COST 526 – Project *CH3*

Final Report

OPTIMIZATION OF THE THERMO-HYDRO-MECHANICAL MODELLING OF GEOMATERIALS

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1. Introduction

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. Model calibration based on laboratory tests faces many difficulties: time and scale effect, sample disturbances or model complexity. Under such circumstances the numerical modelling of geomaterials still is based on computational approximation and empirical knowledge, which may induce some inaccuracy.

This project 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 processes to numerical modelling of THM processes.

2. Goal of the project

The research work was mainly concentrated on the following subjects:

- Mathematical formulation of the THM processes, development of the Finite Element Code and its verification.
- Optimisation algorithms: development and application to themo-hydro-mechanical constitutive law (LTVP model).

The fully coupled three-phase formulation has been developed based on the continuum theory of mixtures using as 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 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. The developed THM mathematical model has been implemented into the Finite Element Code – MHERLIN, which is operational at the moment.

The main tasks in the domain of optimisation was finding of appropriated optimisation strategy and its applicatin to the numerical modelling of the thermo-hydro-mechanical behaviour of clay barriers. The proposed methodology is a combination of quasi-Newton and stochastic methods applicable at local and global levels, respectively. The code ParaID combines these two methods and applies to the thermo-elasto-plastic (LTVP) constitutive model. The procedure and the developed code have been validated for drained as well as undrained triaxial shear tests for three different initial stess states. Comparison between numerical and experimental results clearly shows the capability of the optimisation procedure to derive model parameters correctly.

3. Main scientific outcome

This research work was concentrated mainly on:

- Mathematical formulation of the THM processes and development of the Finite Element Code - MHERLYN.

- Optimisation algorithms: development and application to the 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 development of the THM mathematical model is based on several main steps:

- Conceptualisation 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.

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 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. The formulation of the heat balance equation takes into account thermal coupling with solid and fluid phases. Theoretic analysis and development of a three phase–thermal coupled system, has been done 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 operational at the moment.

The second task of the research concerns the numerical optimisation process applied to the procedure of model calibration. In other words, the goal was to find the optimally accepted combination of model 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.

4. Main technical outcome

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. The Finite Element formulation is presented in the Appendix A of this report.

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.

5. References

Cekerevac C., S. Girardin, G. Klubertanz & L. Laloui, Calibration of an elasto-plastic constitutive model by an unconstrained optimisation procedure. Submitted to Computer and Geotechnics.

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