Numerical Implementation of a Viscoplastic Constitutive Equation for the Modelling of Tailings Heaps

Implémentation Numérique de la Loi Constitutive Viscoplastique pour le Modelage des Terrils

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ABSTRACT
For the modelling and simulation of the time dependent material behavior of rock salt a viscoplastic constitutive equation was developed and implemented into a Finite-Element system at the Institute and the Laboratory of Geotechnics of Technische Universität Darmstadt. The time dependent, three-dimensional constitutive equation is applied for the geotechnical modelling of tailings heaps with heights up to 200 m consisting of deposited rock salt. The deposited rock salt is a waste product of the potassic fertilizer production. The paper shows the theoretical basis, the structure, the implementation and the application of the implemented constitutive equation with the name CAPCREEP.

RÉSUMÉ
Pour la modélisation et la simulation du comportement matériel dépendant du temps du sel gemme une équation constitutive viscoplastique a été développée et mise en application dans un Système d' Eléments Finis à l'Institut et Laboratoire de Géotechnique de Technische Universität Darmstadt. L'équation constitutive tridimensionnelle dépendant du temps est utilisée pour le modelage géotechnique des terrils avec des hauteurs allant jusqu'à 200 m se composant des dépôts du sel gemme. Le sel gemme déposé est un produit de déchets de production d'engrais potassique. L'article montre la base théorique, la structure, l'exécution et l'application de l'équation constitutive mise en application sous le nom de CAPCREEP.

Keywords: constitutive equation, viscoplasticity, rock salt, tailings heap, return-mapping-algorithm

1 INTRODUCTION

The chemical elements potassium, magnesium, sodium and sulphur are for plants, animals and people indispensable mineral substances. Mined potash salts contain the mentioned mineral substances and hence are refined in mechanized processes to fertilizers. Potash salts are materials with a high content of potassium compounds.

The residue not usable at the potash fertilizer production and consisting mainly of rock salt is deposited in granular form on tailings heaps (Lukas 2002).

Figure 1. Tailings heaps close to Magdeburg in Germany.

Such tailings heaps could be found for example in the middle and the east of Germany. For the modelling of such tailings heaps an efficient three-dimensional viscoplastic numerical constitutive equation is essential. Therefore the materialroutine CAPCREEP was developed and implemented in the Finite-Element system ABAQUS via a special interface.

2 MATERIAL PROPERTIES OF ROCKSALT

Rock salt forms crystals in the solid state. In the chemical sense rock salt consists of ion compounds between positively charged sodium ions and negatively charged chlorine anions (Plewinsky et al. 2008).

The high viscoplastic deformability of rock salt is caused by deviations of the pure crystal in form of lattice disturbances. The lattice disturbances allow the flow of different microphysical distortion mechanisms like dislocation glide, dislocation climb and diffusional creep, which are often based on diffusion processes (Munson and Dawson 1984).

The viscoplastic properties of rock salt are macroscopically analyzed at the Institute and the Laboratory of Geotechnics of Technische Universität Darmstadt by performing around 200 triaxial tests. Primarily triaxial compression tests were driven in the form of strain-controlled fracture tests and load-controlled creep tests without fracture in dependence of the compaction state. In a creep test the deformations are investigated with progressive time under constant stress state.

The macroscopic deformation of a rock salt specimen is time and temperature dependent and consists of an instantaneously elastic and plastic part and a viscoplastic part. Instantaneous deformations are independent of time (Figure 2).

The instantaneously plastic deformations depend on the strain rate and hence lead to different yield criterions (Langer 1985). By increasing the temperature the viscoplastic deformation rate goes up by otherwise constant stress state (Comte 1965).

Granular rock salt shows beside the shear strain also a volumetric strain and differs with it from intact rock salt which deforms only by constant volume. For a constant stress state the

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density of granular rock salt fades to the grain density of intact rock salt due to compaction (Zhang et al. 1996).

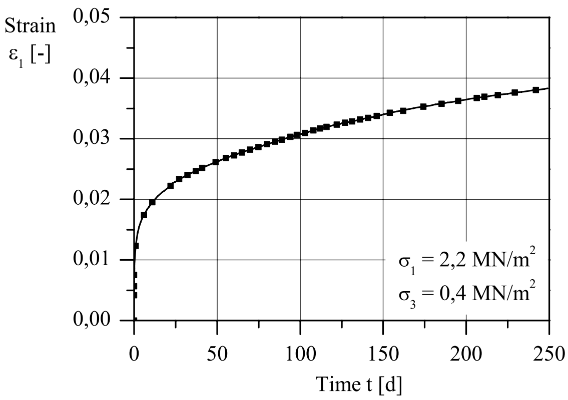

Figure 2. Triaxial creep test.

The compaction state affects also the strength of the granular rock salt. Specimens with low density yield less value for the shear strength then specimens with a higher density (Kappei 1987).

3 CONSTITUTIVE EQUATION

The described constitutive equation was founded on the basis of an extended laboratory test program at the Institute and the Laboratory of Geotechnics of Technische Universität Darmstadt by Boley (1999) and enhanced by Wachter (2009).

The constitutive equation is focussed on the modelling for the research of tailings heaps consisting of granular rock salt. It is formulated as a superposition model and couples additively the different deformation parts.

The elastic deformations are realized by use of HOOKE´s law. Thereby a dependence of the elasticity modulus on the compaction state is considered.

The viscoplastic stationary strain rate is modeled by using the following equation with the material and the regression parameters B_i respectively:

$$\dot{e}^{vpl,st} = e^{-\frac{Q}{R\cdot T}} \cdot \left(B_1 \cdot s + \left[B_2 \cdot s^{B_4} - B_1 \cdot s\right] \cdot \tanh\left(B_3 \cdot s\right)\right) \qquad (1)$$

Equation (1) connects the scalar strain rate $\dot{e}$ with the deviatoric stress s and the temperature T (Katzenbach et al. 2000). The deviatoric stress is defined as the norm of the deviatoric stress tensor:

$$s = \sqrt{s_{ij}\, s_{ij}}\ ,\ s_{ij} = \sigma_{ij} - \frac{\sigma_{kk}}{3}\,\delta_{ij} \qquad (2)$$

The scalar shear strain e is calculated by means of the strain tensor e_{ij} and the volumetric strain ε_{kk} as follows:

$$e = \sqrt{e_{ij}\, e_{ij}}\ ,\ e_{ij} = \varepsilon_{ij} - \frac{\varepsilon_{kk}}{3}\,\delta_{ij} \qquad (3)$$

The exponential function in equation (1) is called the ARRHENIUS-equation and allows the consideration of the influence of the temperature. The symbol Q denotes the activation energy of the microphysical distortion mechanisms, R the universal gas constant. A similar equation is used by Munson and Dawson (1984).

For the viscoplastic transient strain rate a simple formulation is applied in dependence of the porosity n, the time t and the material- and regression parameters C_1, D_1:

$$\dot{e}^{vpl,tr} = \frac{D_1 \cdot n}{C_1} \cdot e^{-\frac{t}{C_1}} \qquad (4)$$

For the mathematical description of the viscoplastic volumetric strain rate an equation based on the work of Zhang et al. (1996) is used. Thereby the influences of temperature, hydrostatic stress state in form of the first stress invariant I_1 and the compaction state are bonded multiplicatively:

$$\dot{\varepsilon}_{kk}^{vpl} = e^{-\frac{Q}{R\cdot T}} \cdot E_7 \cdot e^{E_8 \cdot I_1} \cdot \left(\ln\left(\frac{\varepsilon_{kk,max}}{\varepsilon_{kk,max} - \varepsilon_{kk}}\right)\right)^{-\left(E_5 + E_6 \cdot \varepsilon_{kk,max}\right)} \qquad (5)$$

The symbols E_i characterize further material and regression parameters.

The instantaneously plastic deformations are simulated by means of a cap model. Therefore the rate sensitive strength of the rock salt is according to Wallner (1983) transformed into a strength behavior, which is independent of the strain rate.

The used cap model consists of two yield surfaces. The cone surface is ideal plastic, the cap surface convex and hardening (Figure 3).

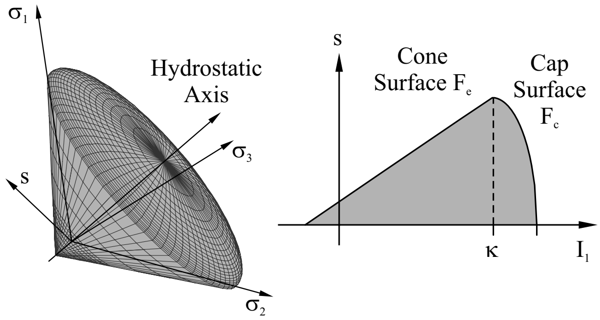

Figure 3. Yield surfaces of the cap model.

Following Desai et al. (1982) the yield criterion for the cone surface is defined using the first stress invariant I_1 as:

$$f_1 = s - F_e(I_1) = s - \left[\alpha - \lambda \cdot e^{-\beta \cdot I_1} + \theta\, I_1\right] = 0 \qquad (6)$$

The elliptic functional form of the yield criterion for the cap surface is (Hofstetter et al. 1993):

$$f_2 = F_c(I_1, \kappa) - F_e(\kappa) = \sqrt{s^2 + \left(\frac{I_1 - \kappa}{r}\right)^2} - F_e(\kappa) = 0 \qquad (7)$$

The symbols α, β, λ, θ, κ und r represent further material parameters. For the consideration of the crossing of the yield surfaces the flow rule according to Koiter (1953) is used, which applies additively instantaneously plastic strain increments for each yield surface, if the corresponding yield surface is activated by means of the yield criterion.

$$d\varepsilon_{ij}^{pl} = \sum_{k=1}^{n} d\gamma_k \frac{\partial f_k}{\partial \sigma_{ij}} \qquad (8)$$

4 IMPLEMENTATION OF THE CAPCREEP MODEL

The above introduced constitutive equation is implemented in the Finite-Element system ABAQUS via a special interface. The developed subprogram CAPCREEP uses the implicit EULER backward integration and the return-mapping-algorithm for the capture of the inelastic deformations. The pattern of the return-mapping-algorithm is shown in Figure 4.

In doing so the so-called trial stress is computed on the basis of the previous converged solution under the assumption of an elastic stress path. If the trial stress lies outside of the yield surfaces, plastic material behavior occurs. In this case the stress point is projected back onto the yield surface using the consistency condition. The projection of the stress point causes the update of the stress and strain tensors as well as further solution dependent state variables (Simo and Taylor 1985).

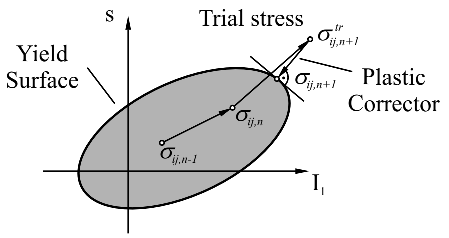

Figure 4. Pattern of the return-mapping-algorithm.

Within the solution algorithm of the Finite-Element-Method the system stiffness is updated. For that purpose the material stiffness as a part of the system stiffness must be computed. On account of the dependence of the material stiffness on the integration process and the return-mapping-algorithm respectively the calculation of the material stiffness should be consistent with the return-mapping-algorithm.

The consistent material stiffness follows as the JACOBI-Matrix of the derivatives of the stress increments after the deformation increments for the updated state. The use of the consistent tangent operator has no influence on the calculation results but on the convergence behavior (Ortiz and Popov 1985).

For the cone surface the equation of the material stiffness follows to:

$$D_{ijkl} = \Xi_{ijkl} - \frac{\Xi_{ijrs} \dfrac{\partial f_1}{\partial \sigma_{rs}} \Xi_{klmn} \dfrac{\partial f_1}{\partial \sigma_{mn}}}{\dfrac{\partial f_1}{\partial \sigma_{ab}} \Xi_{abcd} \dfrac{\partial f_1}{\partial \sigma_{cd}}} \tag{9}$$

The symbol Ξ represents the algorithmic modulus and is computed by using the consistency parameter $\Delta\gamma_1$ coming from the return-mapping-algorithm and the elasticity tensor E to:

$$\Xi_{ijkl} = \left(E^{-1}_{ijkl} + \Delta\gamma_1 \frac{\partial^2 f_1}{\partial \sigma_{ij}\, \partial \sigma_{kl}} \right)^{-1} \tag{10}$$

For the implementation a numerical inversion of the algorithmic modulus is necessary, which is realized numerically by means of an algorithm according to GAUSS (Kolling 2005).

The developed subroutine CAPCREEP consists of 10 calculating steps which are passed through depending on the calculation mode in different variants.

Within the subprogram the stress tensor, the deformation tensor, solution dependent state variables as well as the material stiffness tensor are computed for every integration point of the model and are returned to the master program.

After ensuring of a three-dimensional geometric modelling in step 1 the elastic material stiffness is formed in the following step 2. Afterwards the solution dependent state variables resulting from the previous converged increment are activated in step 3 for the description of the current state. In step 4 and step 5 respectively the cone and cap yield criterions are computed under use of the return-mapping-algorithm.

In step 6 the activation of the model mode is defined. Five modes are distinguished. Four time invariant modes serve for the calculation of the instantaneous strains and are activated on the basis of the yield criterion and the KUHN-TUCKER-conditions respectively (Swan and Seo 2006). The fifth viscous mode is activated in consequence of laboratory test procedure and of the deposition process respectively concerning the tailings heaps. In the steps 7 and 8 the plastic strains are computed.

The updating of the stress tensor, the strain tensor and the solution dependent state variables follows in step 9. In the concluding step 10 of the subprogram CAPCREEP the material stiffness is calculated.

5 VERIFICATION OF THE CAPCREEP MODEL

For the verification and the proof of the suitability of the new numerical model CAPCREEP several triaxial tests and the 34 years lasting stockpiling of an actual tailings heap are simulated.

Figure 5 shows the results of a creep test, which was performed by the Institute and the Laboratory of Geotechnics in order to study the time dependent strain components, and the corresponding results of the Finite-Element-Analysis (FEA) using the material subroutine CAPCREEP.

The dots describe the experimental results in form of the volumetric and shear strain, the lines the corresponding results of the Finite-Element-Analysis.

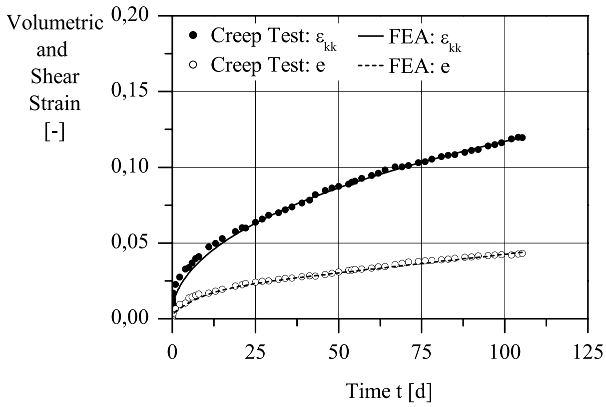

Figure 5. Simulation of a creep test.

In summary these test results but also the results of other very different tests could be simulated quite well with the material subroutine CAPCREEP.

Hence it could be proved on the basis of the laboratory tests, that the mathematical approaches for different strain components are adequate for the simulation of rock salt in the context of tailings heaps.

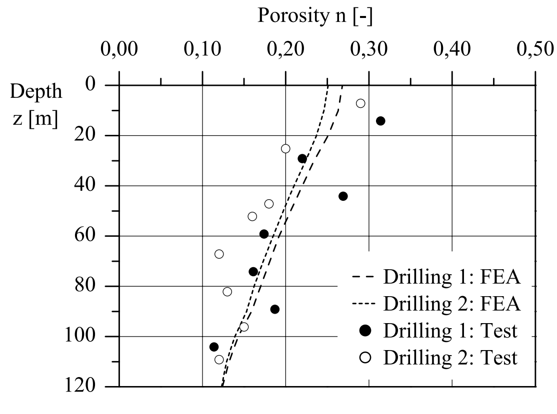

Figure 6. Simulation of a tailings heap.

After simulating the laboratory tests the 34 years lasting stockpiling of the left tailings heap of Figure 1 was simulated.

One of the main calibration and quality feature respectively is the compaction state of the tailings heap after 34 years, which was explored in two new investigation drillings over the whole height of the tailings heap.

Figure 6 shows the results of the Finite-Element-Analysis concerning the compaction state after 34 years plotted over the height of the tailings heap. The dots represent the test results of the specimens of the drillings, the lines the computed results.

Regarding figure 6 it could be summarized, that the compaction state of the tailings heap over the whole height in two different drillings for a special point of time is quite well captured by means of the numerical model CAPCREEP.

6 CONCLUSIONS

To sum up, the numerical model CAPCREEP can be judged as a robust, efficient and purposeful material routine which offers an instrument for the simulation and investigation of complicated, time variant tailings heaps consisting of granular or intact rock salt.

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