A Galerkin Finite Element Scheme for the Analysis of Transient Effects of Heat and Moisture Flow in Porous Media

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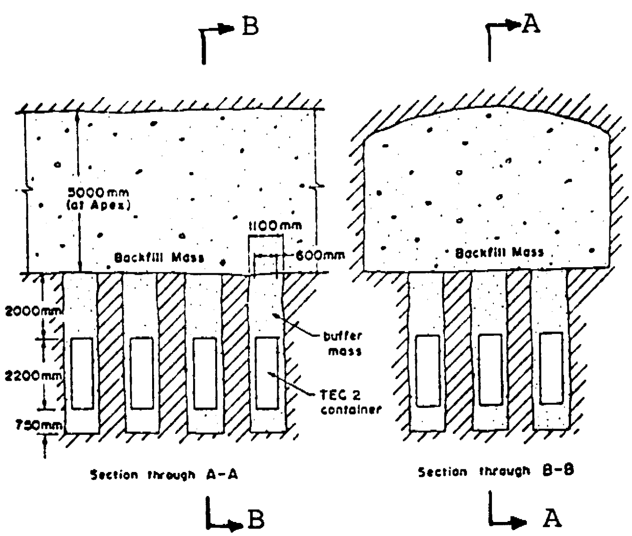
Abstract

This paper focusses on the problem of coupled heat and moisture movement in a porous geological medium. The examination of such processes is of interest in connection with the evaluation of the thermal performance of natural geological barriers which are used to isolate nuclear waste containers from the host rock of a deep vault repository. The mathematical equations governing heat and moisture flow in the porous geological medium are solved by appeal to a Galerkin finite element scheme. The paper focusses on the illustration of the basic features of the numerical scheme. The numerical scheme developed can be used to examine the rate of moisture depletion in the porous medium due to the temperature effects.

Introduction

The study of the coupled processes of heat and moisture flow in porous materials is important to several branches in engineering. The results of such researches have been applied to the study of packed reactor bed technology in chemical engineering, agricultural engineering, drying of foodstuffs and bio-engineering. A more recent application concerns the study of heat and moisture movement in porous geological materials which are proposed for use in nuclear waste disposal endeavours (*Selvadurai* [1], [2]). The Canadian proposals for the disposal of high level nuclear fuel waste specifically concentrates on the deep burial of the waste in plutonic rock masses. The waste repository will be located at a depth of approximately a kilometer and will consist of a series of tunnels which will house the waste forms. The waste will be sealed in containers and placed in boreholes drilled into the floor of the vaults. *Figure 1*. The annular space between the host rock and the waste container will be filled with an engineered barrier, called the "buffer" which is essentially a porous mixture of bentonite clay and sand. The buffer should act as a barrier to suppress the detrimental chemical effects of water in the rock mass and theus enhance the life of the waste container; it should serve as a geochemical filter for the sorption of radio nuclides which may ne released by accidental damage or natural breakdown of the waste container; it should provide sufficient strength to support the self weight of the container and accommodate any detrimental effects of rock deformation; it should be able to absorb water and heal cracks and separation zones which can be created by moisture depletion and, most importantly, it should act as a medium for the efficient conduction of heat from the waste containers to the host rock. Current philosophy concerning the performance of the disposal vault advocates that during the initial stages of the operation of the waste repository, the buffer will communicate the heat from the waste forms into the host rock with a relatively minimum water influx from the host



1 Schematic sectional views of a nuclear waste disposal vault

rock. Such low rates of water influx could be dictated by construction procedures such as dewatering and grouting and the local fissure patterns of the rock in the vicinity of the repository. The exposure of the buffer region to heat conduction with no moisture influx poses a special problem to the performance of the repository. For example it is known that in the performance of buried electrical conduits, the depletion of moisture in the vicinity of the conduit reduces its thermal conductivity and entraps the heat energy resulting in thermal degradation of the electrical conduit. In the context of the performance of the buffer it is imperative that the heat conduction characteristics be maintained even during moisture depletion associated with the heating process of the waste container. A failure to communicate the heat from the waste forms will result in the premature thermal degradation of the disposal vault which presents a problem of high environmental risk.

This research focusses on the problem of coupled heat and moisture flow in porous geological media. The paper discusses the features which govern the processes of heat and moisture flow in porous media. In particular, attention is focussed on the theory of coupled heat and moisture flow proposed by *Philip* and *de Vries* [3]. A weak Galerkin form of a finite element scheme is used to examine the coupled processes. The finite element scheme is used to examine the coupled heat and moisture flow in an axisymmetric waste disposal borehole.

Coupled heat and moisture flow

The mathematical modelling of the process of coupled heat and moisture flow in a porous geological medium is an extremely complicated exercise in continuum mechanics. A comprehensive treatment of such processes must take into consideration (i) the multiphase nature of the porous medium (soil skeleton, the water phase and the vapour phase); (ii) the modes of heat transfer in each separate phase (conduction, convection and radiation); (iii) the occurrence of reversible and irreversible deformations of the soil skeleton associated with moisture influx or moisture loss phenomena; (iv) the presence of moving boundaries within the composite region; (v) occurrence of cracking and damage and (vi) the influences of microstructural forces such as surface tension and other physico-chemical effects. The development of a comprehensive theory to accommodate all of the above processes is expeteed to be a problem of formidable analytical complexity. For this reason, it is prudent to restrict the attention, first; to the study of simplified theories which investigate the process of coupled heat and moisture flow in a porous medium and to assess the reliability of such simplified models by recourse to experimentation. In this paper we focus on the mechanistic theory of coupled heat and moisture flow in a porous medium proposed by *Philip* and *de Vries* [3]. The theory is based on the microscopic interaction processes that exist between the liquid, vapour and porous structure of the medium and employs physical laws governing transport of matter (i. e., diffusion (Fick's Law), saturated flow (Darcy's flow), unsaturated flow (Richard's flow), energy conservation and equilibrium thermodynamics. The developments yield a system of coupled differential equations governing the volumetric moisture content (Θ) and temperature (T). The coupled differential equations take the forms:

$$\frac{\partial \Theta}{\partial t} = \nabla \cdot (D_T \nabla T) + \nabla \cdot (D_\Theta \nabla \Theta) + \frac{\partial K_\Theta}{\partial z} \tag{1}$$

and

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) - \rho L \nabla \cdot (D_{\Theta v} \nabla \Theta) \tag{2}$$

where ∇T and $\nabla \Theta$ denote gradients of the temperature and volumetric moisture content fields; D_T is the thermal moisture diffusivity; D_Θ ist the isothermal moisture diffusivity, $D_{\Theta v}$ is the isothermal vapour diffusivity; λ is the thermal conductivity; L is the latent heat; ρc is the heat capacity and K_Θ is the unsaturated hydraulic conductivity. In general all the thermal properties depend upon the field variables Θ and T. Considering a region $S = S_1 \cup S_2$ the boundary conditions pertaining to temperature on S_1 and heat flux on S_2 can be written as:

$$T = \bar{T} \text{ on } x_i \in S_1 \tag{3}$$

and

$$\lambda \frac{\partial T}{\partial n} - L D_{\Theta v} \frac{\partial \Theta}{\partial n} + a_T T + b_T \Theta + c_T = 0; \tag{4}$$

on $x_i \in S_2$

where a_T, b_T and c_T are constants chosen to fit a certain type of boundary and n is the outward unit normal to S_2. Similarly, considering $S = S_3 \cup S_4$, the boundary conditions for pertaining to moisture constraint and moisture loss takes the forms:

$$\Theta = \bar{\Theta} \text{ on } x_i \in S_3 \tag{5}$$

and

$$D_T \frac{\partial T}{\partial n} + D_\Theta \frac{\partial \Theta}{\partial n} + K_\Theta n_z + a_\Theta T + b_\Theta \Theta + c_\Theta = 0 \tag{6}$$

on $x_i \in S_4$

Also we assume that

$$S_1 \cup S_2 = S_3 \cup S_4 = S \in \Omega$$
$$S_1 \cap S_2 = S_3 \cap S_4 = 0 \tag{7}$$

The description of the problem is completed with the prescription of initial conditions on Θ and T in Ω.

Numerical analysis

In order to perform the numerical analysis of the coupled flow of heat ans moisture within the buffer region we use the developments presented previously and obtain a weak Galerkin form for the governing equations. Avoiding details of calculations it can be shown that the associated integral forms are:

$$\int_\Omega \left\{ \nabla \delta T (\lambda \nabla T - \rho L D_{\Theta v} \nabla \Theta) + \rho c\, \delta T \frac{\partial T}{\partial t} \right\} d\Omega + \int_{S_2} \delta T (a_T T + b_T \Theta + c_T)\, dS = 0 \tag{8}$$

and

$$\int_\Omega \left\{ \nabla \delta \Theta (D_T \nabla T + D_\Theta \nabla \Theta) + \frac{\partial}{\partial z} \delta\Theta K_\Theta n_z + \delta\Theta \frac{\partial \Theta}{\partial t} \right\} d\Omega + \int_{S_4} \delta\Theta \{a_\Theta T + b_\Theta \Theta + c_\Theta\} ds = 0 \tag{9}$$

where δT and $\delta\Theta$ are appropriate weighting functions chosen such that the boundary conditions are satisfied on S_1 and S_3 respectively. These functional forms will be used in the finite element formulations. The basic procedures for the finite element developments are described by *Zienkiewicz* [4] and will also be described fully in [2]. The final coupled matrix equations governing Θ and T take the forms:

$$[K_{TT}]\{T\} + [K_{T\Theta}]\{\Theta\} + [M_T]\{\dot{T}\} = \{P_T\} \tag{10}$$

and

$$[K_{\Theta\Theta}]\{\Theta\} + [K_{\Theta T}]\{T\} + [M_\Theta]\{\dot{\Theta}\} = \{P_\Theta\} \tag{11}$$

where $[K_{TT}]$, $[K_T]$ . . ., etc., are combinations of volume and surface integrals; $\{\cdot\}$ denotes the time derivative and $\{P_T\}$ and $\{P\}$ are "loading" vectors. The time integrations are performed via an implicit finite difference scheme which gives unconditionally stable results (*Zienkiewicz* [4], *Bathe* [5]).

Conclusions

This study focusses on the numerical treatment of the coupled processes of heat and moisture flow in a porous geological material proposed for use in a high level nuclear fuel waste disposal endeavour. The mathematical modelling focusses on a simplified theory which takes into account heat conduction as the basic mode of heat transfer and a diffusion-flow mechanism in the moisture transport process. The resulting system of coupled differential equations are amenable to numerical treatment via a weak Galerkin finite element scheme. The theoretical models are capable of predicting relatively accurately the heat and moisture movement in an experimental situation.

References

[1] *A. P. S. Selvadurai:* Thermal performance of a buffer region developed for use in a nuclear waste disposal vault borehole, I. Experimental modelling (to be published).

[2] *A. P. S. Selvadurai:* Thermal performance of a buffer region developed for use in a nuclear waste disposal vault borehole. II. Comparison of theoretical and experimental resxults (to be published).

[3] *J. R. Philip* and *D. A. de Vries*, Moisture movement in porous materials under temperature gradients, Trans. Amer. Geophys. Union, Vol. 39, pp. 222–231.

[4] *O. C. Zienkiewicz:* The Finite Element Method, McGraw-Hill, New York (1977).

[5] *K.-J. Bathe*, Finite Element Procedures in Engineering Analysis, Prentice-Hall. Englewood Cliffs, N. J. (1982).

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