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Research Paper

A novel parameter identification approach for buffer elements involving complex coupled thermo-hydro-mechanical analyses

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ABSTRACT

Coupled thermo-hydro-mechanical (THM) analyses contain a large set of constitutive parameters and this requires numerous experiments to determine these parameters. This study contributes to the identification of parameters of a coupled THM constitutive model via back analysis of information-rich experiments. An iterative sampling based back analysis approach is proposed comprising both the model parameter identification and the assessment of the reliability of identified model parameters. The results obtained in the context of buffer elements indicate that sensitive parameter estimates generally follow the normal distribution. According to the sensitivity of the parameters and the probability distribution of the samples we can provide confidence intervals for the estimated parameters and thus allow a qualitative estimation on the identified parameters which are in future work used as inputs for computational predictions in high-risk situations.

1. Introduction

Back analysis based on non-linear optimisation techniques is nowadays a well-accepted approach to calibrate models against sets of measured data in geotechnical engineering. Several authors highlight such types of parameter identification approaches as suitable ways to solve geotechnical problems in higher accuracy, including [1–7]. The advantage of using means of non-linear optimisation is that there is no need to invert the governing equations with respect to the involved model parameters, as such inversion is not always easy or possible. The main discussion in the literature with respect to back analysis approaches has so far addressed the formulation of the objective function and the optimisation algorithm. In the field of the optimisation based back analysis, some papers focus on the development of a superior algorithm of the optimisation which has global-search capacity and acceptable computational costs, e.g., [5,8–10]. Other authors worked on the formulation of complex objective functions, so that the parameter set minimising the objective function can be reliably used for numerical simulations and for making predictions based on these simulations [2,3,11].

Generally, there are several challenges while conducting model-based identifications of the constitutive parameters of complex models. One main challenge is that the provided measurements usually cannot be expected to be in the range of the operator linking model input parameters to model output. This is due to noise generally present in the measurements and abstractions during the model building process. Therefore, a direct invertibility of the systems is not possible and we seek for solutions of the inverse (i.e. the calibration) problem in the sense of least-squares solutions. Such solutions always exist, however, there is no guarantee that they will be close to the exact solution and that they are unique. The uniqueness issue can be addressed by restricting search spaces or by providing good initial guesses, if available, and regularisation, for instance according to Tikhonov.

Accepting the concept of a least-squares solution for the inverse problem, it raises another question of how to efficiently find the solution. According to the "no-free-lunch-theorem" [12] there is no strategy which performs better than others on average for all possible optimisation problems. Inspired by good experiences from researchers in the field of geotechnics, we employ meta-heuristic approaches which in particular guarantee good solutions for non-convex complex problems. Besides the above mentioned problems another challenge arises, namely the stable dependency of the solution on the data provided. Assume that there are small changes

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in the data, will this lead to visible changes in the numerical values of the solution? What happens, if we run the applied meta-heuristic search method, which is based on random number generators, several times? To quantify these effects, repeated parameter identifications are performed and statistics on the results are conducted and interpreted.

It is necessary to point out that the applications of estimating the model parameters for a geotechnical problem based on a statistical approaches, e.g. the maximum likelihood method applied by [11] or the Bayesian method applied by [3], have difficulties in the considered models due to the lack of prior information at least about the empirical parameters involved in the constitutive equations. Some researchers suggested that the confidence in the identified parameters can be assessed based on sensitivity measures e.g. [4] or [7]. However, their approaches do not cope with the difficulty of estimating a general sensitivity index for the responses of a model in a multi-field context as studied in this work. For instance, one parameter might be a sensitive parameter in a particular single-field model but it may be a non-sensitive parameter for any other quantity in a coupled system. Therefore, estimating the confidence in identified parameters only based on sensitivity indices for one output quantity might be less reliable for multi-field problems.

Particularly, identifying parameters for the coupled THM analysis in unsaturated soils is a complex problem due to a large set of parameters and a variety of variables in the forward calculation (i.e. displacements, temperature, pore water pressure and air pressure). Some authors attempted to identify constitutive model parameters for unsaturated soils by means of back analysis, for instance [13,14]. They drew an objective function in different subspaces and found the minimum of the objective function assuming that the other parameters are kept constant. In fact, model parameters vary in the search space during searching process, besides that the confidence of the identified parameters has not been assessed. In the paper [10], model parameters for describing the elasto-plastic behaviour have been identified for unsaturated soils. The authors have chosen six parameters for identification based on qualitative arguments. However, the quality of the identified parameters has not been assessed quantitatively.

Therefore, in this paper, a novel back analysis approach is proposed comprising a model parameter identification and an assessment of the reliability of the identified model parameters. Parameter sampling process is carried out based on meta-heuristic optimisation methods, in which parameters are varied under the control of the computational paradigms such as the Particle Swarm Optimisation (PSO) [15]. The confidence intervals are determined based on these parameter samples by means of probability distribution functions, see e.g. [16]. The approach can be applied for back analysing a variety of geotechnical problems, in particular it is well suited for parameter identification problems including large sets of model parameters and multi-physical simulations.

To show the applicability of the proposed method, it is applied to identify the model parameters for the simulation of the behaviour of buffer elements in high-level waste facilities. In proposed designs of repositories for the isolation of high-level radioactive waste, the clayey buffer elements play the role as engineered barriers. The behaviour of the clay barrier is highly complex. It involves coupled THM phenomena, which take place due to the simultaneous heating (generated by the radioactive waste) and hydrating of the barrier (due to the inflow of water from the surrounding rock) and mechanical forces (due to swelling phenomenon of the buffer). It requires a fully coupled non-linear THM numerical analysis for simulating water/vapour transport, heat conduction, and modelling of complex thermo-elasto-plastic stress–strain behaviour.

2. Parameter identification via back analysis

2.1. Back analysis strategy

The back analysis strategy employed in this study is illustrated in Fig. 1. Firstly, the mathematical models for the forward calculation are selected. In coupled THM analysis, we use multi-physical relations described in Table 1, which are implemented in the finite element code, CODE_BRIGHT [17]. Afterwards, the numerical solution of the forward problem is compared with experimental data by means of an objective function i.e. a weighted sum of squared errors. The objective function is minimised by means of non-linear optimisation algorithms, in particular by the PSO method [15]. The initial values of parameters are randomly selected following the uniform distribution within their prescribed ranges of variation. The sampling process generates n_p samples of parameters by means of performing n_p times of the optimisation using the PSO method. Next, a sensitivity analysis is carried out and the confidence intervals are determined. The confidence interval theory is based on assumption that the samples follow a normal distribution, therefore, a normality test has to be performed before calculating the confidence intervals. A model parameter x_j $(j = 1, \ldots, J)$ is called a sensitive parameter when the sum of its sensitivity indices $(\Sigma S^k)_j$ is greater than a predefined value S_0, where k denotes the considered model responses $(k = 1, 2, \ldots, K)$. The confidence intervals are used to assess the reliability of the identified parameters only for those parameters that are sensitive (i.e. $(\Sigma S^k)_j > S_0$) and their samples follow the normal distribution. The normality test is done according to Shapiro–Wilk [18]. The confidence intervals are determined based on the probability distribution of the samples, see [16]. The back analysis procedure is presented in detail in the next subsections.

2.2. Objective function

Let y^{meas} be a set of observed data from an experiment and y^{calc} be a set of obtained data by numerical simulation of this experiment depending on a vector of model parameters

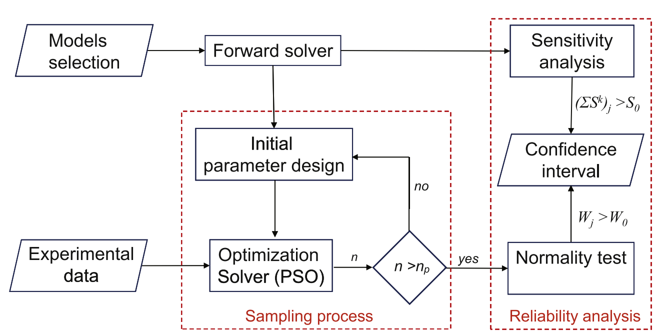

Fig. 1. Schematic presentation of the back analysis strategy.

Table 1
Constitutive relations in coupled THM analysis.

Variables	Constitutive equation	Notation
Liquid and gas advective flux	Darcy's law	q_l, q_g
Vapour and air non-advective fluxes	Fick's law	i_g^w, i_l^a
Conductive heat flux	Fourier's law	i_c
Liquid phase degree of saturation	Retention curve	S_l, S_g
Stress tensor	Mechanical constitutive model	σ