MECHANICAL STABILITY OF BENTONITE BUFFER SYSTEM FOR HIGH LEVEL NUCLEAR WASTE

Antti Lempinen
Helsinki University of Technology
Laboratory of Theoretical and Applied Mechanics

In STUK this study was supervised by **Esko Eloranta**

ABSTRACT

According to present plans, high level nuclear waste in Finland is going to be disposed of in bedrock at a depth of several hundred metres. The spent fuel containers will be placed in boreholes drilled in the floors of deposition tunnels with engineered clay buffer, which is made of bentonite blocks. The tunnels will to be filled with a mixture of bentonite and crushed rock.

Because of the weight of the container and the swelling pressure of the bentonite, there is a possibility that the multibarrier system of the depository is not mechanically stable: the container may move significantly in the bentonite buffer.

For stability calculations a thermomechanical model for compressed bentonite is needed. In this paper a thermomechanically consistent model for reversible processes for swelling clays is presented.

Preliminary calculations were performed. They show that uncertainty in material parameter values causes significantly different results. Therefore, measurements that are consistent with the model are needed.

TIIVISTELMÄ

Nykyisten suomalaisten suunnitelmien mukaan korkeaktiivinen ydinjäte tullaan sijoittamaan perus-kallioon useiden satojen metrien syvyyteen. Ydinjätesäiliöt asetetaan sijoitustunnelien lattiaan porat-tuihin reikiin bentoniittipuskurin ympäröiminä. Sijoitustunnelit täytetään bentoniitin ja kivimurskeen sekoituksella.

Koska ydinjätesäiliö on painava ja bentoniitti on paisuva savi, on mahdollista, että loppusijoituksessa käytettävä puskurisysteemi ei ole mekaanisesti stabiili: ydinjätesäiliöt saattavat liikkua merkittävästi bentoniitin sisällä.

Stabiilisuuslaskelmia varten tarvitaan termomekaaninen malli, joka kuvaa bentoniitin käyttäytymis-tä. Tässä raportissa esitetään termomekaanisesti konsistentti malli paisuvien savien reversiibeleille prosesseille.

Alustavat numeeriset laskut osoittavat, että epävarmuus materiaaliparametrien arvoista aiheuttaa huomattavia poikkeamia laskutuloksiin. Tämän vuoksi on tärkeää tehdä mittauksia, jotka ovat konsis-tentteja termomekaanisen mallin kanssa.

CONTENTS

PREFACE

The present plans of using bentonite as a buffer material in the deposition holes around spent fuel canisters and in tunnels with a mixture of rock crush contain many problems that are not fully treated in the literature so far. Because the swelling characteristics of bentonite is dependent on many factors, and especially because the swelling pressures in the deposition holes and in the tunnels differ greatly from each other there arises doubts that the deposition system will have mechanical instabilities. In Finland the bentonite studies have mainly concentrated so far on chemical and physico-chemical aspects of the bentonite and its function for radionuclide retention. Mechanical aspects have been only dealt with on very general level.

Radiation and Nuclear Safety Authority (STUK) decided to carry out a research to study the mechanical aspects of the bentonite, and especially the mechanical stability of the bentonite buffer system. STUK made a research contract in 1997 with the Laboratory of Theoretical and Applied Mechanics of the Helsinki University of Technology in order to shed light on this problematics.

In the research project it was very soon realized that one of the main problems lies in the material models of bentonite. Therefore, the first part of the project in 1997 concentrated on this topic, and only preliminary modelling results of the mechanical stability could be performed.

This report describes the first part of the project. The second part of Authority's bentonite project has started at the beginning of 1998. The second part will concentrate on the detailed modelling of the stability of bentonite buffer system. Also some experiments have been planned in order to get appropriate material parameter values for the developed material models. The second part belongs to the Publicly Administrated Nuclear Waste Management Research Programme JYT2001. It is financed mainly by the Ministry of Trade and Industry, and it will end at the end of year 2001.

Bentonite buffer is an important component of the multibarrier system, that ensures the safety of spent fuel disposal. The responsibility for the research work needed for the performance assessment of the multibarrier system, rests with the implementator of disposal. The regulator should review the assumptions and data used in performance assessments, and to support this task, verifying studies are often needed. Being crucial to the safety of disposal, the mechanical stability of bentonite buffer was considered as an issue that deserves further clarification through a verifying study.

Esko Eloranta   *Esko Ruokola*

LIST OF SYMBOLS

α	thermal expansion coefficient
α_K	thermal expansion coefficient of fluid K
ε	strain tensor
ε	relative dilation
ε^{ex}	swelling strain
λ	thermal conductivity coefficient
μ	shear modulus
ϕ	porosity
ϕ_K	porous space fraction of phase K
ρ_K	density of phase K
σ	stress tensor
σ	mean tensile stress
ξ	displacement vector
$\mathbf{A}$	thermal stress tensor
$\mathbf{B}_K$	Biot tensors
b_K	Biot coefficients
$\mathbf{C}$	stiffness tensor
C_m	heat capacity
$\mathbf{d}$	strain rate tensor
$\mathbf{d}^*$	virtual strain rate tensor
e	void ratio
$\mathbf{F}$	body force
J	deformation Jacobian
K	bulk modulus
M_{KL}	Biot moduli

m_K	variation in fluid K content
p_K	pressure of fluid K
p_s	suction pressure
$\mathbf{q}$	heat flow vector
r	bulk density
S	entropy density
S_K	entropy mass density of fluid K
S_r	degree of saturation
T	absolute temperature
$\mathbf{T}$	tensile surface force
$\mathbf{V}$	skeleton velocity
$\mathbf{V}^*$	virtual skeleton velocity
$\mathbf{V}_K^r$	relative velocity of phase K
w	water ratio
$\mathbf{w}_K$	relative mass flow vector of fluid K
$\mathbf{X}$	position vector in reference configuration
$\mathbf{x}$	position vector in deformed configuration

Subscripts

g	gas, i.e. air
s	solid
t	trapped interlamellar water
w	free liquid

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1 INTRODUCTION

In Finland, as in many other countries, the high level nuclear waste is planned to be disposed in bedrock at a depth of several hundred metres. The composite copper and steel canisters containing the spent fuel will be placed with engineered clay buffer in boreholes drilled in the floors of deposition tunnels. The clay that forms the buffer is bentonite, which is expansive and considered practically impermeable when saturated. The disposal tunnels are filled with a mixture of sand and bentonite, or crushed rock and bentonite. The planned dimensions of one borehole according to TVO are shown in Figure 1 [Posiva96].

Because of the long activity time of the nuclear waste, it is necessary to carefully examine the stability of this engineered barrier system. One of the stability aspects is that compacted bentonite should retain its high swelling pressure and low permeability properties for thousands of years [Güven90]. Another issue, which is examined in this paper, is the stability of mechanical equilibrium.

A thermomechanical model is needed for calculations. If it is based on models used for non-expansive clays, the corrections for swelling behaviour can lead to thermomechanical inconsistencies. Therefore, the model presented here is based on laws of thermodynamics and observations on the behaviour of bentonite.
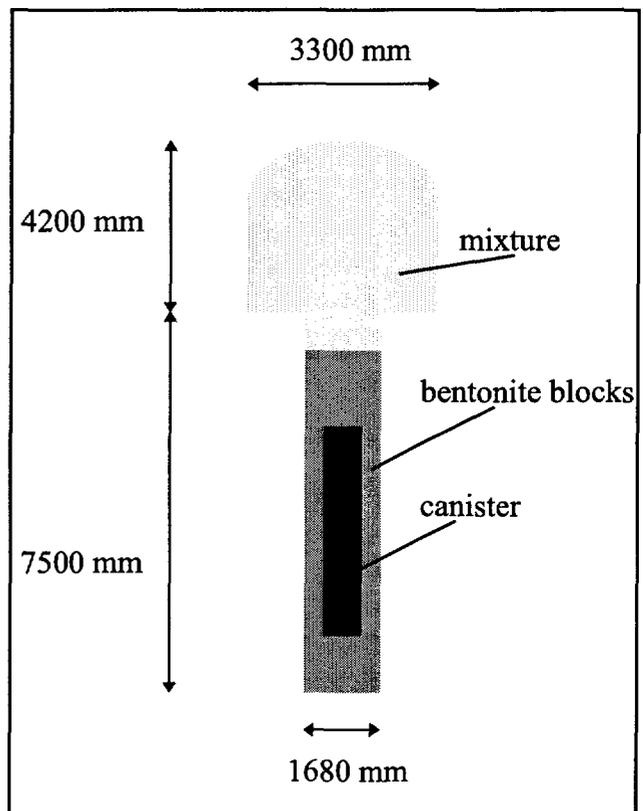

Figure 1. Filled deposition tunnel and the borehole.

2 STRUCTURE OF BENTONITE

Bentonite is an expansive clay, which means that it swells significantly when its water content is increased. The expansive property is caused by montmorillonite, which is the main constituent of bentonite.

Montmorillonites are a group of smectite minerals, and there are two main types: sodium montmorillonite and potassium montmorillonite. The behaviours of Na-montmorillonite and Ca-montmorillonite differ quantitatively, so that there is significant variation in properties of bentonites of different origin.

Bentonite can be considered to have two microstructural levels. First, the mineral platelets form granular elementary particles, where there are porous space between the mineral platelets. Second, the elementary particles form a clay matrix. The intragranular porous space between the mineral platelets is assumed to be always fully saturated with water, even if the intergranular pores are partially saturated, that is, there is no air in the intragranular pores. The active swelling behaviour of bentonite is attributed to the intragranular phenomena, which are observed to be mostly reversible. However, the macroscopic swelling is largely irreversible. This observed fact is caused by clustering of elementary particles, so that there is actually a three-level porous structure: pore space between the mineral platelets, which is filled with water, pore space between the elementary particles and pore space between the clusters of elementary particles. When the clay is strained by the swelling of the elementary particles, the intercluster porous space is irreversibly deformed. The microstructure is drawn schematically in Figure 2. [Gens92]

However, when the clay is compacted with strong enough pressure, the matrix formation is complete in the sense that the bigger pores between the clusters vanish. In this case, the irreversible part of swelling behaviour can be neglected.
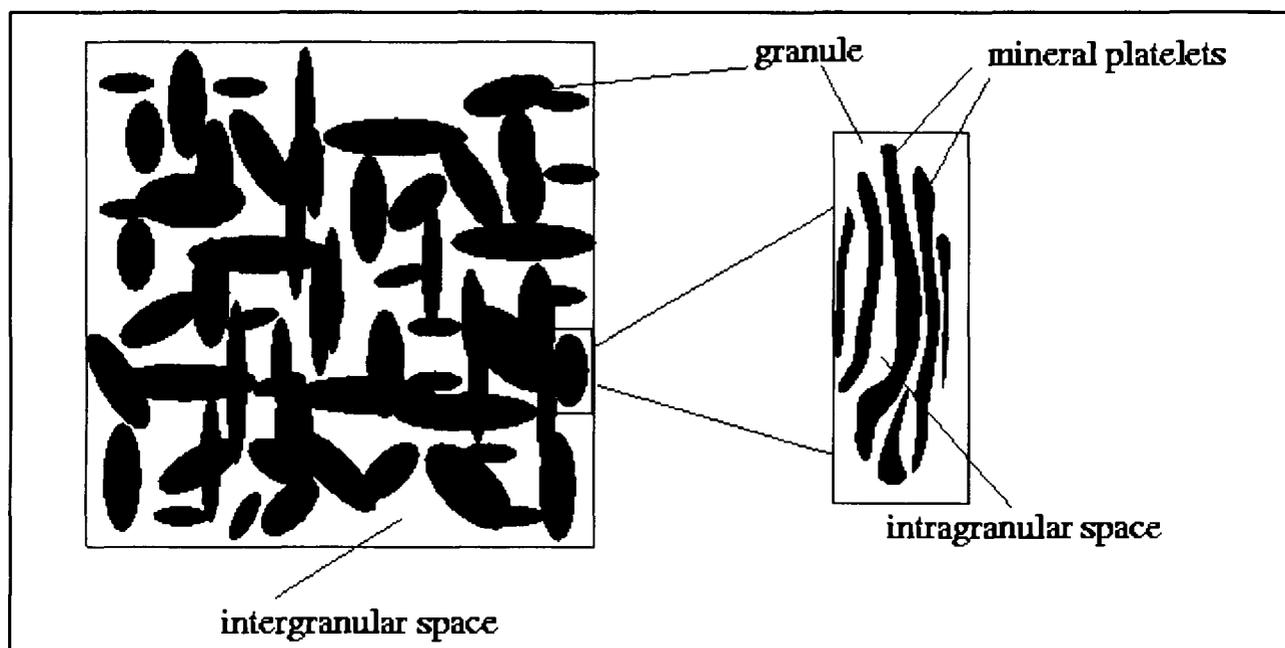

Figure 2. Microstructure of bentonite.

3 DEFINITIONS

3.1 Constituents

With respect to expansive clays, it is assumed that the material consists of four distinct phases: solid matrix (subscript s), which consists of montmorillonite mineral platelets; free liquid (w) in the intergranular porous space; trapped liquid (t), which saturates the intragranular pores; and gas (g), which together with liquid fills the pores between the granules. The gas is a mixture of gases, water is vapour (subscript v), and the liquid is water or brine.

A geometrical point is described here by its location vector in a Cartesian co-ordinate frame of orthonormal basis vectors e_1, e_2, e_3: $x = x_1 e_1 + x_2 e_2 + x_3 e_3$. The Einstein summation convention of repeating tensor indices is also used, so that

$$a_1 b_1 + a_2 b_2 + a_3 b_3 = a_i b_i$$

The solid matrix in an elementary volume $d\Omega = dx_1 dx_2 dx_3$ surrounding a geometrical point x forms the skeleton particle or a material point. The boundary of elementary volume $d\Omega$ is denoted $d\partial\Omega$. Each of the fluid phases in the porous space with the remaining complementary space in the elementary volume form a fluid particle. The volume fraction occupied by the fluid phase $K \in \{w, t, g\}$ in a fluid particle is denoted by ϕ_K. The volume fraction of the porous space is called porosity, denoted by ϕ, so that

$$\phi = \sum_{K \in \{w, t, g\}} \phi_K \qquad (3.1)$$

The density of the solid material that forms the matrix is ρ_s and the density of the fluid K is ρ_K. The density of the whole medium is then

$$r = (1 - \phi)\rho_s + \sum_{K \in \{w, t, g\}} (\rho\phi)_K \qquad (3.2)$$

The skeleton and the fluid particles are assumed to be large enough for the macroscopic properties of the porous medium, which are spatially averaged values over elementary volumes, to be continuous functions of spatial co-ordinates. This means that the scale of elementary volumes is bounded below by the pore size of the material.

3.2 Kinematics

In a reference configuration, a skeleton material point is located by position vector X of components X_α in the Cartesian co-ordinate frame. The volume of the skeleton particle in the reference configuration is $d\Omega_{ref} = dX_1 dX_2 dX_3$. At time t the medium is deformed, and the material point is located by location vector x and its volume is $d\Omega$. This means that the deformation can be expressed as a relation

$$x = x(X, t) \quad x_i = x_i(X_\alpha, t) \qquad (3.3)$$

The deformation gradient P is defined by

$$P = \text{Grad}\, x \quad P_{\alpha i} = \frac{\partial x_i}{\partial X_\alpha} \quad P = P_{\alpha i} e_\alpha \otimes e_i \qquad (3.4)$$

where the symbol $\otimes$ stands for tensorial product.

If an infinitesimal material vector, which is attached to the skeleton, is in reference configuration dX at time t, it can be expressed as

$$dx = dX \cdot P \quad dx_i = dX_\alpha P_{\alpha i} \qquad (3.5)$$

Thus, an elementary volume $d\Omega_{ref}$ transforms into the volume

$$d\Omega = J\, d\Omega_{ref} \qquad (3.6)$$

where J is the Jacobian determinant

$$J = \det(P) \qquad (3.7)$$

Let dX and dX' be two infinitesimal material vectors attached to the skeleton. They are deformed to dx and dx' respectively. Then

$$dx \cdot dx' - dX \cdot dX' = dX \cdot (P \cdot P^T - 1) \cdot dX'$$
$$= dX \cdot (\text{Grad}\xi + (\text{Grad}\xi)^T + \text{Grad}\xi \cdot (\text{Grad}\xi)^T) \cdot dX'$$

(3.8)

where ξ is the displacement vector

$$\xi = x - X$$ (3.9)

If $\|\text{Grad}\xi\| \ll 1$, relation (3.8) can be replaced by

$$dx \cdot dx' - dX \cdot dX' = 2dX \cdot \varepsilon \cdot dX'$$ (3.10)

where ε is the linearized strain tensor

$$2\varepsilon = \text{grad}\xi + (\text{grad}\xi)^T = \frac{\partial \xi_i}{\partial \xi_j} + \frac{\partial \xi_j}{\partial \xi_i}$$ (3.11)

It follows that

$$\frac{d}{dt}[dx \cdot dx'] = 2\,dx \cdot d \cdot dx'$$ (3.12)

where d is the strain rate tensor

$$2d = \text{grad}\,V + (\text{grad}\,V)^T = 2\frac{d\varepsilon}{dt} \quad \text{with} \quad V = \frac{dx}{dt}$$ (3.13)

In the linear case we have also

$$J = 1 + \varepsilon \quad \text{with} \quad \varepsilon = \text{trace}\,\varepsilon = \varepsilon_{ii}$$

so that ε is the relative dilation of the material. This implies

$$\frac{d}{dt}[d\Omega]/d\Omega = \text{trace}\,d = \text{div}\,V$$ (3.14)

The fluid particle movement of fluid K is defined by the fluid mass flow vector with respect to the skeleton w_K. The relative fluid velocity V_K^r of fluid K is defined by

$$w_K = (\rho\phi V^r)_K$$ (3.15)

The trapped fluid is not assumed to form a continuous phase, and therefore it would be ambiguous to define its relative velocity.

3.3 State variables

This thermomechanical model is based on the assumption that every elementary system, that is, the skeleton particle and the fluid particles within the elementary volume, are in thermodynamical equilibrium. This defines an upper bound to the size of elementary volume. This upper bound has to be greater than the lower bound defined by the continuity requirement.

State variables are the physical variables that describe the equilibrium energy state of the elementary systems. Therefore, finding these variables is the link between the macroscopic and microscopic phenomena. State variables cannot be defined without proper knowledge of the basic physical behaviour of the material.

According to general thermodynamics, one of the state variables is the absolute temperature T. Because deformation of an elementary particle needs energy, the strain tensor ε is postulated to be a state variable.

Let ρ_K^0 and ϕ_K^0 be the mass density and the porosity for fluid $K \in \{w, g, t\}$ in the reference configuration, respectively, so that the fluid K mass in an elementary volume is $(\rho^0\phi^0)_K \, d\Omega_{\text{ref}}$. After deformation, the fluid mass of the fluid particle at the same spatial point as the skeleton particle is $(\rho\phi)_K \, d\Omega$. Thus, the variation in fluid K mass content per unit of initial volume of skeleton is defined as

$$m_K = J(\rho\phi)_K - (\rho^0\phi^0)_K$$ (3.16)

Since work is needed to change the fluid mass contents of an elementary particle, variations in fluid mass contents are postulated to be state variables.

The state variables T, ε and m_K are called external variables, because they can be directly measured and they are also the variables that appear in the balance equations. The rest of the state variables cannot be directly measured nor do they appear in balance equations. Therefore, they are called internal state variables. The set of internal state variables ζ includes the plastic or irreversible strain tensor, the irreversible variations in fluid contents and the set of plastic hardening variables.

4 BALANCE EQUATIONS

4.1 Mass balance

It is natural to assume that there is no overall mass creation nor does any mass vanish in the system, i.e.

$$\frac{d}{dt}\int_{\Omega} r\,d\Omega = -\int_{\partial\Omega}(\mathbf{w}_w + \mathbf{w}_g)\cdot\mathbf{n}\,d\partial\Omega \qquad (4.1)$$

for any volume Ω with boundary $\partial\Omega$ and outward normal $\mathbf{n}$. When we assume that there is no mass transformation between the solid mineral and the fluids, (4.1) leads to fluid mass balance equations

$$\begin{aligned}
\frac{dm_w}{dt} + \operatorname{div}\mathbf{w}_w &= \sum_{L\in\{g,t\}}\dot{m}_{L\to w} \\
\frac{dm_g}{dt} + \operatorname{div}\mathbf{w}_g &= \sum_{L\in\{w,t\}}\dot{m}_{L\to g} \\
\frac{dm_t}{dt} &= \sum_{L\in\{w,g\}}\dot{m}_{L\to t}
\end{aligned} \qquad (4.2)$$

where $\dot{m}_{L\to K}$ is the mass transform rate from phase L to phase K such that $\dot{m}_{L\to K} = -\dot{m}_{K\to L}$.

The mass transformation between the gas and the free liquid is caused by condensation of vapour and evaporation of water. Because the equilibrium moisture of the gas depends on the water content and on the temperature, we have

$$\dot{m}_{g\to w} = -(\phi\rho)_g\left(\frac{\partial q_v}{\partial m_w}\frac{dm_w}{dt} + \frac{\partial q_v}{\partial T}\frac{dT}{dt}\right) \qquad (4.3)$$

where q_v is mass fraction of the water vapour in the gas. The mass transformation between the gas and the trapped water can be neglected.

The trapped water content is also assumed to be dependent on water content and on the temperature, so that

$$\dot{m}_{t\to w} = -\left(\frac{\partial m_t}{\partial m_w}\frac{dm_w}{dt} + \frac{\partial m_t}{\partial T}\frac{dT}{dt}\right) \qquad (4.4)$$

It is important to note that the temperature dependence limits the validity of bentonite as buffer material to temperatures below 100°C [Ma92].

4.2 Momentum balance

As usual, we assume that the tensile surface forces $\mathbf{T}$ acting on the surface $\partial\Omega$ of any volume of the material Ω can be derived from the Cauchy stress tensor σ by

$$\int_{\partial\Omega}\mathbf{T}\,d\partial\Omega = \int_{\partial\Omega}\mathbf{n}\cdot\sigma\,d\partial\Omega = \int_{\Omega}\operatorname{div}\sigma\,d\Omega \qquad (4.5)$$

The instantaneous momentum balance, with respect to all matter included in any domain Ω, reads

$$\frac{d}{dt}\int_{\Omega}\left(r\mathbf{V} + \sum_{K\in\{w,g\}}\mathbf{w}_K\right)d\Omega = \int_{\Omega}(r\mathbf{F} + \operatorname{div}\sigma)\,d\Omega \qquad (4.6)$$

where $\mathbf{F}$ is a body force such as gravity, and the angular momentum balance reads

$$\frac{d}{dt}\int_{\Omega}\mathbf{x}\times\left(r\mathbf{V} + \sum_{K\in\{w,g\}}\mathbf{w}_K\right)d\Omega = \int_{\Omega}\mathbf{x}\times(r\mathbf{F} + \operatorname{div}\sigma)\,d\Omega \qquad (4.7)$$

Together the balance equations (4.6) and (4.7) give the symmetry of the stress tensor

$$\sigma^T = \sigma \qquad (4.8)$$

In this context we assume that external load changes so slowly that the system is always in equilibrium and we neglect all the acceleration terms. Therefore, because equation (4.6) is valid for any volume Ω, substitution of the mass balance gives the local form of momentum balance as

$$\operatorname{div}\sigma + r\mathbf{F} = 0 \qquad (4.9)$$

The weak form of the momentum balance reads

$$\forall \mathbf{V}^* \in \mathbf{V} \quad \int_\Omega \left[\mathbf{d}^* : \sigma - r\mathbf{V}^* \cdot \mathbf{F} \right] d\Omega = \int_{\partial\Omega} \mathbf{n} \cdot \sigma \cdot \mathbf{V}^* \, d\partial\Omega$$

$$(\mathbf{d}^* : \sigma = d_{ij}^* \sigma_{ij}) \tag{4.10}$$

where $\mathbf{V}$ is the set of all possible skeleton velocity fields $\mathbf{V}^*$ in Ω and

$$\mathbf{d}^* = \frac{1}{2} \left(\text{grad}\,\mathbf{V}^* + (\text{grad}\,\mathbf{V}^*)^\mathsf{T} \right)$$

is the virtual dilation rate.

4.3 Thermal equation

The first and second laws of thermodynamics can be combined to form an equation called the thermal equation. It describes the thermal balance of the system. When the convective terms are neglected, the local form of the thermal equation for thermoelastic evolutions can be written in the form

$$T \frac{dS}{dt} = -\text{div}\,\mathbf{q} \tag{4.11}$$

where S is the entropy density and $\mathbf{q}$ is the heat flow.

5 STATE EQUATIONS

5.1 General reversible state equations

In this analysis we are interested in deformations that are caused by the weight of the waste overpack and the swelling of the bentonite in the borehole. The pressures involved seem to be smaller than the preconsolidation pressure of the bentonite blocks, so we assume that the deformations are elastic. In that case, any member of the so-called normal set of state variables

$$\left\{\varepsilon, m_w, m_g, T\right\}$$

can be changed in any direction while the other state variables remain unchanged. This, with the laws of thermodynamics, leads to general state equations

$$\sigma = \frac{\partial \Psi}{\partial \varepsilon} \tag{5.1}$$

$$g_w = \frac{\partial \Psi}{\partial m_w} + \frac{\partial m_t}{\partial m_w}\frac{\partial \Psi}{\partial m_t} \tag{5.2}$$

$$g_g = \frac{\partial \Psi}{\partial m_g} \tag{5.3}$$

$$S = -\frac{\partial \Psi}{\partial T} - \frac{\partial m_t}{\partial T}\frac{\partial \Psi}{\partial m_t} \tag{5.4}$$

[Coussy95], where

Ψ is the free energy density available for mechanical work,

g_w, g_g are the mass weighted densities of enthalpies of free liquid and gas, respectively,

S is the entropy density.

Differentiation of equations (5.1)–(5.4) gives the incremental state equations for the stress tensor, free liquid pressure p_w, gas pressure p_g and entropy density:

$$d\sigma = \mathbf{C}:d\varepsilon - \sum_{K=w,g}(\mathbf{MB})_K\frac{dm_K}{\rho_K} - \mathbf{A}\,dT \tag{5.5}$$

$$dp_w = -(\mathbf{MB})_w:d\varepsilon + \sum_{K=w,g}\mathbf{M}_{wK}\frac{dm_K}{\rho_K} + 3(\alpha M)_w\,dT \tag{5.6}$$

$$dp_g = -(\mathbf{MB})_g:d\varepsilon + \sum_{K=w,g}\mathbf{M}_{gK}\frac{dm_K}{\rho_K} + 3(\alpha M)_g\,dT \tag{5.7}$$

$$dS = \mathbf{A}:d\varepsilon - \sum_{K=w,g}\left((3\alpha M)_K\frac{dm_K}{\rho} - S_K dm_K\right) + \frac{C_m}{T}\,dT \tag{5.8}$$

where

$\mathbf{C}$ is the undrained stiffness tensor,

$\mathbf{B}_w, \mathbf{B}_g$ are the Biot tensors,

$\mathbf{M}_w, \mathbf{M}_g$ are the Biot moduli,

$(\mathbf{MB})_K = \sum_{L=w,g}\mathbf{M}_{KL}\mathbf{B}_L$,

$\mathbf{A}$ is the undrained thermal stress tensor,

α_w, α_g are the thermal expansion coefficients of free liquid and gas, respectively,

$(\alpha M)_K = \sum_{L=w,g}\alpha_L\mathbf{M}_{LK}$,

C_m is the undrained heat capacity,

S_w, S_g are the mass weighted entropy densities of free liquid and gas, respectively.

Furthermore, the coefficients above are related by the Maxwell symmetry relations

$$\frac{\partial \mathbf{C}}{\partial m_K} = -\frac{\partial}{\partial \varepsilon}\left(\frac{(\mathbf{MB})_K}{\rho_K}\right) \tag{5.9}$$

$$\frac{\partial}{\partial m_L}\left(\frac{(\mathbf{MB})_K}{\rho_K}\right) = \frac{\partial}{\partial m_K}\left(\frac{(\mathbf{MB})_L}{\rho_L}\right) = \frac{\partial}{\partial \varepsilon}\left(\frac{\mathbf{M}_{KL}}{\rho_K \rho_L}\right) \tag{5.10}$$

$$\frac{\partial \mathbf{C}}{\partial T} = -\frac{\partial \mathbf{A}}{\partial \varepsilon} \qquad (5.11)$$

$$\frac{\partial}{\partial m_L}\left(\frac{3(\alpha M)_K}{\rho_K} - S_K\right) = \frac{\partial}{\partial T}\left(\frac{M_{KL}}{\rho_K \rho_L}\right) \qquad (5.12)$$

$$\frac{\partial \mathbf{A}}{\partial T} = \frac{\partial}{\partial \varepsilon}\left(\frac{C_m}{T}\right) \qquad (5.13)$$

$$\frac{\partial}{\partial T}\left(\frac{3(\alpha M)_K}{\rho_K} - S_K\right) = \frac{\partial}{\partial m_K}\left(\frac{C_m}{T}\right) \qquad (5.14)$$

$$\frac{\partial}{\partial T}\left(\frac{(MB)_K}{\rho_K}\right) = \frac{\partial \mathbf{A}}{\partial m_K} = -\frac{\partial}{\partial \varepsilon}\left(\frac{3(\alpha M)_K}{\rho_K} - S_K\right) \qquad (5.15)$$

$$K, L \in \{\mathsf{w}, \mathsf{g}\}.$$

When we eliminate the variations in fluid contents in equations (5.5)–(5.7), we get the incremental stress state equation in form

$$d\sigma + \sum_{K=w,g} \mathbf{B}_K dp_K = \mathbf{C}^0 : d\varepsilon - \mathbf{A}^0 dT \qquad (5.16)$$

where

$$\mathbf{C}^0 = \mathbf{C} - \sum_{K=w,g} \mathbf{B}_K \otimes (MB)_K$$

is the drained stiffness tensor

$$\mathbf{A}^0 = \mathbf{A} + \sum_{K=w,g} 3(\alpha M)_K \mathbf{B}_K$$

is the drained thermal stress tensor.

Equation (5.16) can be interpreted to be derived from (5.1) so, that the free liquid and gas pressures are state variables instead of variations in free liquid and gas contents. This gives additional Maxwell symmetry relations

$$\frac{\partial \mathbf{C}^0}{\partial p_K} = -\frac{\partial \mathbf{B}_K}{\partial \varepsilon} \qquad (5.17)$$

$$\frac{\partial \mathbf{B}_L}{\partial p_K} = \frac{\partial \mathbf{B}_K}{\partial p_L} \qquad (5.18)$$

$$\frac{\partial \mathbf{A}^0}{\partial p_K} = \frac{\partial \mathbf{B}_K}{\partial T} \qquad (5.19)$$

$$\frac{\partial \mathbf{C}^0}{\partial T} = -\frac{\partial \mathbf{A}^0}{\partial \varepsilon} \qquad (5.20)$$

where $K, L \in \{\mathsf{w}, \mathsf{g}\}$.

5.2 Isotropic state equations

When the material is isotropic, there are no preferential directions in the material and we can write

$$(\mathbf{C})_{ijkl} = (K - 2\mu/3)\delta_{ij}\delta_{kl} + 2\mu\delta_{ik}\delta_{jl} \qquad (5.21)$$

$$(\mathbf{C}^0)_{ijkl} = (K^0 - 2\mu/3)\delta_{ij}\delta_{kl} + 2\mu\delta_{ik}\delta_{jl} \qquad (5.22)$$

$$\mathbf{B}_K = b_K \mathbf{1} \qquad (5.23)$$

$$\mathbf{A} = \alpha K \mathbf{1} \qquad (5.24)$$

$$\mathbf{A}^0 = \alpha^0 K^0 \mathbf{1} \qquad (5.25)$$

where

K, K_0 are the undrained and drained bulk moduli, respectively,

μ is the shear modulus,

α, α^0 are the undrained and drained thermal dilation coefficients, respectively.

Thus, in the isotropic case the incremental state equations can be written in form

$$d\sigma = (K - 2\mu/3)d\varepsilon \mathbf{1} + 2\mu\varepsilon - \sum_{K=w,g} (Mb)_K \mathbf{1}\frac{dm_K}{\rho_K} - \alpha K \mathbf{1} dT \qquad (5.26)$$

or

$$d\sigma + \sum_{K=w,g} b_K \mathbf{1} dp_K = (K^0 - 2\mu/3)d\varepsilon \mathbf{1} + 2\mu\varepsilon - \alpha^0 K^0 \mathbf{1} dT \qquad (5.27)$$

$$dp_w = -(Mb)_w : d\varepsilon + \sum_{K=w,g} M_{wK}\frac{dm_K}{\rho_K} + 3(\alpha M)_w \, dT \qquad (5.28)$$

$$dp_g = -(Mb)_g : d\varepsilon + \sum_{K=w,g} M_{gK}\frac{dm_K}{\rho_K} + 3(\alpha M)_g \, dT \qquad (5.29)$$

$$dS = \alpha K \, d\varepsilon - \sum_{K=w,g}\left((3\alpha M)_K\frac{dm_K}{\rho} - S_K dm_K\right) + \frac{C_m}{T} dT \qquad (5.30)$$

6 CONDUCTION EQUATIONS

The flow of fluids w_K and the thermal flow q are transport phenomena, that can make the evolutions of porous medium irreversible even when the deformations are reversible. The fluid flows are restricted by the fluid mass balance equations and the thermal flow follows the thermal equation.

The hypothesis of normality of these dissipative mechanisms with assumption of no direct coupling lead to usual conduction equations

$$\frac{K_K}{\mu_K}\frac{w_K}{\rho_K} = -\text{grad}\, p_K + \rho_K g \quad K = w,g \tag{6.1}$$

$$q = -\lambda\, \text{grad}\, T \tag{6.2}$$

where K_K and μ_K are the permeability and viscosity of fluid K, respectively, and λ is the thermal conductivity coefficient [Coussy95].

The parameters K_K and λ depend generally on the state variables, but not their gradients nor their change rates.

ed with different initial temperatures and deformations, the dependence of the Biot coefficients on temperature and deformation can be determined. If the coefficients are functions of pressures only, as one could expect at least in the framework of small deformations, an effective stress can be defined as

$$\sigma^* = \sigma - \Pi 1 \quad \text{with} \quad d\Pi = \sum_{K=w,g} b_K \, dp_K \tag{7.9}$$

Note that Maxwell relation (5.17) gives

$$b_K = b_K(p_w, p_g) \Rightarrow K^0 = K^0(\varepsilon, T) \tag{7.10}$$

Now, equation (5.27) becomes

$$d\sigma^* = (K^0 - 2\mu/3)d\varepsilon 1 + 2\mu\varepsilon - \alpha^0 K^0 1 \, dT \tag{7.11}$$

Usually, in models describing saturated clay behaviour the Therzaghi assumption is used. It states that increment of the liquid pressure and increment of the total pressure $p = -\sigma$ have the same effect, so that

$$b_w = 1 \quad \text{and} \quad \Pi = p_w$$

The Therzaghi assumption is often extended to models for the unsaturated state as

$$\Pi = S_r p_w + (1 - S_r)p_g = -S_r p_s + p_g \tag{7.12}$$

It is intuitively clear that a model with definition (7.12) cannot describe the pressure caused by the swelling behaviour. This flaw is often corrected with swelling strain ε^{ex}, also called moisture swelling, so that (7.11) is replaced with

$$d\sigma^* = (K^0 - 2\mu/3)d\varepsilon^* 1 + 2\mu\varepsilon^* - \alpha^0 K^0 1 \, dT \tag{7.13}$$

where ε^* is the effective strain

$$\varepsilon^* = \varepsilon + \varepsilon^{ex} 1 \tag{7.14}$$

In this case the definition of effective strain and the correct expressions for Biot coefficients for expansive clays are related by

$$b_w = \left(S_w + p_s \frac{dS_w}{dp_s} \right) + K^0 \frac{\partial \varepsilon^{ex}}{\partial p_s} \tag{7.15}$$

$$b_w = 1 - \left(S_w + p_s \frac{dS_w}{dp_s} \right) - K^0 \frac{\partial \varepsilon^{ex}}{\partial p_s} \tag{7.16}$$

Table I. Swelling Pressure.

Degree of saturation S_r	Swelling strain ε^{ex}
0.1	0.111
0.2	0.111
0.3	0.105
0.4	0.085
0.5	0.059
0.6	0.025
0.7	0.0
0.8	−0.017
0.9	−0.035
1.0	−0.052

If we assume the definition of effective stress to be consistent with (7.9), relation (7.10) gives

$$\frac{\partial}{\partial T}\left(K_0 \frac{\partial \varepsilon^{ex}}{\partial p_s} \right) = 0 \quad \text{and} \quad \frac{\partial}{\partial \varepsilon}\left(K_0 \frac{\partial \varepsilon^{ex}}{\partial p_s} \right) = 0 \tag{7.17}$$

and we can use as a definition for effective stress expression

$$\sigma^* = \sigma + (-S_r p_s + p_g)1 - K^0(\varepsilon^0, T^0)\varepsilon^{ex}(p_s, \varepsilon^0, T^0)1 \tag{7.18}$$

where the bulk modulus and the swelling strain curve are measured at a reference temperature T^0 with a constant reference strain ε^0.

In Table I are the swelling strain values given in [Börgesson95b].

7.3 Porous elasticity

According to [Börgesson95a], under isothermal conditions, the change of logarithm of the mean effective stress $\sigma^* = 1/3 \, \text{trace}(\sigma^*)$ of preconsolidated bentonite is proportional to the logarithm of reversible void ratio $e = \phi/(1-\phi)$, that is

$$\log \frac{e}{e_{ref}} = -\beta \log \frac{\sigma^*}{\sigma_{ref}} \quad \text{or} \quad e = e_{ref}\left(\frac{\sigma^*}{\sigma_{ref}} \right)^{-\beta} \tag{7.19}$$

where β, e_{ref} and σ_{ref} are constants. The values for Na-bentonite MX80 preconsolidated at 100 MPa are given to be

$$\beta = 0.187$$

$$e_{ref} = 1.0$$

$$\sigma_{ref} = 2.0 \text{ MPa}$$

In order to see the how equation (7.19) is related to the more often used porous elasticity (see e.g. [ABAQUS]), it can be rewritten as

$$de = -\beta e \, d\left(\log \frac{\sigma^*}{\sigma_{ref}}\right) = \frac{-\beta e \, d\sigma^*}{\sigma^*} \qquad (7.20)$$

where the porous bulk modulus $\kappa = \beta e$ can be considered constant in small deformations.

Because the mass content of the solid per initial volume does not change, we have, assuming an incompressible mineral,

$$d(J\rho_s\phi_s) = \rho_s(1-\phi)d\varepsilon - \rho_s \, d\phi = 0 \qquad (7.21)$$

Integration of equation (7.21) gives

$$e = (e_0 + 1)\exp(\varepsilon) - 1 \qquad (7.22)$$

where e_0 is the void ratio of the unstrained state. Substitution of (7.22) into (7.19) and differentiation gives

$$d\sigma^* = -\frac{\sigma_{ref}(e_0 + 1)}{\beta e_{ref}}\left(\frac{(e_0 + 1)\exp(\varepsilon) - 1}{e_{ref}}\right)^{-(1+\beta)/\beta} \exp(\varepsilon) d\varepsilon$$

$$= -\frac{\sigma^*(e_0 + 1)}{\beta e_{ref}}\left(\frac{(e_0 + 1)\exp(\varepsilon) - 1}{e_{ref}}\right)^{-1} \exp(\varepsilon) d\varepsilon$$

$$(7.23)$$

We cannot identify the drained bulk modulus as

$$K^0 = -\frac{\sigma_{ref}(e_0 + 1)}{\beta e_{ref}}\left(\frac{(e_0 + 1)\exp(\varepsilon) - 1}{e_{ref}}\right)^{-(1+\beta)/\beta} \exp(\varepsilon)$$

$$= -\frac{\sigma^*(e_0 + 1)}{\beta e_{ref}}\left(\frac{(e_0 + 1)\exp(\varepsilon) - 1}{e_{ref}}\right)^{-1} \exp(\varepsilon)$$

$$(7.24)$$

and, if we know the Poisson ratio ν, the shear modulus as

$$\mu = \frac{3}{2}\frac{(1-2\nu)}{(1-\nu)}K^0 \qquad (7.25)$$

In the range of small deformations we can approximate the drained bulk modulus as

$$K^0 \approx -\frac{\sigma_{ref}(e_0 + 1)}{\beta e_{ref}}\left(\frac{e_0(1+\varepsilon) + \varepsilon}{e_{ref}}\right)^{-(1+\beta)/\beta} d\varepsilon \qquad (7.26)$$

When we take the temperature changes into account, we replace the volume dilation in (7.24) with

$$\varepsilon - \alpha_0 \, \Delta T$$

where ΔT is the temperature change from the reference state and the thermal dilation coefficient α_0 is assumed to be constant.

8 NUMERICAL EXAMPLES

The preliminary numerical calculations presented here show no signs of mechanical instability, because they are simplified isothermal axisymmetric cases. However, they show that the uncertainty of parameter values leads to significantly different results.

The calculations were performed with a general purpose finite element program, described in [Freund94], which is linked to Scilab, an application for matrix computations [Scilab].

Because of the difference in scales, the radial and vertical displacements were solved separately, and the bulk modulus was taken from the previous time step. The finite element mesh of 6-node triangular elements that was used in the calculations is in Figure 3.

The calculations were performed with uniformly increasing saturation starting from $S_r = 0.7$. The waste overpack was assumed to be 6000 kgm^{-3} heavier than the bentonite, the density of which was given to be 1900 kg m^{-3}.

The properties of the mixture of bentonite and crushed rock are so far unknown, because there are no specifications yet. Therefore, the mixture was simply modelled as bentonite with no swelling property. This is, of course, an oversimplification.

According to equation (7.19), the mean effective stress at void ratio $e = 0.7$ is -13.4 MPa. When these are used as the reference values, the calculations show that the waste overpack is lifted by the reversible swelling 1.2 mm.

In [Johannesson95], the tensile strength, that is the maximum tensile mean stress that causes a reversible deformation is given to be approximately 1.3 MPa. According to equation (7.4) and Table I, the effective mean pressure at $e = 0.7$, $S_r = 0.7$ is 542 kPa. When the sum of these is used as the reference pressure, i.e. $\sigma_{ref} = -1.84$ MPa, the calculations show that the overpack is lifted by the reversible swelling 7.3 mm, about six times as much as according to the previous calculation.
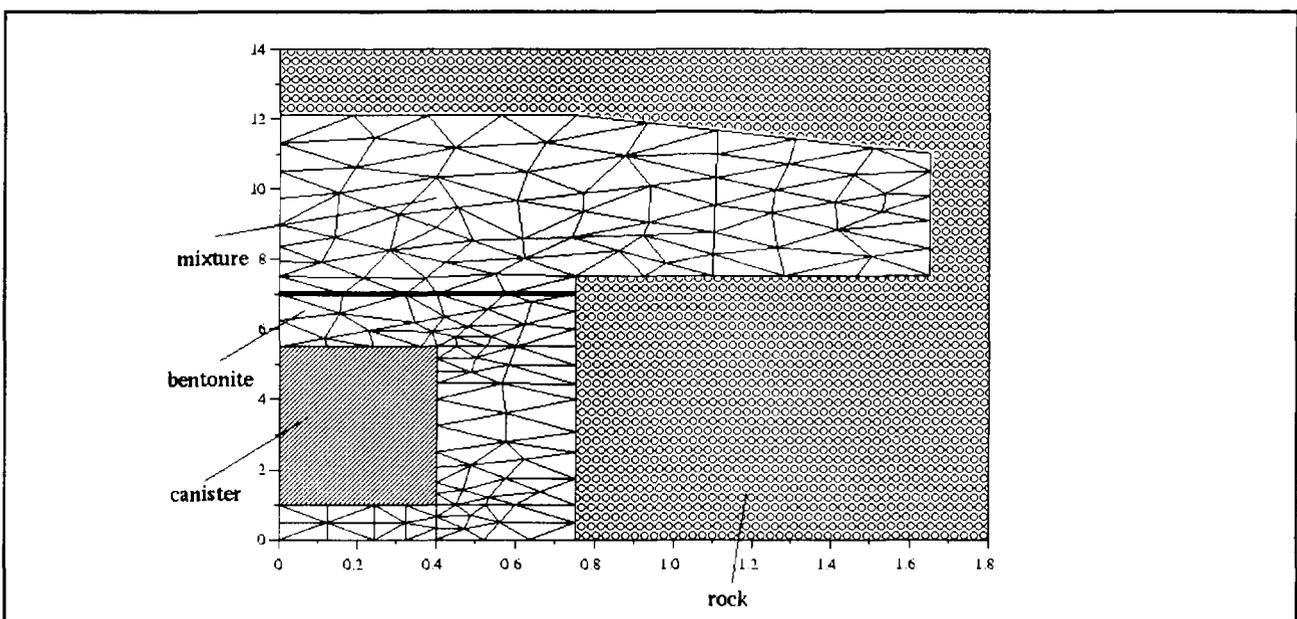

Figure 3. *Finite element mesh.*

9 CONCLUSIONS

The deformation of the calculation with σ_{ref} = −1.84 MPa is shown in Figure 4. No conclusions about the mechanical instability can be made, although there are no signs of such behaviour. The mechanical stability calculations need axially asymmetric perturbed analysis, but the difference in calculated overpack elevations shows that reliable results require more accurate measurements for parameter values.

The basic difficulty with the parameter values given in literature is that they are often calculated from measurements made for thermodynamically inconsistent models. The models are usually modified from material models, which can not describe the expansivity property of bentonite. The corrective terms can become very complex or the given information is inadequate: for example, to use the swelling strain, one needs the correct bulk modulus of the reference state, when only suction dependence is given.
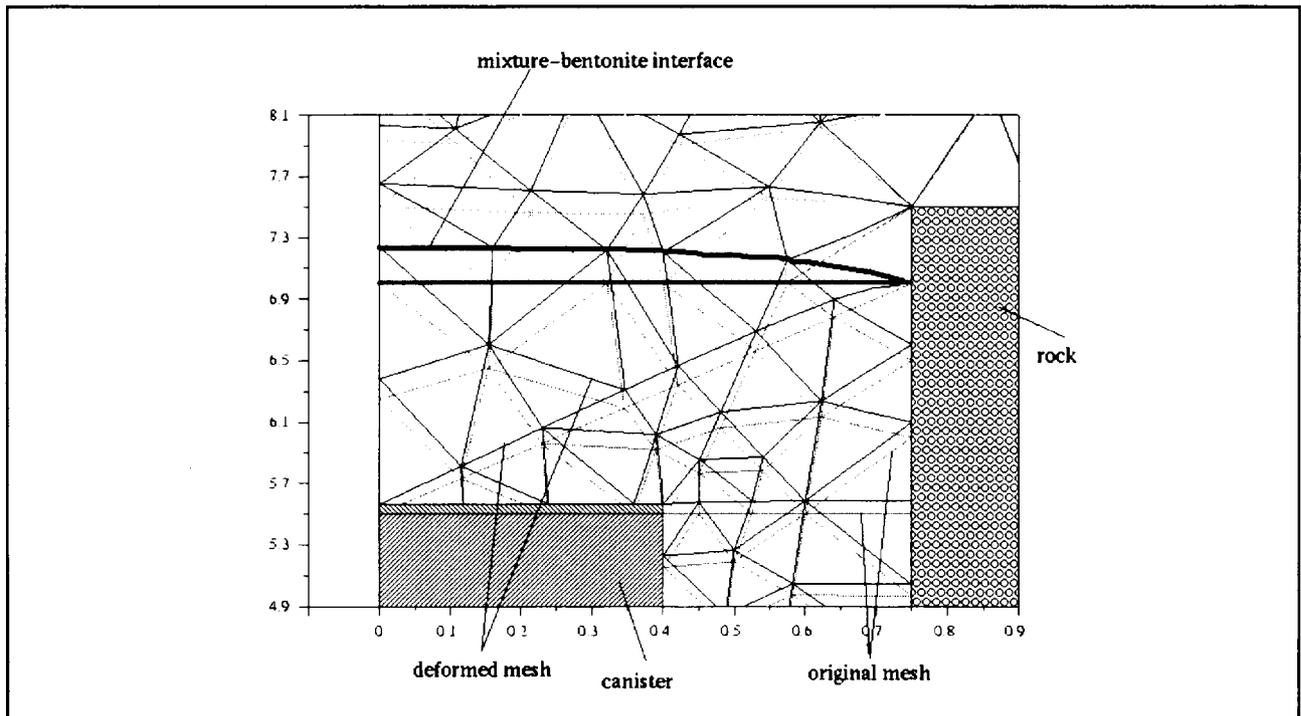

Figure 4. Calculated deformation, magnification factor 10.

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