

COST 526

**Automatic Process Optimization in Materials Technology
(APOMAT)**

Title:

Process Optimization of numerical Modeling of Geomaterials

Keywords: Numerical optimization, constitutive modeling, natural materials, underground structures

Organization/Company:

**Swiss Federal Institute of Technology
EPF Lausanne
LMS-DGC
EPFL
CH-1015 Lausanne
Switzerland**

Project leader: **Dr. Lyesse Laloui**

Tel.: ++ 41 21 693 23 14

Fax: ++ 41 21 693 41 53

E-mail: Lyesse.Laloui@epfl.ch

1. Duration / run time of the project

- Starting date: 1st January 2002
- Finishing date: 31rd August 2004

2. Overall cost

- 135 kEURO

3. Funding situation

- As soon as the project is accepted by the MC of the COST action, the Swiss Federal Office of Education and Science will support our project with the needed fund

4. Project partners indicated to participate

- The main partner is:

Colenco Power Engineering - NE
Dr. G. Klubertanz

Mellingerstr. 207
CH-5405 Baden / Schweiz

Tel. ++41 56 483 15 88

Fax ++41 56 493 73 57

www.colenco.ch/de/grundwasserschutz_und_entsorgung.html

5. Project partners to be found

Not specified yet

6. Short description of the material process to be optimized

As in mechanical engineering, large civil engineering projects often encounters situations where complex material behaviour has to be modelled numerically. Whereas engineering faculties can handle artificial material with perfectly controlled parameters, for underground structures and natural materials, one often faces natural variability and inhomogeneity of the material under consideration.

Parameters for material models generally are obtained via laboratory or small scale field test while the problem is on a much larger spatial scale: this often makes it difficult to apply the laboratory result directly to the problem under consideration. In some cases, e.g. for the sealing of waste disposal in deep geological layers, it is virtually impossible to obtain undisturbed, good quality samples for testing.

Finally, the material models themselves tend to become tremendously complex as soon as some coupling is to be modelled: for example the few existing material models taking into account a deformable porous skeleton and two interstitial fluids have up to several dozens of parameters.

Consequently, there is an urgent need for an optimization of the numerical modelling of the natural materials with good and robust constitutive laws, most efficient computer codes and adapted parameter identification algorithms.

7. Material(s) involved:

- Natural materials such sand and clay will be considered in this project. This kind of material is known as geomaterials. From mechanical point of view, geomaterials have the following characteristics: i. They are influenced by the mean pressure, temperature, suction and chemistry; ii. They have plastic hardening behaviour with dilatancy (non-associative flow rule); and iii. They are constituted by several phases (solid with multi-porosity), liquid and air.

8. Optimization potential of the process or process step

- The optimization of the numerical modeling of geomaterials is an important topic for several geomechanical applications. In this project, we will focus on the numerical modeling of the engineered barrier system for nuclear radioactive waste disposal in deep soils.

The safety and long-term performance of underground permanent repositories rely on a combination of several engineered and geological barriers. The properties of the geological barrier depend on the natural conditions of the formation considered to host the repository, but the performance of the engineered barriers is a result of their design and construction, and of the interaction between both barriers in response of the conditions expected in a high level waste repository. These interactions need to be identified and fully understood for input in models realistically describing the behaviour of the near field to predict reliably the long-term performance and safety of a repository.

9. Specified material properties to be achieved

- The heat produced in the nuclear waste repository has the potential to influence the performance of the engineered and to some extent the geological barrier. Due to the higher thermal gradient and to the particular sealing material used, the engineered barrier system may be more seriously affected than the host rock. It is therefore necessary to optimize the process of identification of the material parameters and the numerical simulation of coupled THM (thermo-hydro-mechanical) phenomena developing in the sealing or filling material (bentonite or concrete) when heated. A more precise identification of the critical issues of THM processes is to be performed.

10. Process parameters to be optimized

- Not applicable

11. Material laws including material dependent coefficients

- The LTVP model will be used here as the material law. This is a thermo-viscoplastic constitutive law developed by this proposed project leader (Laloui, 1993, 2001) and Modaressi & Laloui (1992, 1997) for the numerical modelling of the cyclic elasto-thermoplastic and elasto-thermoviscoplastic behaviour of geomaterials. This model is based on non-linear elasticity and four kinematic plastification mechanisms: one isotropic and three deviatoric. Temperature acts on the essential rheological parameters. With this structure, the LTVP model can be distinguished from other models since:

- it is the first cyclic thermo-viscoplastic constitutive models able to represent principal thermo-mechanical characteristics of geomaterials over a wide range of loading (such as cyclic behaviour, even at high temperatures) and initial conditions (such as initial and induced anisotropies);
- it handles overconsolidated as well as normally consolidated clays in the same framework,
- elasto-thermoplastic formulation, when applicable, is robust and needs less model parameters

but results in heavier computations,

- the isotropic thermo-plastic mechanism is able to distinguish the thermal hardening introduced by the irreversible compaction of NC clays which results in yield surface shrinkage, and the effect of the modification of the mechanical parameters which can either induce a shrinkage or a dilation of the deviatoric yield limit.

Parametric studies carried out with the help of this model show that the coupling of elasto-plastic parameters with temperature produces qualitatively different results from those of a thermo-elastoplastic model without coupling (Félix et al. 1996).

12.Simulator

- The hydro-mechanically coupled FE code MEHRLIN developed at Colenco Power Engineering (CH) will be used.
- It will be extended to a thermo-hydronechanical formulation for modelling thermal responses of a clay-based sealing material on a thermal disturbance under non-isothermal conditions. Validation will be undertaken with respect to available data from small scale laboratory and medium scale field tests.

13.Optimizer

Not specified yet

14. Competence / activities of proposer:

- The proposer of this project could be considered as a specialist in the field of numerical and constitutive modeling in geomechanics. He has contributions in the areas of material modeling, testing and computational methods. These include theoretical modeling based on fundamental principles of thermodynamics, mechanics and physics, laboratory testing, field verifications, and development and application of up-to-date computational procedures and algorithms for problems involving linear and nonlinear behavior, static and quasi-static loads, and flow and heat transfer (in geoenvironmental engineering) through deformable media. Large experience in planning, development and management of research and consulting projects. He is a project leader in COST P4 and was active member of the MC of COST 337. A brief CV is attached.