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(*) Not shown in INIS Thesaurus 1985.

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SUMMARY

Numerical results are obtained for the local effects produced by the emplacement of a high-level waste repository in a granitic rock. These results imply considering the coupled thermal-flow problem in a porous media. The method described herewith is based in the solution of the governing equations by boundary-fitted finite differences, with a special treatment of the heat sources. The calculations are performed in terms of primitive variables by two solution techniques, namely iterative and direct, the latter employing a sparse matrix solver. An extension of the technique aimed at including discrete fractures is also discussed.

1. INTRODUCTION

The multiple scales associated with the modelling of the local effects of the emplacement of a nuclear waste repository have been discussed in detail by Ferreri and Ventura /1/, with reference to the thermal history of the system. In this reference the authors showed that proper treatment of the heat sources lead to significant economy and accuracy in the predictions. The conventional approach to the modelling of flows with concentrated heat sources imply generous grid refinements in the vicinity of the sources and, consequently, a large number of nodes (of the order of 10^4) in the three-dimensional (3D) case. If it is considered that one must usually deal with a large number of heat sources and/or a large number of time steps, then, keeping a low number of nodes (of the order of 2,000 in 3D) makes the computations attainable with a "general purpose" computer (as the one available at CNEA).

A natural extension to the results of reference /1/ is shown in this paper, namely considering the simulation of the flow-field evolution as time elapses. In this case, the governing equations are solved by means of a boundary-fitted, finite-difference technique, in terms of the so called "primitive variables" in a porous media; i.e., velocity-pressure for the Navier-Stokes equations and temperature for the energy equation. The momentum equations are solved under Darcy's approximation with the fluid considered as almost incompressible, allowing for a thermal driving source -obtained from the Boussinesq expansion- for the fluid density. We considered that the rock was in thermal equilibrium with the fluid, thus in turn allowing to consider a single energy equation for a media with equivalent properties.

Results for some cases of interest, to be shown later, were obtained from two versions of the code. The first one was of the iterative type (running an adaptation of the code of Martínez and Ferreri /2/) with explicit advancement of the energy equation and a semi-implicit solution algorithm for the momentum and mass conservation equations. The second version was based in the same approximation to the governing equations, although a direct solver was employed instead. In this way, a fully implicit approximation to the flow equations, together with the characteristics of the solver, allowed for the obtention of a robust code. A recent extension of this method permitted to include discrete fractures in the field.

In what follows, consideration is given to the numerical approximation to the governing equations, the computational algorithms are described and some calibration results are shown, although for the two-dimensional (2D) case.

2. GOVERNING EQUATIONS

The equations for natural convection in a porous media have been discussed by many authors. Among them, Ene and Sánchez-Palencia /3/ considered the validity of the usual approximations to the Navier-Stokes equations in general terms and Hodkingson et al. /4/ considered the thermal aspects of a repository behaviour, including the validity of the governing equations, in the context of repository modelling.

Then, under Darcy's approximation for the momentum, under Boussinesq's expansion for fluid density and considering an equivalent porous media, the equations governing the flow are:

$$\bar{u} = - \frac{k}{\nu_f} (\nabla P + \beta \bar{g} \Delta T) \qquad (1)$$

$$\nabla \bar{u} = 0 \qquad (2)$$

$$\frac{\partial T}{\partial t} + \alpha \bar{u} \nabla T = \nu_t \nabla^2 T + Q \qquad (3)$$

In equations 1-3, $\bar{u}$ is the volume-averaged fluid velocity, P is the fluid static pressure plus the static head, β is the volumetric thermal expansion coefficient of the fluid, T is the temperature of the system, g is the gravity acceleration, ρ_0 is the fluid reference density, k is the permeability of the rock,

ν_f is the momentum diffussivity (fluid kinematic viscosity divided by ρ_0) and Q represents the heat sources. If the average properties of the solid are defined as $\{\}_{av} = (1 - \phi)\ \{\}_s + \phi\ \{\}_f$, where ϕ is the porosity, s means the solid and f means the fluid, then, ν_t is the average thermal diffussivity. Finally, α is the ratio between the thermal capacity of the fluid and the average thermal capacity of the porous media.

In equations 1-3 it is assumed that ν_f and ν_t are not temperature dependent, the extension to the general case being straight-forward.

The presence of Q in equation (3) imposes some difficulties for the numerical solution of the system of equations because the temperature variations in the neighbourhood of the sources are quite steep.

3. RESOLUTION METHODS

The numerical solution of 1-3 was obtained by means of boundary-fitted finite-difference techniques. The discrete version of these equations can be easily found from previous work by J. F. Thompson (see reference /5/, for instance) and by one of the authors /2/. As the present approach is somewhat different from the usual one in boundary-fitted coordinates, some algebraic details are provided in what follows.

Figure 1 shows a cell belonging to a hypothetical grid in the physical plane and illustrates the location of the variables. As can be seen, we consider velocities located at the cell corners and cell-centered pressures. Temperatures are located at cell corners. D_{ij} is a discrete representation of the flow divergence and is also located at the cell center. The meaning of u_f and v_f will be cleared up later.

The equations obtained, after the transformation of the original equations in terms of U,V, are:

$$u = - \Delta t_f \left(AUX \frac{\partial P}{\partial U} + AVX \frac{\partial P}{\partial V} \right) \tag{4}$$

$$v = - \Delta t_f \left(AUY \frac{\partial P}{\partial U} + AVY \frac{\partial P}{\partial V} + \beta\ g\ \Delta T \right) \tag{5}$$

$$BUX \frac{\partial u}{\partial U} + BVX \frac{\partial u}{\partial V} + BUY \frac{\partial v}{\partial U} + BVY \frac{\partial v}{\partial V} = 0 \tag{6}$$

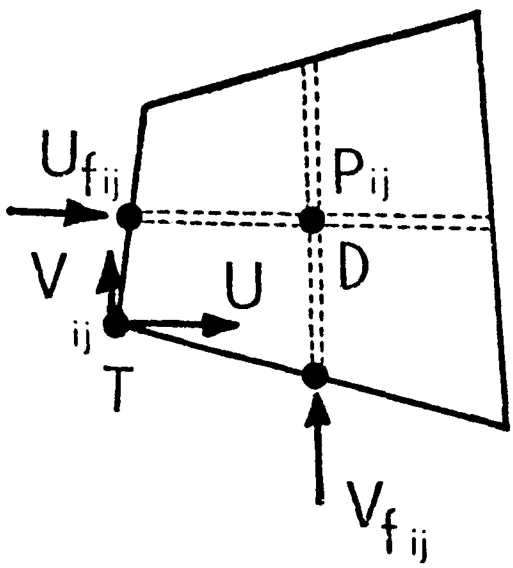

Figure 1. A computational cell illustrating the centering of variables

$$\frac{\partial T}{\partial t} + \alpha\, u\, (AUX\, \frac{\partial T}{\partial U} + AVX\, \frac{\partial T}{\partial V}) + \alpha\, v\, (AUY\, \frac{\partial T}{\partial U} + AVY\, \frac{\partial T}{\partial V}) =$$

$$= \nu_t\, (AUU\, \frac{\partial^2 T}{\partial U^2} + AVV\, \frac{\partial^2 T}{\partial V^2} + AUV\, \frac{\partial^2 T}{\partial U\, \partial V} + AU\, \frac{\partial T}{\partial U} + AV\, \frac{\partial T}{\partial V} + Q \qquad (7)$$

where $\Delta t_f = k/\nu_f$.

The coefficients in equations 1-7 determine the influence of the grid variations and are numerically calculated from the following expressions:

$AUX = U_x$		$AUU = U_x^2 + U_y^2$
$AVX = V_x$		$AUV = 2\,(U_x\, V_x + U_y\, V_y)$
$AUY = U_y$	and	$AVV = V_x^2 + V_y^2$
$AVY = V_y$		$AU = U_{xx} + U_{yy}$
		$AV = V_{xx} + V_{yy}$

The expressions for BUX... are the same as the corresponding ones for AUX..., the difference between them is that BUX...

are evaluated at cell centers and AUX... are evaluated at cell corners.

The discrete version of equations 4-7 is obtained by means of centered-difference expressions, implying appropriate averaging of the variables in the cell.

As an example, the pressure term on the right-hand side of equation 4 is calculated as:

$$AUX_{ij}\ (P_{i-1\ j-1} + P_{i-1\ j} - P_{i j-1} - P_{ij})/2 +$$
$$AVX_{ij}\ (P_{i-1\ j-1} + P_{i j-1} - P_{i-1\ j} - P_{ij})/2$$

with similar expressions for the remaining terms of equations 4-7.

The treatment of the heat sources in equation 7 is accomplished by the technique in reference /1/. In this reference it was shown that concentrated heat sources can be adequately treated if the solution of the problem:

$$L\ \{T\} = Q$$

is obtained from:

$$L_h\ \{T\} = L_h\ \{S\}$$

where S is the analytical solution of $L\{S\} = Q$ in the neighbourhood of the heat source and L_h is the discrete version of L.

We are now in a position to consider the differences between the solution algorithms. The first one, as stated previously, was of the semi-implicit type. In this version, temperatures were advanced explicitly from time $n\Delta t$ to time $(n+1)\Delta t$; this step produced new driving forces in the momentum equations which were "solved" to produce tentative values for u and v. Pressures and velocities were iteratively adjusted to simultaneously satisfy equations 4-6 through the repeated application of the following steps:

i) The discrete analogue of the cell divergence D_{ij} is evaluated as follows:

$$\begin{aligned} D_{ij} = \{\ & (u_{i+1 j+1} + u_{i+1 j} - u_{i j+1} - u_{ij})\ BUX_{ij} + \\ & (u_{i+1 j+1} + u_{i j+1} - u_{i+1 j} - u_{ij})\ BVX_{ij} + \\ & (v_{i+1 j+1} + v_{i+1 j} - v_{i j+1} - v_{ij})\ BUY_{ij} + \\ & (v_{i+1 j+1} + v_{i j+1} - v_{i+1 j} - v_{ij})\ BVY_{ij}\ \}/2 \qquad (8) \end{aligned}$$

ii) The pressure in the cell is adjusted to bring cell divergence to zero, as follows:

$$P_{ij}^{(k+1)} = P_{ij}^{(k)} + \delta P_{ij} \tag{9}$$

where:

$$\delta P_{ij} = -\beta_{ij}\ D, \tag{10}$$

$$\beta_{ij} = \frac{\omega}{\Delta t_f}\ \{\ BUU_{ij} + BVV_{ij} + CT\ \} \tag{11}$$

and CT means Cross Terms (i.e., higher order terms implying crossed derivatives of the transformation coefficients).

ω is an overrelaxation parameter whose typical value is 1.4 for this type of problems.

iii) The velocity of components at the cell corners are accordingly modified as follows:

$$u_{i+1\,j+1}^{(k+1)} \leftarrow u_{i+1\,j+1}^{(k)} + C\ (AUX_{i+1\,j+1} + AVX_{i+1\,j+1}),$$

$$u_{i+1\,j}^{(k+1)} \leftarrow u_{i+1\,j}^{(k)} + C\ (AUX_{i+1\,j} - AVX_{i+1\,j}),$$

$$u_{i\,j+1}^{(k+1)} \leftarrow u_{i\,j+1}^{(k)} + C\ (-AUX_{i\,j+1} + AVX_{i\,j+1}),$$

$$u_{ij}^{(k+1)} \leftarrow u_{ij}^{(k)} + C\ (-AUX_{ij} - AVX_{ij}),$$

$$v_{i+1\,j+1}^{(k+1)} \leftarrow v_{i+1\,j+1}^{(k)} + C\ (AUY_{i+1\,j+1} + AVY_{i+1\,j+1}),$$

$$v_{i+1\,j}^{(k+1)} \leftarrow v_{i+1\,j}^{(k)} + C\ (AUY_{i+1\,j} - AVY_{i+1\,j}),$$

$$v_{i\,j+1}^{(k+1)} \leftarrow v_{i\,j+1}^{(k)} + C\ (-AUY_{i\,j+1} + AVY_{i\,j+1}),$$

$$v_{ij}^{(k+1)} \leftarrow v_{ij}^{(k)} + C\ (-AUY_{ij} - AVY_{ij})$$

and $C = \Delta t_f\ \delta P_{ij}\ /2$

Boundary conditions were appropriately applied after each iteration sweep and convergence was usually reached. This convergence and subsequent pressure smoothing allowed us to start a new time step.

The other version of the code implied a fully coupled solution of the system 4-7. This version was originally intended to test the proper posing of boundary conditions, because it was not always clear whether or not the system of equations was over-determined. A careful arrangement of equations was necessary in order to avoid a large fill-in; scaling of the coefficient was sometimes inevitable.

For a general computational cell, the ordering of the equations was:

i) u momentum (from which u was obtained)

ii) continuity (from which v was obtained)

iii) v momentum (from which P was obtained)

iv) energy equation (from which T was obtained)

Boundary conditions were incorporated explicitly in the system of equations.

For an arbitrary Raleigh's number, the problem is fully non-linear in nature, due to the presence of the advective terms in equation 7. In the typical applications of repository modelling, advective terms are not too important. So, it was decided to linearize the problem by menas of suitable extrapolation of velocities as obtained from two previous time steps. No attempt was made to iterate the solution because some comparisons between the codes showed close agreement between the computed solutions. However, in other applications, the iteration may be inevitable.

The algebraic system of linear equations was solved with a library sparse matrix solver named MA28AD from the Harwell package /6/, which proved to be efficient in most cases. However, one must be careful concerning the relative weight of the coefficients, if willing to obtain meaningful results.

It is interesting to point out that, after proper scaling, the direct version was far more robust than the iterative one and, as a consequence, some generalizations were implemented. The first one was considering permeability as variable.

The second and most important modification was allowing for the consideration of discrete fractures in the granitic mass.

This version, implied the definition of one-dimensional paths among cell centroids and a whole set of fracture fluid velocities, shown in figure 1 as u_f and v_f. If the fractures are constrained to follow the lines of centroids (i.e., lines of constant U or V in the plane of reference), then:

$$u_f = - \Delta t'_f \left\{ \frac{1}{J(CUU)^{1/2}} \frac{\partial p}{\partial U} + \beta g_V \Delta T \right\} \tag{13}$$

$$v_f = - \Delta t'_f \left\{ \frac{1}{J(CVV)^{1/2}} \frac{\partial p}{\partial V} + \beta \, g_U \, \Delta T \right\} \qquad (14)$$

The coefficients CUU and CVV are similar to AUU and AVV, except for the fact that they are evaluated at the corresponding points for u_f and v_f. J is the Jacobian of the transformation and g_U, g_V are the components of $\bar{g}$ along the U and V directions in the physical plane.

4. RESULTS

In this section we show several calibration results of interest in the context of our assessments for the nuclear safety of high-level waste repository.

The first case consists in an isolated, infinitely long line source located in the center of the integration domain, assumed to be semi-infinite. The local analytical approximate solution was obtained from a limiting solution for a plane rectangular source with its strength decaying in time. The computational grid is shown in figure 2a; the integration domain is 1500 m as per x and 2000 m as per y. The source is located at x = 0, y = 0 and the earth surface is located at y = 500 m.

The transport parameters were $\nu_t = 0.11 \; 10^{-5} \; m^2/s$ and $\nu_f = 6.58 \; 10^{-7} \; m^2/s$; the thermal expansion coefficient of the fluid was $\beta = 3.85 \; 10^{-4} \; K^{-1}$; the permeability of the rock was $k = 1.7 \; 10^{-15} \; m^2$. These values gave $\Delta t_f = 2.58 \; 10^{-9}$ s. The time step for the integration was first fixed at $\Delta t = 1$ y, as a test. The integration domain was discretized in 12 x 12 rectangular cells (note the low number!). The Raleigh's number of the flow, defined as $Ra = k \; \beta \; g \; L \; \Delta T \; \alpha \; / \; \nu_f \; \nu_t$ /7/ was in the order of 0.5. This low value permitted to neglect the effects of advection in the analytical solution for the source. The codes gave identical results and the fully-coupled version, with fully-implicit time integration for T and $\Delta t = 10$ y, was finally adopted.

Figure 2b shows a vector plot of velocities as obtained for t = 500 y and figure 2c shows a zoom of the vector plot in the vicinity of the source.

The results for temperatures are quite similar to those obtained with a fully analytical, decoupled solution.

A second example is shown in figure 3, which shows the calculations corresponding to a case with specified input flow and heat input from a plane source of finite width. The parameters are similar to those of the previous case. Figure 3a shows the grid and figure 3b shows a vector plot for t = 500 y, considering the heat emmited by the sources.

5. CONCLUSIONS

A description has been made of the results obtained with codes developed on the basis of a boundary-fitted finite-difference technique, as applied to the problem of natural convection in a porous media. The code work in terms of primitive variables.

The method allows for considering singularities of heat generation and fractures in the bulk of the porous media (this version is being calibrated at the time of writing). The codes incorporate the proper consideration of the heat sources by means of local semi-analytical solutions.

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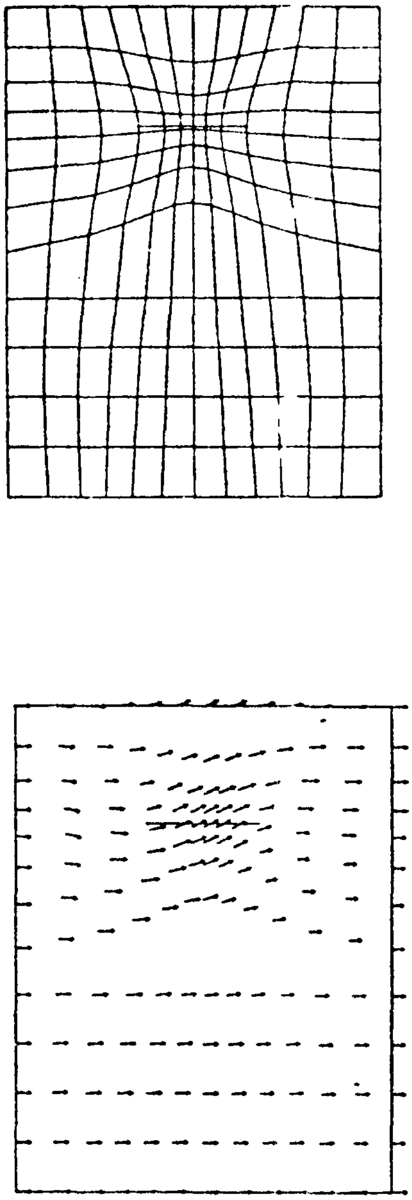

Figure 3. The flowfield originating in a plane heat source, Q = 5.25 W/m^2

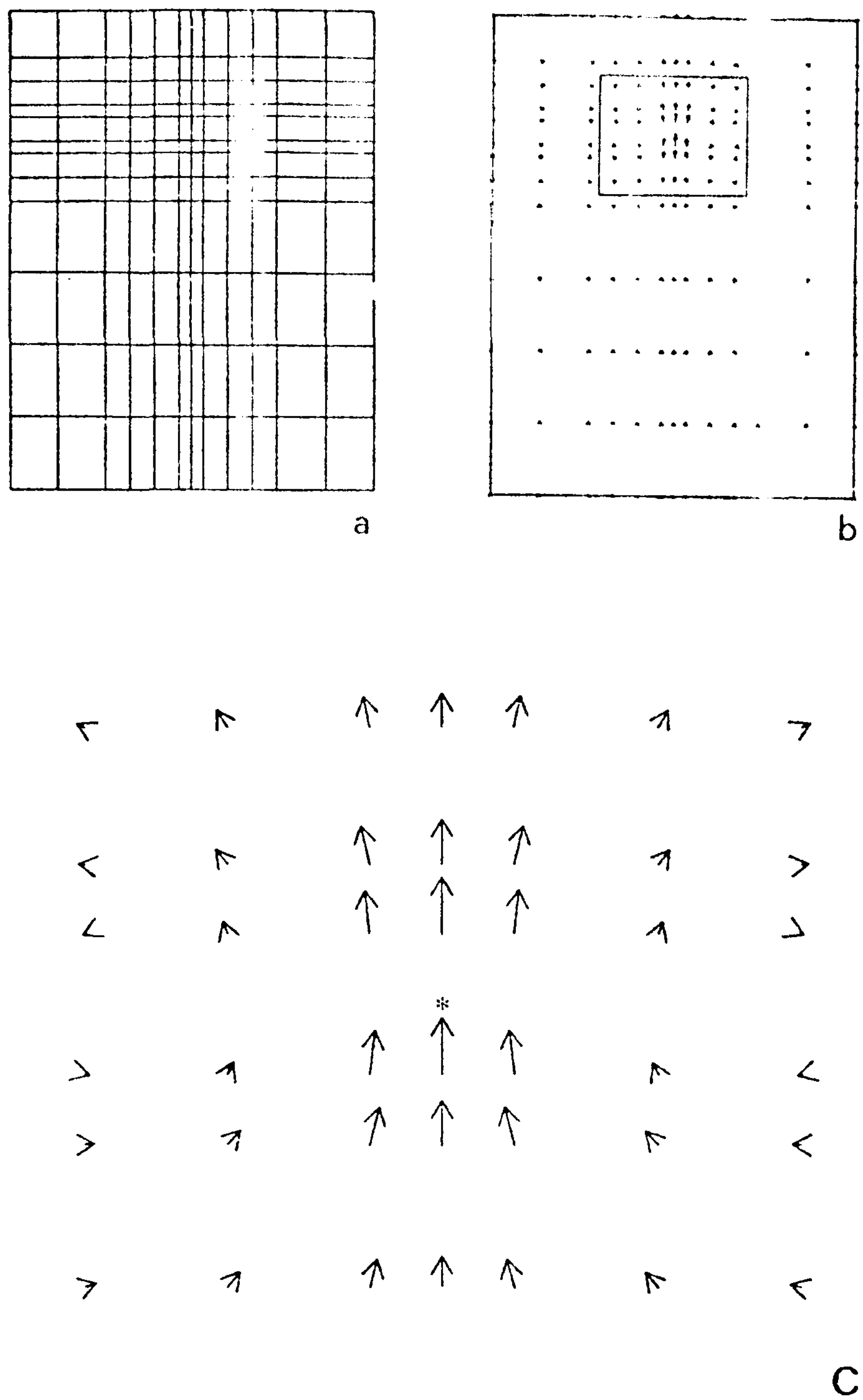

Figure 2. The flowfield originating in an infinitely long line heat source, Q = 100 W/m

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