COST 526

"Automatic Process Optimization in Materials Technology"

(APOMAT)

Half-Yearly Report

1. Reporting Period	**1.7.2002 – 31.12.2002**
Project title Project leader Organization Main collaborators involved	**Optimization of Cooling Processes in Geomaterials** **Dr. Lyesse Laloui** **Swiss Federal Institute of Technology, EPF Lausanne** **Dr. G. 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 Budapest + 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

As in mechanical engineering, large civil engineering projects often encounter situations where complex material behaviour has to be modeled numerically. Whereas engineering faculties can handle artificial material with perfectly controlled parameters, for underground structures and natural materials (geomaterials), 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 effect between the constituents 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 still based on computational approximation and empirical knowledge. Such an approach may induce some inaccuracy.

In this project, we would to contribute to the improvement of the numerical modeling of the thermo-hydro-mechanical (THM) behaviour of geomaterials by:

i. The extend of the capability of our numerical tool (Finite element code)
ii. The validation of the THM numerical approach;
iii. The introduction of some numerical optimization processes.

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 keeping 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 behaviour 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, work concentrated on several subjects:

- concept development and mathematical formulation of the THM - system
- code development
- literature research on optimization algorithms suitable for the problem at hand

The development of the THM mathematical model is based on several main steps:

- Conceptualization of expected processes, identification of proper existing THM-laws to model the main features. In particular anisotropic thermal and hydraulic properties of the rock, thermal influence on rock parameters can be included, where this can be expected to be relevant

- Formulation of the heat balance equation that is to be implemented in the MHERLIN code, accounting for thermal coupling with solid and fluid phases (theoretic analysis and development of a three phase –thermal coupled system) under the following assumptions:
    - no phase change (i.e. no steam)
    - anisotropic thermal properties (conduction)
    - thermoelastic (in a first stage) and thermoplastic behaviour

The fully coupled three phase formulation is based on the continuum theory of mixtures and treats the unsaturated soil as a superposed continuum of solid, liquid and gas. Principal variables are consequently the temperature, the solid deformation, the liquid pressure and the gas pressure. The two fluid phases are in motion and a nonlinear pore pressure - saturation relation is used. The resulting system of equations is discretized in space using the finite element technique and in time by the Θ - method. A simplified version of the full equations is proposed.
Main effort in the domain of optimization was spend on finding a strategy for the optimization that would allow handling the problem defined above. It turned out that apparently no standard optimization strategy is likely to be well suited. Several options where considered for the algorithm, but no final choice has been made jet.

RESULTS

Model development and code programming progressed according to schedule; the project is still at its beginning and work focused on gathering information and establishing the bases for a successful scientific work. Therefore, no tangible results in form of conclusions are available jet.
The project is currently in a phase of code development and preparation on the one hand, and of evaluation and definition of the optimization approach. Code development and implementation proceed as planned, accounting for the 3 months delay in project attribution. The code will be available and operational early 2003.
Concerning the optimization procedure, research concerning the appropriate algorithm has been started. It seems, following the discussions at the working group meetings of this COST 526 Action, appropriate to proceed in two steps, first to consider a parameter optimization of the THM parameters of the material, and to approach the overall structure in a second step.

CONCLUSIONS/PERSPECTIVES

As far as code development is concerned, all necessary tools will be available and verified as planned. No major problems are expected.
On the optimization side, finding a suitable algorithm seems to be a rather non-trivial task and most likely several methods will have to be tested on simple but representative problems in order to evaluate them. This step was not planned originally, but seems to be necessary. This will be the focus of work in the next months.

7. List of publications

a) Published

As the project just started, no publications have been produced so far.

b) Submitted for publications

c) In preparation