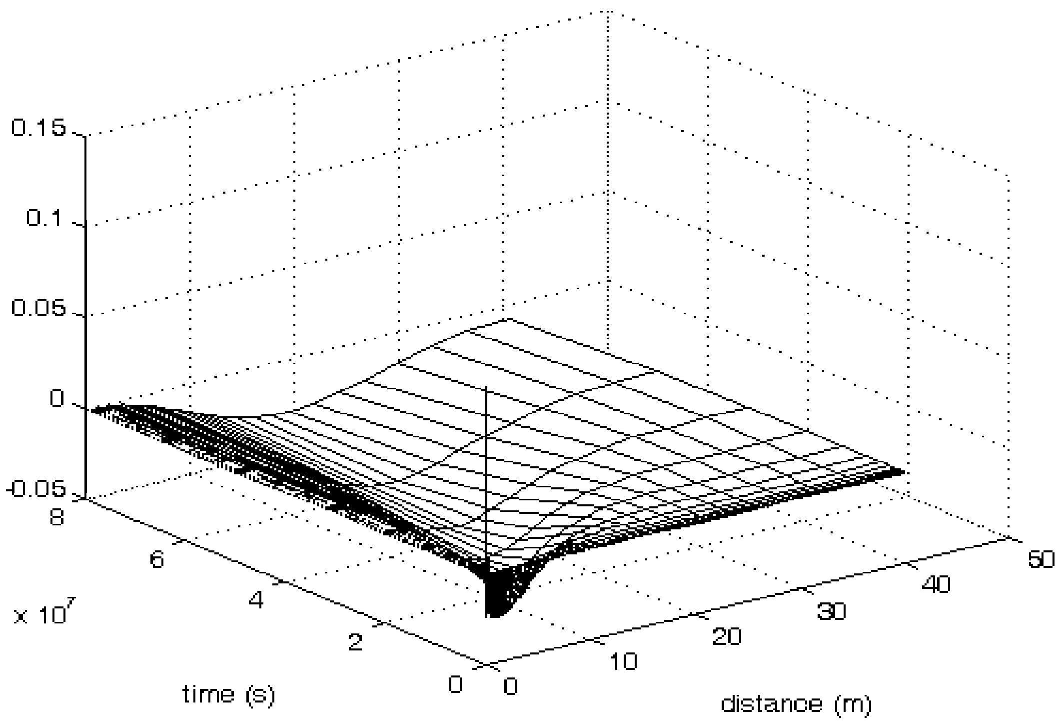

Fig. 3: Variation of difference between temperature field of matrix elements and the temperature field given by the analytical solution of Carslaw and Jaegar CASE 1

APPLICATION OF IDENTIFIED PROPERTIES TO DIFFERENT BOUNDARY CONDITIONS

Four comparison tests were made to check how well the identified properties k_{eff} and α_{eff} in problems under different boundary conditions perform. The rock domain was kept unchanged using the same porous material properties in NUFT according to Table I. The boundary condition at $x = 0$ was changed from 1st kind temperature boundary condition to 3rd kind convective boundary condition assuming four different surface heat transport coefficients: 1, 2, 4 and 8 W/(m^{2}K). Numerical analysis using NUFT with the four convective boundary conditions were carried out to generate baseline results for comparison. This work was performed as part of the software qualification activities of MULTIFLUX V2.0 [6], a hydrothermal ventilation code that uses NUFT by coupling its results to a CFD with convective boundary condition. The NUFT-based temperature variations were compared with the analytical solution to the convective boundary condition problem. The analytical results are generated using the solution from Carslaw and Jaeger(*1986*).

$$T_{cond}(t)\Big|_{x=0} = \frac{T_{wall}}{h\sqrt{\pi\alpha_{eff}t}} \qquad \text{(Eq. 6)}$$

The k_{eff} and α_{eff} are substituted with rounded values determined by parameter identification:
k_{eff} = 1.37 W/(mK)
α_{eff} = 0.539×10^{-6} m^2/s

The results of the NUFT-MULTIFLUX and the Carslaw and Jaeger calculations are shown in Fig. 4

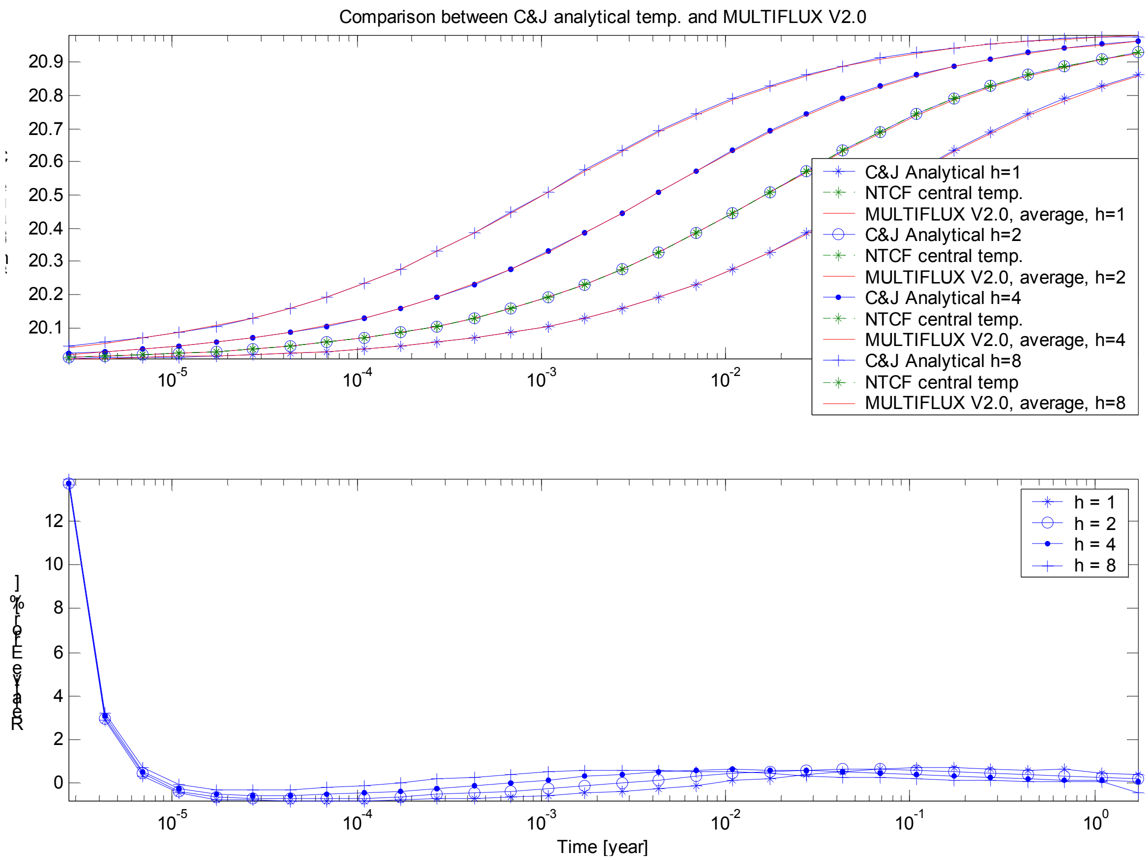

Fig. 4 Comparison between Carslaw and Jaeger Analytical Results and those from MULTIFLUX V2.0

CONCLUSIONS

1. Effective thermophysical parameters were identified successfully based on the transport code NUFT. Both the effective heat conductivity and the effective thermal diffusivity fell in the expected regime.
2. The effective parameters were used for various convective boundary conditions to find the boundary surface temperature variation. The results show close agreement with the known analytical solution.
3. The identified parameter can be used in a simple conduction-only model with effective properties. Such a model is faster to solve. Parameter identification can be advantageous for providing a simple and efficient representation of the transport code.
4. Although an advective, convective media was used, the identification of the effective heat conductivity and effective thermal diffusivity was done under the assumption of a dual-porosity, fractured, and partially saturated medium.

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