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NUMERICAL MODELLING OF EXPANSIVE CLAYS

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Abstract: *The paper deals with the hypoplastic model for expansive clays which takes into account the double structure of clays. The model is formulated in the rate form which requires integration in time. Several integration schemes based on the Runge-Kutta-Fehlberg (RKF) methods of different order have been investigated. The RKF methods have been implemented in the FE code SIFEL and there is a comparison of their performance on a benchmark example of triaxial test. The mechanical model is accompanied with the model of one-phase water flow in the porous medium.*

Keywords: Expansive clays, Hypoplasticity, Runge-Kutta-Fehlberg method, Water flow in porous medium, Coupled problem.

1. Introduction

Expansive clays are known for their large swelling/shrinkage capacity which is influenced by the water content namely. Bentonites are also known for their very low permeability coefficient whose typical magnitude ranges from 10^{-14} to 10^{-12} $m.s^{-1}$ according to void ratio. Swelling accompanied with low permeability comprises self-sealing properties of bentonites that have been exploited in the sealing of dams for example. The bentonites are also assumed to be a part of engineering barrier at deep geological repositories in high level radioactive waste disposals. The engineering barrier is composed from the special containers for spent nuclear fuel sealed by the bentonite layer which should able to stop the radionuclides migration in the case of container failure. Obviously, it is crucial for the design of engineering barrier to use the proper model of bentonite behaviour.

In the soil modelling, two major groups of models are exploited. One large (older) group of models is based on theory of elasto-plasticity (Hughes 1987) where the model assumes plastic strains in the form

$$\dot{\boldsymbol{\varepsilon}} = \dot{\lambda} \frac{\partial f(\boldsymbol{\sigma}, \mathbf{h})}{\partial \boldsymbol{\sigma}}, \tag{1}$$

$$\boldsymbol{\sigma} = \mathbf{D}_e : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p\right), \tag{2}$$

where $f(\boldsymbol{\sigma}, \mathbf{h})$ represents selected yield function. In the above equations, $\boldsymbol{\sigma}$ stands for the stress tensor, $\mathbf{h}$ is the vector of hardening parameters, λ is the consistency parameter, $\mathbf{D}_e$ is the fourth-order elastic stiffness tensor, $\boldsymbol{\varepsilon}$ is the total strain tensor and $\boldsymbol{\varepsilon}_p$ is the tensor of plastic strains. Several models for the partially saturated soils have been proposed (e.g. Alonso, 2011). Advantages of the mentioned elasto-plastic models is the pressure dependent loading, direct incorporation of the state boundary surface and, in the case of extended model, the taking into account the influence of suction pressure. But they have also important shortcoming related to the elastic unloading which is not in agreement with the observed soil behaviour.

To avoid of these shortcomings, a relatively new group of hypoplastic models has been developed by Gudehus, 2004 and Herle, 20011. They have involved different loading/unloading moduli directly in the rate form of stress-strain relation:

$$\dot{\boldsymbol{\sigma}} = \mathcal{M}(\boldsymbol{\sigma}, \Delta\boldsymbol{\varepsilon}, \mathbf{v}) : \dot{\boldsymbol{\varepsilon}}, \tag{3}$$

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where $\mathcal{M}$ is the is the fourth-order generalized stiffness tensor which depends on the actual stresses $\boldsymbol{\sigma}$, increment of strains $\Delta\boldsymbol{\varepsilon}$ and other state variables denoted by vector $\mathbf{v}$. The rate from of stress-strain relation of the hypoplastic models thus constitutes the system of ordinary differential equations. The total stress needed at the equilibrium conditions have to be obtained by the integration of Eq. (3) in time. Additionally, the state variables are also given in the rate from and therefor they have to be integrated too.

2. Hypoplastic model for expansive clays

The advanced hydro-mechanical model based on hypoplasticity has been proposed in Mašín, 2013. The model takes into account the double structure of the aggregated clayey soils and it exploits separated formulation of macro and micro behaviour according to well established models (Alonso, 2011 and Romero, 2011) but there is added dependence of water retention on volumetric deformation. Coupling between macro and microstructure levels depends on size of macropores (interaggregate pores) and there is assumed that the shear strength of soil is attributed to the macrostructure and it is given by effective stress measure independent on microstructural quantities. Hydraulic equilibrium is assumed between both structure levels.

The model assumes additive decomposition of the total strain rate $\dot{\boldsymbol{\varepsilon}}$ in the form

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^M + f_m \dot{\boldsymbol{\varepsilon}}^m, \qquad 0 \leq f_m \leq 1 \tag{4}$$

where f_m stands for the factor that quantifies the level of occlusion of macro-porosity by aggregates ranging from 0 to 1. Similarly, the total void ratio e together with the consistent definition of the porosity measures for particular structural levels are defined in the model. Two different mechanical models for macro and microstructure level are defined in the model. Assuming local hydraulic equilibrium and the Bishop's effective stresses concept, the following terms for the rates of effective stresses at macro and micro levels are given

$$\dot{\boldsymbol{\sigma}}^M = f_s - (\mathcal{L}: \boldsymbol{\varepsilon}^M + f_d \mathbf{N} \|\boldsymbol{\varepsilon}^M\|) + f_u \mathbf{H}, \tag{5}$$

$$\dot{\boldsymbol{\sigma}}^m = \mathbf{I} \frac{p^m}{\kappa_m} \varepsilon_V^m \tag{6}$$

where f_s is the barotropy factor, $\mathcal{L}$ is the hypoelastic fourth-order tensor, f_d is the pyknotropy factor, $\mathbf{N}$ is the second order tensor defined according to the failure condition, the factor f_u and the second order tensor $\mathbf{H}$ control wet induced collapse. In the microlevel stress term, $\mathbf{I}$ is the second order identity tensor, p^m is the mean stress at the microlevel, κ_m is the model parameter and ε_V^m is the volumetric strain at microlevel. It should be noted, that the reversible behaviour linear in $\ln p^m$ vs. $\ln(1 + e^m)$ plot is adopted at the microstructure level. The more details about the model can be found in Mašín, 2013.

3. Model of water flow in deforming porous medium

In this case, the assumption of isothermal one-phase flow is adopted for the model based on Lewis and Schrefler (Lewis, 1971). Neglecting the water vapour exchange and assuming the dependency of the degree of saturation on the pore water pressure results in continuity equation for one-phase (liquid water) flow in deforming medium

$$\left(\frac{\alpha - n}{K_g} S_r^2 + \frac{n\, S_r}{K_w}\right) \frac{\partial u_w}{\partial t} + \left(\frac{\alpha - n}{K_g} S_r u_w + n\right) \frac{\partial S_r}{\partial u_w} \frac{u_w}{t} + \alpha S_r \operatorname{div} \dot{\mathrm{u}} +$$

$$+ \frac{1}{\rho^w} \operatorname{div} \left[\rho^w \frac{k^{rw}\, \mathbf{k}_{sat}}{\mu^w} (-\operatorname{grad} u_w + \rho^w \mathbf{g})\right] = 0, \tag{7}$$

where α is the Biot's constant, n is the porosity, S_r is the degree of saturation, K_g and Kw are bulk moduli of water and grains respectively, u_w is the pore water pressure, ρ^w is the density of water, k^{rw} stands for the relative permeability which depends on the degree of saturation, $\mathbf{k}_{sat}$ is the matrix of intrinsic permeability of the fully saturated medium, μ_w is the coefficient of dynamic viscosity and $\mathbf{g}$ is the gravity acceleration vector.

4. Time integration of hypoplastic model

Recall that in hypoplasticity model described in Section 2, the total stress rate $\dot{\boldsymbol{\sigma}}$ is defined. Additionally, the hypoplastic model involves state variables given by vector $\mathbf{v}$ that can be also formulated in the rate form and thus generally, the stress rate can be defined by

$$\dot{\boldsymbol{\tau}} = \boldsymbol{\mathcal{M}}\dot{\boldsymbol{\epsilon}} = \boldsymbol{\Psi}(\boldsymbol{\tau}(t), \Delta\boldsymbol{\epsilon}(t)), \tag{8}$$

where $\boldsymbol{\tau}$ is the generalized stress vector $\boldsymbol{\tau} = \{\boldsymbol{\sigma}, \mathbf{v}\}^T$, $\boldsymbol{\mathcal{M}}$ represents the generalized stiffness matrix and $\boldsymbol{\epsilon}$ is the generalized strain vector $\boldsymbol{\epsilon} = \{\boldsymbol{\varepsilon}, s\}^T$ where s is the suction and $\boldsymbol{\Psi}$ represents the model response function on the given input of strain increment $\Delta\boldsymbol{\epsilon}$ of the actual time step and attained stress level $\boldsymbol{\tau}$. With respect to experiences and conclusions in Sloan, 2014, the explicit integration Runge-Kutta-Fehlberg algorithm with substepping has been selected and implemented in SIFEL. Eq. (8) represents initial value problem given by the set of ordinary differential equations. These equations can be written in generic substep *k* at time interval $[t_n;\ t_{n+1}]$ formally as follows

$$\boldsymbol{\tau}_{k+1} = \boldsymbol{\tau}_k + \Delta t_k \sum_{i=1}^{s} b_i\, \boldsymbol{k}_i(\boldsymbol{\tau}_k\, \Delta\boldsymbol{\epsilon}(t_{n+1}), \Delta t_k), \tag{9}$$

where $\boldsymbol{k}_i(\boldsymbol{\tau}_k, \Delta\boldsymbol{\epsilon}(t_{n+1}), \Delta t_k)$ represents the function $\boldsymbol{\Psi}$ evaluated for the given strain increment of the actual time step $\Delta\boldsymbol{\epsilon}(t_{n+1}) = \boldsymbol{\epsilon}(t_{n+1}) - \boldsymbol{\epsilon}(t_n)$ and attained stress levels at the prescribed points of time interval. In Eq. (9), dimensionless step length $\Delta t_k \in (0; 1]$ has been introduced with the following definition

$$\Delta t_k = \frac{t_{k+1} - t_k}{t_{n+1} - t_n}\,. \tag{10}$$

In RKF method, the step length Δt_k is constructed according the difference between solution of two embedded Runge-Kutta algorithms of different order of accuracy obtained by the set of coefficients $\bar{b}_i$ and $\tilde{b}_i$. These coefficients may be summarized in the form of Butcher table whose generalized example is given in Tab. 1. According to this table, coefficients $\boldsymbol{k}_i$ can be evaluated in selected times and corresponding stress values

$$\boldsymbol{k}_i(\boldsymbol{\tau}_k, \Delta\boldsymbol{\epsilon}(t_{n+1}), \Delta t_k) = \boldsymbol{\Psi}\big(\boldsymbol{\tau}_k + \Delta t_k \sum_{j=1}^{i-1} \tilde{a}_{i,j} \boldsymbol{k}_j, \Delta\epsilon(t_{n+1})\big). \tag{11}$$

Coefficients $\tilde{a}_{i,j}$, $\bar{b}_j$, $\tilde{b}_j$ $\tilde{c}_i$ are selected so that the method provides the numerical approximation of the solution of order *s* and *s*+1.

Tab. 1: Generalized example of the Butcher table.

0	0	0	$\cdots$	0	0
$\tilde{c}_2$	$\tilde{a}_{2,1}$	0	$\cdots$	0	0
$\vdots$	$\vdots$	$\ddots$	$\ddots$	$\vdots$	$\vdots$
$\tilde{c}_{s-1}$	$\tilde{a}_{s-1,1}$	$\tilde{a}_{s-1,2}$	$\cdots$	0	0
$\tilde{c}_s$	$\tilde{a}_{s,1}$	$\tilde{a}_{s,2}$	$\cdots$	$\tilde{a}_{s,s-1}$	0
	$\tilde{b}_1$	$\tilde{b}_2$	$\cdots$	$\tilde{b}_{s-1}$	$\tilde{b}_s$
	$\bar{b}_1$	$\bar{b}_2$	$\cdots$	$\bar{b}_{s-1}$	$\bar{b}_s$

Several time integration RKF schemes have been implemented and their description in the form of Butcher's tables is given in Tabs. 2, 3 and 4. Should be noted that the algorithm RKF-23bs is the Bogacki-Shampine coefficient pairs proposed in Shampine, 1987 and the advantage of the method is that it provides the better estimate of error with the minimum cost because the $\boldsymbol{k}_4$ can be used as $\boldsymbol{k}_1$ in the next step - First Same As Last (FSAL) concept.

Tab. 2: Butcher table for RKF-23 (left) and RKF-23bs Bogacki-Shampine (right).

0			
1/2	1/2		
1	-1	2	
	1/6	2/3	1/6
	0	1	0

0				
1/2	1/2			
3/4	0	3/4		
	2/9	1/3	4/9	
	7/24	1/4	1/3	1/8

Tab. 3: Butcher table for RKF-45.

0						
1/4	1/4					
3/8	3/32	9/32				
12/13	1932/2197	-7200/2197	7296/2197			
1	439/216	-8	3680/513	-845/4104		
1/2	-8/27	2	-3544/2565	1859/4104	-11/40	
	16/135	0	6656/12825	28561/56430	-9/50	2/55
	25/216	0	1408/2565	2197/4101	-1/5	

5. Performance comparison of various integration schemes

The implemented hypoplasticity model was tested on a benchmark example with axisymmetrical specimen 1x1 m subjected by triaxial drained test with constant confining pressure and gradually increasing axial load, initial stress -200 kPa, constant suction -1.9 MPa. Comparison of integration schemes for various tolerances on benchmark example is given in Tab. 4.

Tab. 4: RKF schemes comparison.

ϑ		RKF-23	RKF-23bs	RKF-45
10^{-7}	σ_{err}	1.57e-2	2.08e-3	0
	t [s]	34.6	21.1	84.7
10^{-6}	σ_{err}	1.85e-2	2.37e-3	1.89e-3
	t [s]	19.3	13.2	10.7
10^{-5}	σ_{err}	2.23e-2	5.78e-3	2.97e-3
	t [s]	11.95	8.81	8.41
10^{-4}	σ_{err}	3.67e-2	9.45e-3	6.07e-3
	t [s]	7.70	6.44	8.11
10^{-3}	σ_{err}	–	1.34e-2	8.92e-3
	t [s]	–	6.43	8.07

In Tab. 4, the relative error between two solutions of RKF is denoted by ϑ, σ_{err} stands for relative error of stress vector compared to RKF-45 with the minimum ϑ value and there are also elapsed times of particular benchmarks denoted by *t*.

The constitutive fourth-order tensor exhibited high nonlinearity and high computational demands in the selected benchmark example and therefore selection of suitable integration scheme plays important role. Comparison revealed that RKF-23bs can be regarded as be optimum choice for this benchmark.

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