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Formulation of Natural Convection around Repository for Dual Reciprocity Boundary Element Solution

L. Vrankar
SNSA, Slovenian Nuclear Safety Administration, Vojkova 59, SI–1000 Ljubljana, Slovenia

B. Šarler
Laboratory for Fluid Dynamics and Thermodynamics, Faculty of Mechanical Engineering,
University of Ljubljana, Aškerčeva 6,
SI–1000 Ljubljana, Slovenia

Abstract

The disposal of high-level radioactive wastes in deep geological formations is of pronounced technological importance for nuclear safety. The understanding of related fluid flow, heat and mass transport in geological systems is of great interest. This article prepares necessary physical, mathematical and numerical fundamentals for computational modelling of related phenomena. The porous media is described by the simple Darcy law and momentum-energy coupling is due to Boussinesq approximation. The Dual Reciprocity Boundary Element Method (DRBEM) is used for solving coupled mass, momentum and energy equations in two-dimensions for the steady buoyancy-induced convection problem in an semi-infinite porous media. It is structured by weighting with the fundamental solution of the Laplace equation. The inverse multiquadrics are used in the DRBEM transformation. The solution is obtained in an iterative way.

1. Introduction

The understanding of transport phenomena in porous media [1] is of great importance. For example, this class of phenomena are encountered in hydrology, petroleum geology, underground disposal of nuclear wastes, etc.

The disposal of high–level radioactive wastes in deep geological formations (e. g. clay, salt and granite) are of pronounced technological importance for nuclear safety. The aim of disposal is to prevent the radionuclides to return to the biosphere (soil, surface waters). To assess a long term safety of such radioactive waste disposal system, mathematical models are used to describe the complicated groundwater flow, chemistry and potential radionuclide migration through these formations [2]. Recommendations for this analytical safety assessment work for underground disposal have been prepared by the IAEA as a publication in their Safety Series. Agency differentiates the safety assessment into two major components: scenario analysis (involving identification and definition of phenomena which could initiate and/or influence the release and transport of radionuclide from the source to men) and consequence analysis.

The ability to define acceptability criteria against which a disposal facility design can be put to test may only leave the 'as low as reasonably achievable' principle for developing as overall disposal system with a minimum of detriments on the long–term.
However, it is necessary for the safety assessment to understand the complex behaviour of flow and species transfer in the vicinity of a repository. These phenomena are being studied with relevance to disposal of wastes in several countries. Until now stochastic approaches, hydrologic modelling, laboratory research, computational modelling, etc. were used. The transport phenomena in spectra of geological systems could be described as equivalent porous media with respect to fluid flow and solute transfer.
Shortly after disposal the temperature near the repository will increase and thermal stresses will occur, which may have an influence on the permeability of rock mass. Furthermore, the buoyancy induced fluid flow will occur in the rock mass around the repository due to the temperature differences.
This paper discusses the solution of steady natural convection problem in semi–infinite porous media by the Dual Reciprocity Boundary Element Method [3]. Its main goal is in preparing the necessary physical, mathematical and computational fundamentals for development of related computer programme. Computer programme will make possible a simulation of steady natural convection in unbounded media. This physical situation represents simple first step in computational modelling of the repository–soil system.

2. Physical Model

The porous medium is assumed to be rigid, homogeneous, isotropic, with both, the porous media matrix and the saturated fluid incompressible. It is also assumed that the fluid and the matrix are in thermal equilibrium ($T_{solid} = T_{fluid} = T$) and the fluid motion can be described by Darcy's law. Permeability, viscosity, effective thermal diffusivity, and coefficient of thermal expansion are assumed constant.
The equations describing the conservation of mass (1), Darcy's law (2) and energy (3) are:

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$0 = -\nabla P - \frac{\mu}{K}\mathbf{v} + \mathbf{f} \tag{2}$$

$$\rho_0 c_p \nabla \cdot (\mathbf{v}T) = k\nabla^2 T + q \tag{3}$$

where $\mathbf{v} = (u, v)$, K, μ, $\mathbf{g}$, P, k, q, c_p are seepage velocity vector, permeability of the medium, dynamic viscosity of the fluid, acceleration vector due to gravity, pressure, thermal conductivity of the medium, internal heat generation per unit volume and specific heat at constant pressure of the fluid.
The change of density with temperature is in present physical model included only in body force term $\mathbf{f}$ (gravitational force per unit volume of the fluid) through Boussinesq approximation (4):

$$\mathbf{f} = \mathbf{g}\rho_0[1-\beta(T-T_0)] \tag{4}$$

In equation (4) ρ_0 is density of the fluid, T is temperature, β is the volumetric coefficient of thermal expansion, and the subscript $_0$ refers to the reference values.

Boundary Conditions:
The coupled set of equations can be solved only if the conditions are specified along the entire boundary (around repository and at infinite region) that bounds the flow field:

1. Around the source region (repository) Γ the impermeable and slip velocity boundary conditions are assumed (the normal component of the seepage velocity $\mathbf{v} = (u,v)$ must vanish and other components of the seepage velocity can have arbitrary values):

$$\mathbf{v} \cdot \mathbf{n}_\Gamma = 0 \tag{5}$$

where $\mathbf{n}_\Gamma$ stands for the normal on the boundary Γ directed into repository.

2. At semi–infinite region:

$$\mathbf{v} \Rightarrow 0;\ T \Rightarrow T_0;\ \text{when } r \Rightarrow \infty$$

$$\frac{\partial T}{\partial \mathbf{n}_\Gamma} = 0 \quad \text{when } r \Rightarrow \infty \tag{6}$$

The solution of the equations (1,2) is constructed by assuming the impermeable velocity boundary conditions on the whole boundary Γ. The solution of the equation (3) is constructed by assuming the division of the boundary Γ into necessarily parts Γ^D and Γ^N with the Dirichlet and Neumann boundary conditions, respectively

$$-k\frac{\partial T}{\partial \mathbf{n}_{\Gamma^N}} = b_{\Gamma^N}\ ;\ T = T_{\Gamma^D} \tag{7}$$

with T_Γ and b_Γ representing known functions. The solution of the posed natural convection problem represents the velocity, pressure, and temperature distribution over domain Ω and boundary Γ.
The above mentioned equations are solved numerically by DRBEM which is relatively novel numerical procedure. It is particularly suitable for semi–infinite domains, typical for the repository–environment system.

3. Solution Procedure

3.1 Overview

The boundary element method is a weighted residual technique for solving partial differential equations, characterized by choosing an appropriate fundamental solution as a weighting function and by using the generalized Green's formula for complete transfer of one or more partial differential operators on the weighting function. The main comparative advantage of the boundary element method over other discrete approximate methods is demonstrated in cases where all of the resultant domain integrals could be represented by the boundary integrals. This turns out to be possible only for some partial differential equations. When dealing with the boundary element method for the transport equation structured by weighting with the fundamental solution of Laplace equation, domain integrals appear at least from the transience, convective, and source terms.
The Dual Reciprocity Boundary Element Method represents one of the possibilities for transforming the resultant domain integrals into a finite series of boundary integrals. The key point of the DRBEM is approximation of the field in the domain by a set of global approximation functions and subsequent representation of the domain integrals of these global approximation functions by the boundary integrals.

3.2 Integral Equations

The construction of the solution is represented in two steps. Only basic elements are represented. The details can be found in [4]. The first step involves the conversion of the partial differential equations into integral equations as well basic elements of the iterative procedure [5]. The second step focuses on the discretization and solution of the algebraic systems of equations.
The momentum equation is coupled with the energy equation through the body force. The energy equation is coupled with the momentum equation through the velocity field. Respectively, the solution inherently involves iterations.
Let us assume the velocity, pressure and temperature fields are all known at iteration level m. The discussion of iteration cycle that follows explains how the velocity, pressure and temperature field are calculated at the next iteration level m+1.
The solution of the momentum equation at the iteration level m+1 is constructed in the following way:
The Pressure Poison Equation (PPE) is constructed by taking the divergence of the Darcy's law (2):

$$\nabla^2 P^{m+1} = \nabla \cdot (-\frac{\mu}{K}\mathbf{v}^m + \mathbf{f}^m) \tag{8}$$

The PPE is simplified into:

$$\nabla^2 P^{m+1} = \nabla \cdot \mathbf{f}^m \tag{9}$$

by taking into account the mass conservation (1). The Neumann pressure boundary conditions can be defined on the whole boundary Γ by taking the scalar product of the Darcy's equation with the normal on the boundary. This gives:

$$\nabla P^{m+1} \cdot \mathbf{n}_\Gamma = (-\frac{\mu}{K}\mathbf{v}^m + \mathbf{f}^m) \cdot \mathbf{n}_\Gamma \tag{10}$$

Since the impermeable velocity boundary conditions (5) are valid, upper equation reduces to :

$$\nabla P^{m+1} \cdot \mathbf{n}_\Gamma = \mathbf{f}^m \cdot \mathbf{n}_\Gamma \tag{11}$$

The PPE together with the boundary conditions (11) is solved by weighting the equation (9) with the fundamental solution of the Laplace equation $T^*(\mathbf{p};\mathbf{s})$ (where **s** stands for the source position vector and **p** stands for the position vector) over the domain Ω. The related boundary–domain integral expression for the calculation of the pressure field is (after application of the Green's second identity):

$$\int_\Gamma \frac{\partial P^{m+1}}{\partial \mathbf{n}_\Gamma} T^* d\Gamma - \int_\Gamma P^{m+1} \frac{\partial T^*}{\partial \mathbf{n}_\Gamma} d\Gamma - c_s^* P_s^{m+1} = \int_\Omega \nabla \cdot \mathbf{f}^m T^* d\Omega \tag{12}$$

Superscript s denotes evaluation of a quantity at the source point **s**. Coefficient c_s equals 0 for point **s** outside Ω, ½ for s on the smooth boundary, and 1 for **s** in the domain. In this case:

$${}_2T^*(\mathbf{p};\mathbf{s}) = \frac{1}{2\pi}\log\frac{r_0}{r} \tag{13}$$

is two dimensional fundamental solution of Laplace equation, where r_0 represents reference radius and $r^2 = (p_x - s_x)^2 + (p_y - s_y)^2$.

Equation (12) is first used for determining the pressure distribution on the boundary Γ and subsequently explicitly in the domain Ω. The pressure gradients in interior points are explicitly calculated from the Pressure Gradient Poisson Equation (PGPE [4]):

$$\int_{\Gamma}\frac{\partial P^{m+1}}{\partial \mathbf{n}_{\Gamma}}\nabla T^{*}d\Gamma - \int_{\Gamma}P^{m+1}\nabla\frac{\partial T^{*}}{\partial \mathbf{n}_{\Gamma}}\,d\Gamma + \nabla(c_s^{*}P_s^{m+1}) = \int_{\Omega}\nabla\cdot\mathbf{f}^{m}\nabla T^{*}d\Omega \qquad (14)$$

obtained by taking the gradient of the PPE acting on the Fundamental solution source point.

After calculating the pressure gradient field the velocity field at iteration level m+1 could be explicitly calculated from the Darcy's equation:

$$\mathbf{v}^{m+1} = \frac{K}{\mu}(-\nabla P^{m+1} + \mathbf{f}^{m}) \qquad (15)$$

The iteration cycle is completed by calculating the temperature field at iteration level m+1 (and with this also $\mathbf{f}^{m+1}$). This is accomplished by weighting the energy conservation equation by the fundamental solution of the Laplace equation and by using the Green's second identity:

$$\int_{\Gamma}\frac{\partial T^{m+1}}{\partial \mathbf{n}_{\Gamma}}T^{*}d\Gamma - \int_{\Gamma}T^{m+1}\frac{\partial T^{*}}{\partial \mathbf{n}_{\Gamma}}\,d\Gamma - c_s^{*}T_s^{m+1} = \int_{\Omega}\frac{1}{\alpha}\nabla\cdot(\mathbf{v}^{m+1}T^{m+1})\,T^{*}d\Omega + \int_{\Omega}\frac{q}{k}T^{*}d\Omega \qquad (16)$$

with $\alpha = k/(\rho_0 c_p)$ denoting thermal diffusivity.

Equation (16) is used to simultaneously solve the unknown temperature distribution in the Neumann part of the boundary, the unknown temperature derivative in the normal boundary direction in the Dirichlet part of the boundary and unknown temperatures in the domain.

The iteration cycle is completed with calculation of the updated body force $\mathbf{f}^{m+1}$. The iterations are stopped when conditions: $|T^{m+1}| - |T^{m}| < T_\varepsilon$, $|\mathbf{v}^{m+1}| - |\mathbf{v}^{m}| < v_\varepsilon$ are satisfied, with v_ε and T_ε representing the velocity and pressure convergence tolerances.

When the above iteration conditions are not satisfied, new iteration cycle starts with the relaxed value of body force:

$$\mathbf{f}^{m+1} = \mathbf{f}^{m} + c_{rel}(\mathbf{f}^{m+1} - \mathbf{f}^{m}) \qquad (17)$$

with c_{rel} representing the heuristic relaxation factor.

The detailed information of discretization of the involved boundary–domain integral equations and respective formation of the algebraic equation systems for the solution of the unknowns can be found in [4].

3.3 Conversions of Domain Integrals into Boundary Integrals

As was mentioned in chapter introduction the key point of the DRBEM [3] is approximation of the field in the domain by a set of global approximation functions and subsequent representation of the domain integrals of these global approximation functions by the boundary integrals. This discussion is limited to the involved domain integrals:

$$I_1 = \int_{\Omega}F(\mathbf{p})\,T^{*}(\mathbf{p};\mathbf{s})d\Omega;\quad I_2 = \int_{\Omega}\nabla\cdot\mathbf{G}\,(\mathbf{p})T^{*}(\mathbf{p};\mathbf{s})d\Omega;\quad I_3 = \int_{\Omega}\nabla^{2}F(\mathbf{p})\,T^{*}(\mathbf{p};\mathbf{s})d\Omega \qquad (18)$$

The integral type I_1 arises when weighting the transience and source terms, I_2 when weighting the convective term, and I_3 when weighting the diffusive term. Arbitrary scalar and vector valued functions are denoted with F(**p**) (scalar valued function) and **G(p)** (body force in equation (12))respectively.
Boundary geometry is approximated by N_Γ straight line segments and spatial variation of the fields on each of the boundary segments is represented by constant interpolation functions with meshpoints coinciding with the geometrical centers of the straight line segments (see Figure 1).
Spatial variation of the fields in Ω is represented by the N_ψ global interpolation functions [3] of the form:

$$F(\mathbf{p}) = \psi_n(\mathbf{p})\,\varsigma_n \tag{19}$$

The coefficients of the global shape functions could be expressed from the values of function F at points n = 1,2, ... $N_\Gamma+N_\Omega$ where the first N_Γ points n coincide with the nodes of the boundary elements and the last N_Ω points n are distributed in the domain Ω.
Coefficient ς_n are calculated by constructing a system of N_ψ algebraic equations:

$$\psi \cdot \varsigma = \mathbf{F} \tag{20}$$

F represents vector of collocation points $\mathbf{p}_n$. Coefficients ς_n follow by inverting the system of algebraic equations:

$$\varsigma = \psi^{-1}\mathbf{F} \tag{21}$$

Usually, for the global interpolation function ψ_n in a two dimensional case (closed region) conical functions and augmented thin plate splines [6], are chosen.

For unbounded problems, however, it is not appropriate to chose the same functions. In this way, the boundary element mesh is limited to internal boundary of the semi–infinite domain which encloses the repository. So it is suitable to use the interpolation function (inverse multiquadrics) which has to be employed in order to make negligible the contribution of points far away from the region of the interest (infinity).

These functions have a special decay and form :

$$\psi_n(\mathbf{p}) = \frac{1}{\sqrt{r_n^2 + C^2}} \tag{22}$$

where r_n is distance between field point **p** and collocation point $\mathbf{p}_n$, C is an arbitrary constant.
The first two integrals (18) are calculated by defining the harmonic functions φ_n :

$$\varphi_n(\mathbf{p}) = \sqrt{r_n^2 + C^2} - C\ln(C + \sqrt{r_n^2 + C^2}) \tag{23}$$

obtained after solving the equation:

$$\nabla^2 \varphi_n(\mathbf{p}) = \psi_n(\mathbf{p}) \tag{24}$$

4. Typical Input Parameters

Performance of the resulting method is compared with the results in reference [7] and [8]. As necessary condition for getting good results is to propose good real input data. The goal of this chapter is performed what kind of data can be included in the programme. Figure 1 shows a circular cavity embedded in an infinite medium as an example of underground repository geometry.

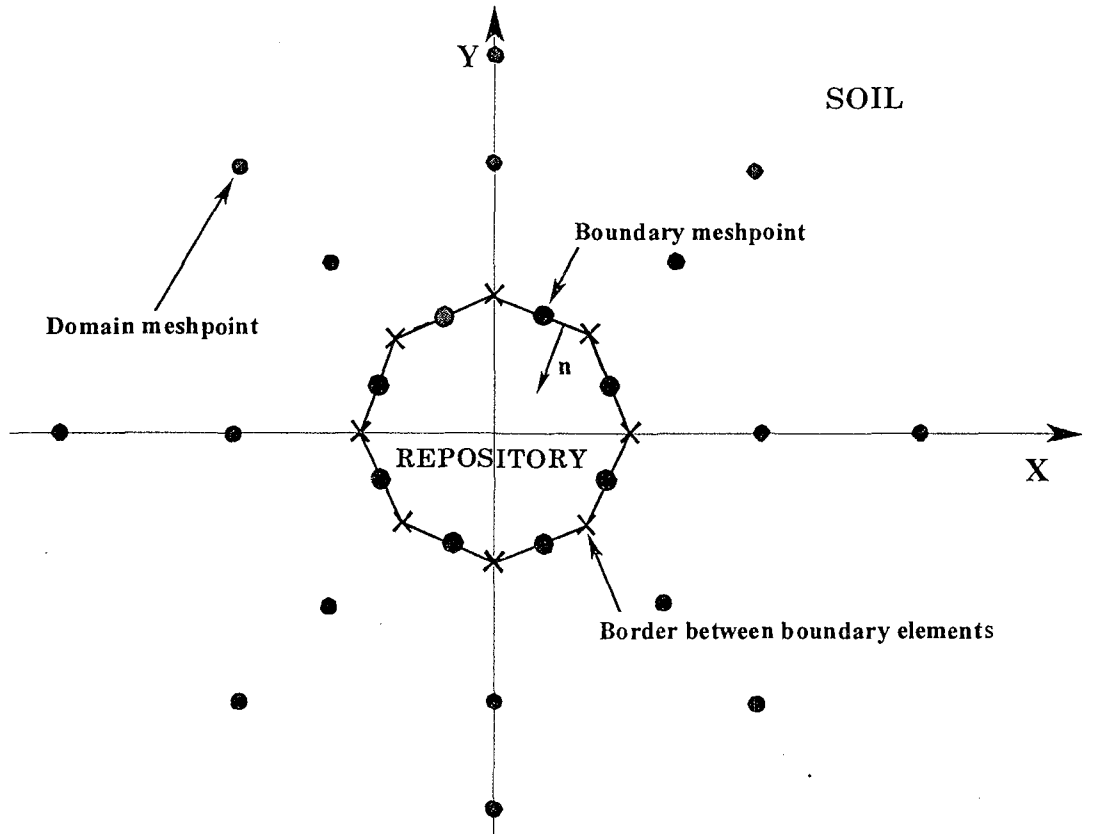

Figure 1. Cavity in infinite medium

The following typical data have been extracted from sources (thermal characteristics for tuff) [9,10]:

- Thermal conductivity k [W/(mK)]: 1.875
- Bulk density ρ_0 [kg/m^3]: 2297
- Thermal capacitance [J/(m^{3}K)]: 3358 at 114 °C
- Specific heat at constant pressure c_p[J/(kgK)]: 1460
- Reference temperature T_0 [°C] at repository depth: 26
- Coefficient of thermal expansion β [°C^{-1}]: $6.8.10^{-6}$
- Static pressure P [MPa] at repository depth 300m : 6.6
- Waste package data (initial area power) [W/m^2] : 18.8
- Permeability of the medium K [m^2]: clay:1.10^{-9}, Sandstone:1.10^{-5}, Granite:1.10^{-7}

The calculations will be performed at generic depth where source region (repository) is subject to Dirichlet conditions. It is proposed that the surface maintains approximately a temperature of 50 [°C] .

5. Conclusions

This preliminary study gives basic elements for computational modelling of the natural convection around repository. It is based on simplest Darcy porous media physical concept. The numerical solution, based on the Dual Reciprocity Method, has been already successfully tested in standard differentially heated rectangular cavity benchmark situation [4]. It is particularly suitable for use in the present semi–infinite domain context due to trivial discretization. Next steps will include the buildup of the specific models and computer runs in geometry's, relevant for the possible repositories. The geometry data will be provided by the SNSA. For this purpose, an axisymmetric version of the code is in development. One of the main difficulties represents the analytical integration (see [6]) of the inverse multiquadric functions ψ_n and φ_n which are currently not known.

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