COST 526

"Automatic Process Optimization in Materials Technology"

(APOMAT)

Half-Yearly Report

1. Reporting Period	**1.1.2003 – 31.6.2003**
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. G. Klubertanz Colenco Power Engineering 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)

x YES
❒ NO

Participation in the Working Group Meeting in Brussels + project progress report

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

Colenco Power Engineering
Baden / Switzerland

5. Meetings, visits, exchange of scientists, short-term scientific missions	**Location, date** Lausanne, August 27, 2003

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

Project Overview

As in mechanical engineering, large civil engineering projects often encounter situations where complex material behavior has to be modeled 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 modeled: 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. In such conditions, the numerical modeling of geomaterials is still based on empirical knowledge and such an approach may induce some inaccuracy.
In this project, we contribute to the improvement of the numerical modeling of the thermo-hydromechanical (THM) behavior of geomaterial by

i. extending the capabilities of an existing code
ii. validating of our THM numerical approach
iii. introducing a numerical optimization process

The methodology of numerical optimization will be applied to the numerical modeling 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.
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 behavior of the near field to predict reliably the long-term performance and safety of a repository. Parameters to be optimized are mainly:

thermal parameters of sand/clay mixture by determining an appropriate mixing ratio
heat generation of the waste (via dilution or delayed burying)

Validation of the whole numerical approach (mechanical modeling and optimization process) will be undertaken with respect to available data from small scale laboratory and medium scale field tests.

Work Accomplished

In the reporting period, we focused mainly on the development of an optimization procedure for the material model LTVP to be used. This is a thermo-viscoplastic constitutive law developed by the project leader (Laloui, 1993, 2001) and Modaressi & Laloui (1992, 1997) for the numerical modeling 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.

The model was carefully analyzed in order to identify possibilities for an efficient optimization algorithm. Finally, it was decided to use a combined procedure of quasi-Newton and stochastical methods, including parameter separation according to physically distinguished domains to be optimized.
This optimization approach for the LTVP-model has been implemented in a Fortran code called ParaID. This code finds an optimized set of all 27 parameters of the material model, or a subset of those, according to the users requirements, corresponding to a given set of laboratory measurements of triaxial tests. The code can handle multiple test results for different initial conditions for each optimization procedure. The code has been tested and validated using available laboratory data.
Work on the THM-simulator has been continued, the thermo-hydraulic part can be considered as stable. Work continues on some aspects of the thermo-mecanical implementation.

Results

An adequate optimization procedure for the problem at hand has been identified. This procedure has been implemented, and a Fortran code is operational. Some validation tasks are still ongoing.

The THM simulator is progressing well and most work there is accomplished.

Conclusions / Perspectives

A powerful optimization tool adapted to the LTVP model is available as planned. Work there progressed rapidly and was finished, accounting for the 3 months delay in project start - ahead of schedule. The THM simulator should be available with full planned functionality within the next months.
The project is overall running on schedule and progresses as planned.

No major problems are expected. Focus of the work in the second half 2003 will be on the one hand on the optimization of a boundary value problem and on the other hand on the continued validation of the optimization procedure.

7. List of publications

a) Published

b) Submitted for publications

c) In preparation

A paper on the optimization algorithm is in preparation.