COST 526

"Automatic Process Optimization in Materials Technology"
(APOMAT)

Half-Yearly Report

1. Reporting Period	**1.7.2003 – 31.12.2003**
Project title	**Optimization of Cooling Processes in Geomaterials**
Project leader Organization	**Dr. Lyesse LALOUI** Swiss Federal Institute of Technology, EPF Lausanne
Main collaborators involved	**Dr. Georg KLUBERTANZ** Colenco Power Engineering – NE Baden / Switzerland

2. Funding Situation

Amount of money received specifically for COST	107.- kEuros
Other resources partially used for the project	47.- kEuros

3. International Collaboration
(mention group and type of work done in collaboration during the reporting period)

Participation in the Working Group Meeting in Krakow + project progress report
x YES
❐ NO

4. Industry participation
(mention name of companies and work done in collaboration during the whole project)

Colenco Power Engineering – NE
Baden / Switzerland

5. Meetings, visits, exchange of scientists, short-term scientific missions	**Location, date**

6. Progress within the reporting period
(Not exceeding 3 pages, including tables and figures)

PROJECT OVERVIEW

Large civil engineering projects very often encounter situations where complex behaviour of (polyphasic) materials has to be modelled numerically, while most available numerical tools are designed to handle artificial materials with perfectly controlled parameters. For underground structures and geomaterials we have to take into account natural variability and inhomogeneity of the material under consideration. Model parameters generally are obtained via laboratory tests while the problem is on a much larger spatial scale. Moreover, laboratory-testing time is quite short while the phenomena considered can take place over long time, as in the case of creep of soil. These two effects (time and scale) give rise to difficulties to apply the laboratory results to in-situ phenomena.

In the particular case of the sealing of radioactive waste in repository tunnels, located several hundred meters deep into the ground, it is impossible to obtain absolutely undisturbed samples for testing. Efficiency of numerical modelling depends also on complexity of problems: the material models tend to become tremendously complex as soon as some coupling effect between the constituents is to be modelled. For example, modelling of thermo-hydro-mechanical behaviour requires many parameters that can be classified as: elastic, plastic, hardening and thermal and their number grows up to few dozens of parameters. Determination of this huge number of parameters is difficult and sometimes impossible based only on experimental results. In such circumstances the numerical modelling of geomaterials still is based on computational approximation and empirical knowledge, which may induce some inaccuracy.

In this project, we contribute to the improvement of the numerical modelling of the Thermo-Hydro-Mechanical (THM) behaviour of geomaterials by:

i. Extension of the capability of our numerical tool (Finite Element Code);
ii. Validation of the Thermo-Hydro-Mechanical (THM) numerical approach;
iii. Introduction of numerical optimisation process to numerical modelling of THM processes.

The Finite Element Code MHERLYN, is extended, including formulation of the heat balance equation accounting for thermal coupling with solid and fluid phase (theoretic analysis and development of a three phase–thermal coupled system). In particular anisotropic thermal and hydraulic properties of the rock and thermal influence on rock parameters can be included, where this can be expected to be relevant.

The methodology of numerical optimisation will be applied to the numerical modelling of the engineered barrier system for nuclear radioactive waste disposal in deep soils in order to assess material properties and variability that allow to keep repository performance within a predefined range. Validation of the whole numerical approach (mechanical modelling and optimisation process) will be undertaken with respect to available data from small scale laboratory and medium scale field tests.

WORK ACCOMPLISHED

In the reporting period, work concentrated mainly on:

- Mathematical formulation of the THM processes and development of the Finite Element Code - MHERLYN.
- Optimisation algorithms: development and application to themo-hydro-mechanical constitutive law - LTVP model (Laloui and Cekerevac 2003). A part of the work has been concentrated to the validation of the method used.

The fully coupled three-phase formulation has been developed based on the continuum theory of mixtures using as a principal variables the temperature, the solid displacement, the liquid pressure and the gas pressure. The formulation of the heat balance equation takes into account thermal coupling with solid and fluid phases, under following assumptions:

- There is no phase change (i.e. no steam);
- Anisotropic thermal properties (conduction);
- Thermo-elastic and thermoplastic behaviour.

The developed THM mathematical model has been implemented into the Finite Element Code – MHERLIN, which is partially operational at the moment. Validation of the mathematical modelling and the developed code is in progress and will be continued with respect to available data from small scale laboratory and medium scale field tests (for example FEBEX project or CACTUS poject).

The second task of the research concerns the numerical optimisation process applied to the procedure of model calibration. In other words, the goal is to find the optimally accepted combination of parameters, which gives *the best* model response. To do that, we have to establish optimisation criteria that will be used as a "measure" between numerical and experimental results. Based on the literature review, we found that for this specific problem, the most appropriate approach is a quadratic objective function having the possibility to give different "weights" on points in different domains of behaviour. Using this approach, we have transformed our problem to a minimisation problem in n-dimensional space, where n is number of model parameters.

The important task was to find a strategy for the minimisation that would allow us to handle the problem defined above. Several options where considered for the algorithm, and finally we concluded that optimisation should be done by two methods:

i) Local method and

ii) Global method.

Optimisation at the local level is done by the quasi-Newton method, which combines advantages of the gradient method with the Newton's approach. The method uses gradients of the objectives functions giving an inverse of Hessien matrices indicating the precision of obtained parameters. The other advantage of the quasi-Newton method is that there is no need for a resolution of the system of linear functions that rapidly increases computation time. To obtain direction of decrease of objective function, we employed the quasi-Newton method and gradient method to treat inactive and active variables, respectively. The number of optimisation to be done is equal to the number of variables.

The global method is needed to insure that optimised model parameters correspond to a minimum of the objective function over the whole considered domain. Among the tested strategies, the stochastic method is the most appropriated one for problems where the dimension of the space in which the optimisation takes place, constituted of model parameters, is high. It requires fewer evolutions of the objective functions in comparison with deterministic methods. Starting from the initially imposed parameters, we generate randomly variables trying to minimise objective function and compare the resulting value to the original one, restricting the admissible parameter ranges further and further as we go on.

These two optimisation techniques are coupled and implemented in the code ParaID devoted to the parameters optimisation. ParaID enables us to use combination of the employed techniques or only one of them. The most common and recommend approach is to start with the stochastic method and to use the obtained variables as an input for the quasi-Newton method and finally again verify the found optimum by the stochastic method. According to parametric study on objective functions, the variables can be classified as: smooth, neutral and irregular. The smooth and neutral variables can be easily optimised by the quasi-Newton method while for irregular the only method that can be used is the stochastic.

Finally, the procedure has been validated for drained as well as undrained triaxial shear tests for three initial states (Cekerevac and Laloui 2004). Comparison between numerical and experimental results clearly shows capability of the optimisation procedure to derive model parameters correctly.

References

Cekerevac, C., and Laloui, L. 2004. Experimental study of thermal effects on the mechanical behaviour of a clay. *International Journal for Numerical and Analytical Methods in Geomechanics incorporating Mechanics of Cohesive-frictional Materials*, **28**(3): 209-228.

Laloui, L., and Cekerevac, C. 2003. Thermo-plasticity of clays: An isotropic yield mechanism. *Computers and Geotechnics*, **30**(8): 649-660.

RESULTS

This Project progressed according to the time schedule in the reporting period. The fully coupled three-phase formulation has been developed based on the continuum theory of mixtures using as a principal variables the temperature, the solid displacement, the liquid pressure and the gas pressure. The formulation of the heat balance equation takes into account thermal coupling with solid and fluid phases. The developed THM mathematical model has been implemented into the Finite Element Code – MHERLIN, which is partially operational at the moment. Validation of the mathematical modelling and developed code is well under way and will be continued with respect to available data from small scale laboratory and medium scale field tests (for example FEBEX project or CACTUS poject).

The methodology of numerical optimisation has been applied to the numerical modelling of the thermo-hydro-mechanical behaviour of the clays. The proposed methodology is a combination of a quasi-Newton and a stochastic method applicable at local and global levels, respectively. The code ParaID, developed by using Visual Fortran, is devoted to the optimisation of the LTVP model parameters. The code is “open” and can be easily implemented for any other constitutive model. Finally, the procedure has been validated for drained as well as undrained triaxial shear tests for three different initial states. Comparison between numerical and experimental results clearly shows capability of the optimisation procedure to derive model parameters correctly.

The optimisation procedure is planned to be done to the overall structure after validation of the mathematical THM model and Finite Element Code – MHERLYN.

CONCLUSIONS/PERSPECTIVES

The fully coupled three-phase formulation has been developed based on the continuum theory of mixtures. The formulation has been implemented into the Finite Element Code – MHERLIN, which is partially operational. The programme is currently under validation with respect to available experimental results (laboratory and in-situ medium scale tests).

On the optimisation task, an appropriated optimisation strategy has been developed and applied to the numerical modelling of the thermo-hydro-mechanical behaviour of clay barriers. The procedure and developed code have been validated for drained as well as undrained triaxial shear tests for three initial states. Comparison between numerical and experimental results clearly shows capability of the optimisation procedure to derive model parameters correctly.

Both tasks required an additional time to be finished, and no major problems are expected!

PERSPECTIVES

According to the decision made by the Committee of Senior Officials of COST, this COST Action will be prolonged for 12 months. With respect to the importance of the project, the obtained results, work progress and required time to finish the project, we will ask the Federal Office for Education and Science (OFES) financial prolongation of six months.

7. List of publications a) Published
b) Submitted for publications
c) In preparation
A Journal Paper is actually in the phase of preparation, entitled: ***"Elasto-plastic model parameters identification by numerical optimisation"*** by S. Girardin, C. Cekerevac, G. Klubertanz and L. Laloui.