

Numerical Methods for Transient and Coupled Problems

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ON NUMERICAL MODELS FOR THE ANALYSIS OF
NUCLEAR WASTE DISPOSAL IN GEOLOGICAL CLAY FORMATIONS

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ABSTRACT

A study of disposal in clay formation of long lived radioactive wastes requires an analysis of coupled thermal, mechanical and hydraulic fields.

In this paper a mathematical description of clay behaviour under combined actions of heating, elastoplastic deformations and groundwater flow is presented and related numerical models are discussed.

1. INTRODUCTION

One of the hypotheses for disposal of nuclear waste of long live radioactivity is a construction of repositories in deep clay formations. Principal candidates in Italy are largely diffused pliocenic clays.

Heating of clay due to radioactive decay induces: heat transfer through the geologic formation, development of pore water pressure and its dissipation via water seepage together with stress and strain effects due to heating and seepage. Clearly, a simultaneous development of these phenomena leads to their mutual interdependence and to necessity of coupled analyses.

Due to their complex microstructural properties clay exhibits both non-linearity of hydraulic and thermal behaviour and non-linearity and irreversibility of mechanically induced deformation. In the present model the aforementioned effects are intended to be taken into account. For the mechanical part a Cam-Clay type model is adopted and generalized to thermoplastic effects.

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Preliminary results of experimental verification of the model indicate high non-linearity of tested clays.

2. MECHANICAL, HYDRAULIC AND THERMAL PROPERTIES OF CLAYS AND THEIR MATHEMATICAL DESCRIPTION

2.1 GENERAL REMARKS

Italian pliocenic clay formations are sediments consisting of finest grains of soils and mineral products of rock degradation deposited under marine conditions.

Due to subsequent geologic agents such as environment condition during deposition, lithostatic pressures, cementation, etc, clays exhibit a particular complexity of microstructure. Unlike in some other granular materials, in clays a separation of solid and liquid phase is impossible under normal conditions. In fact, it is known, that water in clay may appear in four categories of conditions i.e. pore water, adsorbed water, solvate water and structural one [1]. Water of the two first categories only may migrate freely due to hydraulic gradients. Chemical bond energy between solid and water of other two categories is recognized to vary with temperature in different manner. It leads to exchanges of quantities of water between the categories. It results then in necessity of introduction of two distinct thermal expansion coefficients (Mitchell, Campanella), [2]. In the model the above microstructural effects are described phenomenologically by employing global behaviour measures.

Simple intuition indicates that mechanical behaviour of clays depends on temperature and on pore water pressure rise induced by it. Flow and pressure of water depend on the other hand on permeability of clay and water thermal expansion. Thermal properties, perhaps to the least extent, are function of stress or porosity variation.

In what follows we shall examine one by one deformational, hydraulic and thermal local behaviour relationships underlining their interdependences.

2.2 MECHANICAL LOADING RESPONSE

Analogously to isothermal conditions, only a part of

strain of clay under combined mechanical and thermal action is reversible. The other, permanent part of strain due to both kind of agents is significant.

The reversible part of strain is assumed to be composed of solid grain compression due to pore water pressure, p , effective stress induced deformation of clay skeleton and thermal isotropic expansion both of grains themselves and of skeleton which involves also possible structural and/or adsorbed water changes in a following way, [2,3]:

$$\underline{\varepsilon}^e = \frac{1}{3} \left[C \ln \frac{\bar{\sigma}'}{\bar{\sigma}'_0} + C^* p - (\alpha^* + \alpha^{st}) \Delta T \right] \underline{m} + \frac{1}{2G} \underline{s} \quad (1)$$

where $\bar{\sigma}'$ is effective mean stress connected to pore water pressure p via effective stress relationship: $\bar{\sigma}' + p = \bar{\sigma}$. $C = C(\Delta T)$ is known as effective elastic compression index and is supposed to depend on temperature. $C^* = \text{const.}$ is the grain solid (mineral) compliance modulus. Also the coefficient of cubic thermal expansion of grain solid α^* , is assumed as constant; this is not the case of α^{st} , referred to as coefficient of thermal expansion of soil structure, after Mitchell and Campanella [2]. It varies with effective mean stress and temperature and moreover may take on both positive and negative values, as for soft seabed clays [2,4], and for rocks [5]. For strongly isotropically consolidated clays under 6 MPa, preliminary results are obtained. Fig.1 shows volumetric strains due to heating and cooling from 20°C to 81.5°C under two different isotropic pressure in drained conditions ($p=0$). Note a significant difference of thermal curves. The difference in their performance, considered as elastic for the strong overconsolidation may be attributed both to variation of $C = C(\Delta T)$ and of $\alpha^{st} = \alpha^{st}(\bar{\sigma}')$. The absence of plastic effects is confirmed by the closure of the loading cycle.

In equation (1), G is shear modulus, whereas \underline{m} is one-zero column vector, \underline{s} is the stress deviator vector.

The plastic part of strain $\underline{\varepsilon}^p$ due to its loading history dependence is expressed in terms of increment. Plastic flow, refers to the soil structure skeleton, while grains are supposed to deform elastically. The former occurs if the effective stress state reaches the yield condition: [9]

$$f = f(\bar{\sigma}', K, \Delta T) \quad ; \quad K = K(\varepsilon_v', \Delta T) \quad (2)$$

In what follows the dependence of a plastic flow on pore pressure hardening domains: (ductile)

The variation of plastic flow is poorly understood under temperature condition, of the isotropic hardening and brittle to ductile stress deviator

Consider now

$$df = \frac{\partial f}{\partial \bar{\sigma}'} d\bar{\sigma}'$$

from which it can be determined the thermal condition of the plastic flow hardening

$$d\varepsilon^p = \lambda \frac{\partial f}{\partial \bar{\sigma}'}$$

where λ is the plastic multiplier. The plastic flow hardening modulus depends on the plastic flow. A respect to the plastic flow of all that is hardening both to the plastic flow and to the plastic flow hardening. In the absence of plastic flow $d\bar{\sigma}' > 0$, requires

This finding is in agreement with the plastic flow hardening modulus of consolidated clays. The total mean stress is the sum of the plastic flow hardening modulus and the plastic flow hardening modulus ($\underline{s}=0$)

$$f_{,T} = \left[\frac{df}{dT} \right] +$$

In what follows a generalization to thermal dependence of a Cam Clay type model will be used. It employs a closed yield surface in the stress deviator, pressure invariant plane, Fig.2. It divides, via a hardening rule, the admissible stress range into two domains: that of softening (brittle) and hardening (ductile) behaviour.

The variation of the yield surface with temperature is poorly known for clay. It is supposed to shrink under temperature elevation in isotropic pressure condition, and to exhibit a decrease with temperature of the isotropic pressure required for ductile - brittle transition (or critical state) at constant stress deviator (observed also for rocks).

Consider now the consistency equation at yielding,

$$df = \frac{\partial f}{\partial \bar{\epsilon}'} d\bar{\epsilon}' + \frac{\partial f}{\partial K} \frac{\partial K}{\partial \bar{\epsilon}_v'} d\bar{\epsilon}_v' + \left(\frac{\partial f}{\partial K} \frac{\partial K}{\partial \Delta T} + \frac{\partial f}{\partial \Delta T} \right) dT = 0 \quad (3)$$

from which the plastic strain increment may be determined if by analogy with clay behaviour in isothermal conditions a non-associated flow rule is assumed

$$d\bar{\epsilon}_v^p = \lambda \frac{\partial g}{\partial \bar{\epsilon}'} = \frac{1}{H} \left(\int_{\bar{\epsilon}'}^T d\bar{\epsilon}' + \int_{,T} dT \right) \frac{\partial g}{\partial \bar{\epsilon}'} ; \int_{,T} = \frac{\partial f}{\partial K} \frac{\partial K}{\partial \Delta T} + \frac{\partial f}{\partial \Delta T} \quad (4)$$

where λ is plastic multiplier, $g = g(\bar{\epsilon}', T) = 0$ is the plastic potential, $H = - \int_{,K} (\partial K / \partial \bar{\epsilon}_v^p)^T g_{, \bar{\epsilon}'}$ is the hardening modulus, while T as a superscript means transpose. A comma denotes a partial derivative with respect to following subscript variable. Note first of all that plastic strain increment is proportional both to the effective stress and temperature increments. In the hardening range, $H > 0$, a heating in the absence of the effective stress increment, $d\bar{\epsilon}' > 0$, requires through eq.(3) that $\int_{,T} > 0$.

This finding has been qualitatively confirmed in plastic deformation due to heating of normally consolidated Orto clay (Tiber Valley) under constant total mean stress, in undrained isotropic conditions. From the eq.(3) with the Cam Clay criterion $f = \bar{s}^T \bar{s} / \bar{\epsilon}' + M \ln(\bar{\epsilon}' / \bar{\epsilon}'_c) = 0$; $\bar{\epsilon}'_c = \exp(\bar{\epsilon}' / \lambda - K)$, being $\lambda - K$ a hardening modulus, it results that for such path ($\bar{s} = 0$)

$$\int_{,T} = \left[\frac{dp}{dT} + (\bar{\epsilon}' - p)^3 \frac{1}{\lambda - K} \frac{d\bar{\epsilon}_v^p}{dT} \right] \frac{1}{(\bar{\epsilon}' - p)^2} ; dp = -d\bar{\epsilon}' \quad (3a)$$

A preliminary result on variation of the pore pressure with temperature under various confining pressure is shown in Fig. 3. Irreversible volumetric strain associated with this variation has been found positive (consolidation) thus all terms in (3a) are positive, and thus $f_{,T} > 0$ for $\underline{s} = 0$. Note, that due to the heating, soil in undrained conditions is not any more incompressible.

In the softening range, $H < 0$, the material behaviour is stress uncontrolled, and thus $d\bar{\sigma}' = 0$ is not admissible under heating. Moreover, two contrasting effects of heating must be taken into account, that of yield criterion reduction and hardening modulus increase (bigger ductility). The former is described via $\partial f / \partial \Delta T > 0$, whereas the latter via $\partial f / \partial \Delta T < 0$. Since for $H < 0$, $f_{, \bar{\sigma}'} d\bar{\sigma}' < 0$, (4), the effect of temperature induced bigger ductility, requires that $|\partial f / \partial K \cdot \partial K / \partial T| > \partial f / \partial \Delta T$. This is met by assuming a coupled strain-temperature hardening variable in $K = K(\underline{\epsilon}^{pl}, \Delta T)$ in eq.(2), see also [10].

Summing the elastic and plastic strain increments (see (1) and (4)) one arrives at the following expression:

$$d\underline{\epsilon} = \underline{\underline{C}}^{ep} d\underline{\sigma}' + \frac{1}{3} C^* \underline{m} dp - \underline{m}_1 dT \quad (5)$$

where

$$\underline{\underline{C}}^{ep} = \underline{\underline{C}}^e + \frac{1}{H} \underline{g}_{, \bar{\sigma}'} \left(\underline{f}_{, \bar{\sigma}'} \right)^T \quad (6)$$

and $\underline{\underline{C}}^e$ is the thermoelasticity matrix derivable from (1)

$$\underline{m}_1 = \frac{1}{3} (\alpha^* + \alpha^{st} - C_{, T} \ln \frac{\bar{\sigma}'}{\bar{\sigma}_0} + \alpha_{, T}^{st} \Delta T) \underline{m} - \frac{1}{H} \underline{f}_{, T} \frac{\partial g}{\partial \bar{\sigma}'} \quad (7)$$

Clearly $d\underline{\epsilon}^{pl}$ is non zero in loading conditions only, i.e. when

$$\underline{f}_{, \bar{\sigma}'}^T d\bar{\sigma}' + \underline{f}_{, T} dT > 0 \quad \text{at} \quad \underline{f} = 0 \quad (8)$$

Otherwise $d\underline{\epsilon}^{pl}$ is zero.

After some algebra it is easy to find an inverse relation to (5) which reads;

$$d\underline{\sigma}' = \underline{\underline{D}}^{ep} d\underline{\epsilon} + \underline{\Delta}_t dT - \underline{\Delta}_p dp$$

where

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$$\alpha_T = \alpha^* + \alpha^{st} - C_{,T} \ln \frac{\bar{\epsilon}'}{\bar{\epsilon}'_0} + \alpha_{,T}^{st} \Delta T \quad (10)$$

$$\underline{\underline{D}}^{epl} = \underline{\underline{E}} - \frac{1}{H-H_c} \underline{\underline{E}} \underline{\underline{g}}_{, \bar{\epsilon}'} (\underline{\underline{f}}_{, \bar{\epsilon}'})^T \underline{\underline{E}} ; H_c = - \underline{\underline{f}}_{, \bar{\epsilon}'}^T \underline{\underline{C}} \underline{\underline{g}}_{, \bar{\epsilon}'}$$

$$\underline{\underline{\Delta}}_v = \frac{1}{3} C^* \underline{\underline{D}}^{epl} \underline{\underline{m}} ; \underline{\underline{\Delta}}_t = \alpha_T \underline{\underline{D}}^{epl} \underline{\underline{m}} - \frac{1}{H-H_c} \underline{\underline{C}}^{el} \underline{\underline{g}}_{, \bar{\epsilon}'} \underline{\underline{f}}_{, \bar{\epsilon}'} \quad (11)$$

whereas loading condition expressed in terms of $d\underline{\underline{\epsilon}}$, corresponding to (8) is now:

$$\underline{\underline{f}}_d^T d\underline{\underline{\epsilon}} > \delta_T dT - \delta_p dp \quad (12)$$

where

$$\underline{\underline{f}}_d = (\underline{\underline{f}}_{, \bar{\epsilon}'})^T \underline{\underline{C}}^{el} ; \delta_T = \alpha^T \underline{\underline{f}}_{, \bar{\epsilon}'} + \underline{\underline{f}}_{, T} ; \delta_p = C^* \underline{\underline{f}}_{, \bar{\epsilon}'}$$

For further developments of flow continuity equation it is important to know deformation of soil pores. It is assumed first of all, that such deformation consists of skeleton structure minus grain compression, pore change due to homothetic mechanical and thermal grain deformation, being its n-th fraction, and finally structure rearrangement both elastic, thermally induced and plastic as specified in incremental form in what follows:

$$dn = \frac{1}{1 + C^* p + \alpha^* \Delta T} \left\{ - \left(\frac{C}{\bar{\epsilon}'} - C^* - \alpha_{, \bar{\epsilon}'}^{st} \Delta T \right) d\bar{\epsilon}' - n C^* dp + \right. \\ \left. + (n \alpha^* + \alpha^{st}) dT - \left(C_{, T} \ln \frac{\bar{\epsilon}'}{\bar{\epsilon}'_0} - \alpha_{, T}^{st} \Delta T \right) dT - \right. \quad (13)$$

$$\left. - \frac{1}{H} \left(\frac{\partial \underline{\underline{f}}}{\partial \bar{\epsilon}'} d\bar{\epsilon}' + \underline{\underline{f}}_{, T} dT \right) \frac{\partial \underline{\underline{g}}}{\partial \bar{\epsilon}'} - \frac{1}{H} \frac{\partial \underline{\underline{g}}}{\partial \bar{\epsilon}'} \left(\frac{\partial \underline{\underline{f}}}{\partial \underline{\underline{s}}} \right)^T d\underline{\underline{s}} \right\}$$

The rhs denominator in most cases may be approximately taken as equal to 1.

2.3 MASS FLOW CONTINUITY EQUATION. THERMO-HYDRAULIC CLAY PROPERTIES.

Suppose at the beginning that the water flow through clays is in condition of full saturation and continuity. Then the continuity equation reads:

$$- \nabla (\rho^w \underline{\underline{v}}) = \frac{d}{dt} (n \rho^w) \quad (14)$$

where ρ^w is the water density while v is water flow velocity and ∇ is divergence operator. The water flow through the soil is governed by a generalized Darcy law:

$$v = -K \nabla \left(\frac{p}{\rho^w g} + h \right) \quad (15)$$

where K is the permeability and $(p/\rho^w g + h)$ the elevation head.

The permeability K is known to depend on the material porosity and water viscosity. The latter depends on temperature. Following Koženy [6], Bažant [7] and Kézdi [1] the resultant permeability may be written as follows:

$$K = \frac{\gamma^w}{\mu_0} \frac{T - T^r}{K_0 S^2} \left(\frac{n}{1-n} \right)^2 n \quad (16)$$

where μ_0, K_0, T^r are experimental coefficients, and S is specific surface area.

The right hand side of (14) may be made explicit as follows:

$$\frac{d}{dt} (n \rho^w) = \rho^w \frac{\partial n}{\partial t} + n \left(\rho^w C^w \frac{\partial p}{\partial t} - \rho^w \alpha^w \frac{\partial T}{\partial t} \right) \quad (17)$$

denoting by C^w and α^w water bulk compliance modulus and its thermal cubic coefficient. Neglecting spatial variation of K in lhs of (15) and substituting (13, 15, 17) to (14) one reaches a definite form of the flow continuity equation:

$$\begin{aligned} & \frac{\gamma^w}{\mu} \nabla \left\{ K (T - T^r) \left(\frac{n}{1-n} \right)^2 n \nabla \left(\frac{p}{\rho^w g} + h \right) \right\} = \\ & = t_\varepsilon \left(\frac{d\varepsilon}{dt} \right) + \frac{1}{3} C^* \frac{d\bar{\varepsilon}'}{dt} + \left[(1-n) C^* + n C^w \right] \frac{dp}{dt} + \\ & + \left[(n-1) \alpha^* - n \alpha^w \right] \frac{dT}{dt} \end{aligned} \quad (18)$$

Note that (18) is valid if (12) or (8) are fulfilled i.e. in the case of plastic, thermal or joint loading conditions. In the opposite case the plastic terms, i.e. these containing $1/H$ should be suppressed ($1/H \equiv 0$), since purely thermoelastic deformation takes place.

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2.4 HEAT BALANCE EQUATION

The heat transport through the clay formation is affected by the seepage of pore water and by soil porosity changes due to mechanical loads.

The energy transport equation thus reads:

$$\nabla(\lambda \nabla T) = \rho^w c^w \underline{v} \nabla T + \frac{\partial}{\partial t} (\rho c \Delta T) \quad (19)$$

where λ is thermal conductivity of soil, $\rho^w c^w$ and ρc are specific heat capacities of water and of soil.

Assuming that clay is fully saturated and that water and solid densities are constant

$$\rho = n \rho^w + (1-n) \rho^* \quad ; \quad d\rho = c \Delta T (\rho^w - \rho^*) dn \quad (20)$$

one may obtain the following equation

$$\nabla(\lambda \nabla T) = \rho c \frac{\partial T}{\partial t} + \rho^w c^w \underline{v} \nabla T + c \Delta T (\rho^w - \rho^*) \frac{dn}{dt} \quad (21)$$

The second term of the rhs represents coupling of the thermal problem with the hydraulic one, whereas the third term is the coupling with the mechanical one.

Moreover, preliminary results on Boom clays show that the coefficient of thermal conductivity increases with temperature, and similarly does the specific heat [8]. These data require anyway a larger experimental confirmation.

In the case in which there is no mechanical loading and no inflow of external water both the porosity changes and the water velocities are purely temperature induced.

The real loading situation in the case of nuclear waste repositories is not far from the one described above. In fact in some important practical case, the loading may be idealized as restricted to radioactive decay heating only, at constant mechanical and hydraulic loads. It may lead to certain simplifications in the numerical procedures as discussed in the following section.

3. FINITE ELEMENT APPROXIMATION

A F.E. element discretization of the above equation system is described below. By introducing a piecewise representation of the primary unknowns p, T and δ , the mass flow eq.(18) in plane strain becomes:

$$\begin{aligned} & \left[\int_A \underline{B}_F \underline{K}_P \underline{B}_F dA \right] \underline{p} + \int_A \underline{B}_F \underline{K}_P [\rho^{\omega} g] dA - \int_r \underline{N} \underline{v} d\Gamma = \quad (22) \\ & = \left[\int_A \underline{N}^T \underline{I} \underline{B}_s dA \right] \underline{\delta} + \left\{ \int_A \underline{N}^T [(1-n)C^* + nC^{\omega}] \underline{N} dA \right\} \underline{\dot{p}} + \\ & + \left\{ \int_A \underline{N}^T [(n-1)\alpha^* - n\alpha^{\omega}] \underline{N} dA \right\} \underline{\dot{T}} \end{aligned}$$

where $\underline{\dot{p}}, \underline{\dot{T}}, \underline{\dot{\delta}}$ are the nodal rate vectors, and a standard finite element notation is used.

The heat flow eq.(21) takes now the following form:

$$\begin{aligned} & \left[\int_A \underline{B}_F \underline{K}_t \underline{B}_F dA \right] \underline{T} + \int_r \underline{N}^T \phi d\Gamma = \left[\int_A \underline{N}^T \underline{U} \underline{B}_F dA \right] \underline{T} + \\ & + \left[\int_A \underline{N}^T \rho c \underline{N} dA \right] \underline{\dot{T}} - \left[\int_A \underline{N}^T c \Delta T (\rho^{\omega} - \rho^*) \underline{N} dA \right] \underline{\dot{n}} \quad (23) \end{aligned}$$

where

$$\underline{B}_F = \begin{bmatrix} \frac{\partial \underline{N}_x}{\partial x} \\ \frac{\partial \underline{N}_y}{\partial y} \end{bmatrix} ; \quad \underline{N} = \begin{bmatrix} \underline{N} \\ \underline{N} \end{bmatrix} ; \quad \underline{U} = \rho^{\omega} c^{\omega} \begin{bmatrix} v_x & 0 \\ 0 & v_y \end{bmatrix} \quad (24)$$

The equilibrium equation is then:

$$\underline{K} \underline{\delta} + \underline{f} = \underline{o} \quad (25)$$

with

$$\underline{f} = \left[\int_A \underline{B}_s^T (\underline{\Delta}_P + \underline{I}) dA \right] \underline{\dot{p}} + \int_A \underline{B}_s^T \underline{\Delta}_t dA \underline{\dot{T}} - \int_r \underline{N}^T q d\Gamma - \int_A \underline{N} b dA$$

and

$$\underline{B}_s^T = \begin{bmatrix} \frac{\partial \underline{N}^T}{\partial x} & 0 & \frac{\partial \underline{N}^T}{\partial y} \\ 0 & \frac{\partial \underline{N}^T}{\partial y} & \frac{\partial \underline{N}^T}{\partial x} \end{bmatrix} \quad (26)$$

where \underline{K} is a non-symmetric elastoplastic incremental stiffness matrix.

Note that eq.(24) is accompanied by the yield condition equation and by a set of loading condition inequalities, (12) omitted here for brevity. The above equations may subsequently be discretized in time in a manner described already elsewhere [3,11].

The system of non-linear equations can be solved in principle with well established procedures. Due to the considerable numerical effort required, it is worthwhile to analyze whether any simplification may be introduced by taking into account the specific application we have in mind. In particular, we would like to uncouple the thermal problem by neglecting the first and third term of the rhs of eq.(23). This seems justified everywhere in the repository except very close to the canisters where large hydraulic gradients could be generated.

By reducing the number of independent unknowns to be solved simultaneously, it is possible to introduce the above discretized model into an already developed general purpose program for non-linear stress analysis. Work along these lines is currently in progress.

4. CONCLUSIONS

In the paper coupled, non-linear thermal, hydraulic and mechanical properties of clays have been presented and a mathematical model has been described. The model has been formulated on the basis of a preliminary experimental data. Systematic laboratory studies are now in progress guided by the above theory. Note, that some traditional simplifications of Soil Mechanics should be renounced and modifications are called for in existing software to allow implementation of the model. It may be seen for example that water and soil compressibilities have to be taken into account for undrained conditions, due to pronounced thermal expansion of water.

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where

$$\underline{B}_f = \begin{bmatrix} \frac{\partial \underline{N}}{\partial x} \\ \frac{\partial \underline{N}}{\partial y} \end{bmatrix}$$

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with

$$\underline{f} = \left[\int_A \underline{B}_s^T \right]$$

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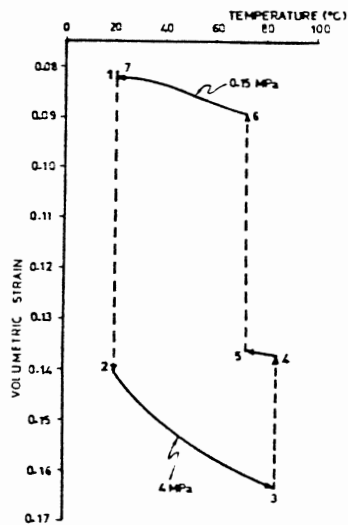


Fig. 1

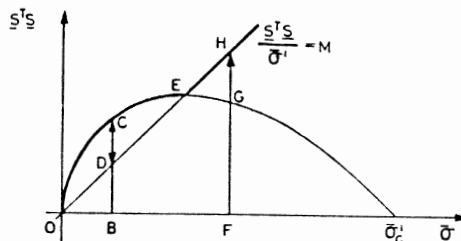


Fig. 2

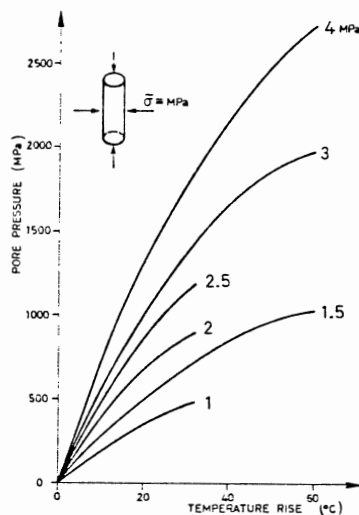


Fig. 3

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TRANSIENT AND
CONSTRUCTION

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ABSTRACT

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