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PARAMETER IDENTIFICATION APPLYING IN COMPLEX THERMO-HYDRO-MECHANICAL PROBLEMS LIKE THE DESIGN OF BUFFER ELEMENTS

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Abstract. *This study contributes to the identification of coupled THM constitutive model parameters via back analysis against information-rich experiments. A 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 obey 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 prognosis computations of buffer elements. These elements play e.g. an important role in the design of nuclear waste repositories.*

1 INTRODUCTION

Identifying parameters for coupled THM analysis in unsaturated soils is a complicated 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 [1, 2]. 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 the searching process. Beside that the confidence of the identified parameters have not been assessed. In [3] 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 model parameter identification and an assessment of the reliability of the identified model parameters. Parameter samplings are carried out based on metaheuristic optimization methods, in which parameters are varied under the control of the computational paradigms such as the Particle Swarm Optimisation (PSO) [4]. The confidence intervals are determined based on these parameter samplings by means of probability distribution functions, see e.g. [5]. 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-response measurements.

This proposed strategy is applied to identify the model parameters for the simulation of the behaviour of buffer elements in high-level nuclear waste facilities. The clayey buffer elements in nuclear waste repository 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 nonlinear THM numerical analysis for simulating water/vapour transport, heat conduction, and modelling of complex thermo-elasto-plastic stress-strain behaviour. The results of the back analysis approach are finally compared and discussed considering experimental data in this paper.

2 PARAMETER IDENTIFICATION VIA BACK ANALYSIS

2.1 Back analysis strategy

The back analysis strategy 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 finite element code, CODE_BRIGHT [6]. 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 approach, where the latter is minimised by means of nonlinear optimisation, in particular by PSO method [4]. The sampling process is carried out based on the replication of optimisations. Each optimisation begins by an initial values of parameters. The initial values of parameters are uniformly distributed within their prescribed ranges. The sampling process generates n_p samples of parameters by means of iterating n_p times of the optimisation with the PSO method. Next, a sensitivity analy-

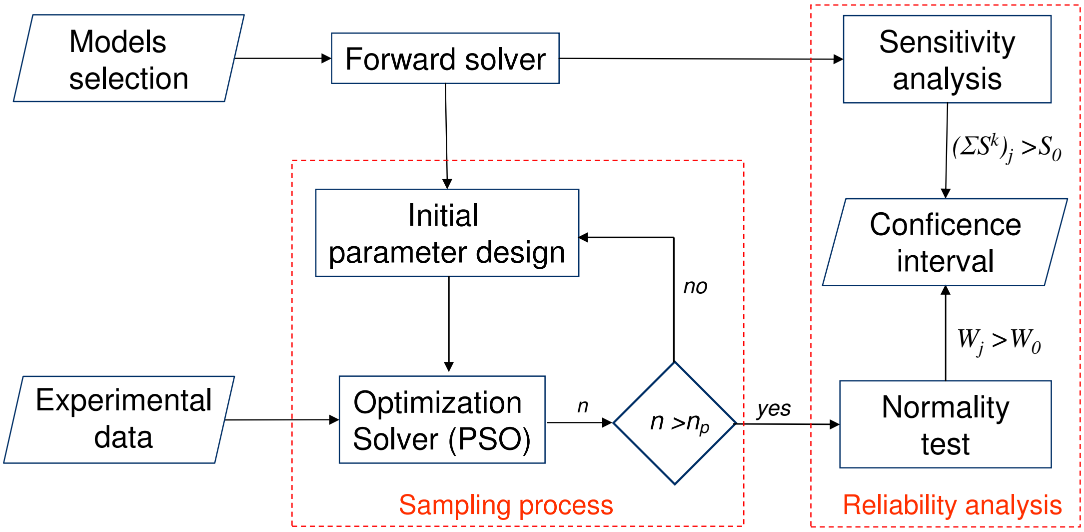

Figure 1: Schematic presentation of the back analysis strategy.

sis and a normality test are performed. A model parameter x_j $(j = 1, ..., J)$ 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 is a number of model responses (k=1,2,...,K). Only if one parameter is a sensitive parameter (i.e. $(\Sigma S^k)_j > S_0$ with $S_0 > \epsilon > 0$) and the distribution of its samples generated by sampling process follows a normal distribution $(W_j > W_0)$, the confidence interval will be used to assess the reliability of the parameter. The normality test is done according to Shapiro-Wilk [7]. Certainly, the reliability of the identified parameters is higher in general, when n_p is greater. The confidence intervals are determined based on the probability distribution of the samples, see [5].

3 BACK ANALYSIS OF THM COLUMN EXPERIMENTS

3.1 Summary of forward THM analysis

Back analysis based parameter identification is used widely for calibrating parameters for geotechnical models. There are still few works in literature on the identification of the model parameters for coupled THM model based on back analysis approaches. The coupled THM phenomenon is recently attracting the attention of the researchers and engineers involved in the conceptual design of engineered barriers for storage of spent nuclear fuel and nuclear waste. The effects of the THM phenomena play an important role to optimise performance of the buffer system for the nuclear waste containers. In the following subsections, the constitutive models used for the coupled THM analyses are presented.

The solution of the coupled THM problems is performed via the finite element method. The constitutive relations are summarised in Table 1. Due to the complexity of the constitutive model there is a large number of model and material parameters involved in it. The material model parameters in the THM analysis are classified in groups depending on their relation to the stress-strain response (net stress driven processes), hydraulic loading (suction driven processes), and to the temperature change. The aim is to clarify the influence of each group of parameters on the coupled THM response of the soil. The input parameter vector $\boldsymbol{x}$ is composed of the following parameter sets:

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

- Parameters involved in modelling net stress driven processes (d$\boldsymbol{\sigma} \neq 0$):
  $\mathcal{M} = (k_{io}, \alpha_i, p_{ref}, \lambda(0), r, \beta, k, p_{s0}, p^c, M, \alpha, e_o, p_o^*)$
- Parameters involved in modelling suction driven processes (d$s \neq 0$):
  $\mathcal{H} = (P_0, \lambda, \phi_0, k_o, k_{s0}, \alpha_{ss}, \alpha_{sp})$
- Parameters involved in modelling temperature driven processes (d$T \neq 0$):
  $\mathcal{T} = (\tau, D, n_D, \lambda_{sat}, \lambda_{dry}, \alpha_0, \alpha_1, \alpha_3, \rho)$

Therefore the vector of model parameters reads:

$$\boldsymbol{x} = (\mathcal{H}, \mathcal{T}, \mathcal{M}) \tag{1}$$

The vector of model response $\boldsymbol{y}^{calc}$ is composed as follows:

$$\boldsymbol{y}^{calc} = (y_{tm}^d(\boldsymbol{x}))^{calc} = (S_l(tm), \sigma_{yy}(tm), T(tm), s(tm))^{calc} \tag{2}$$

where $S_l(tm)$ is the degree of saturation over time t at observation point m, $\sigma_{yy}(tm)$ is the vertical stress, $T(tm)$ is the temperature, and $s(tm)$ is suction.

3.2 Results

Figure 3 presents the histograms and scaled Student probability density distribution (PDF), in which model parameters are normalised from 0 to 1 corresponding to their minimum and maximum boundaries, respectively. From Figure 3, it is clear that these parameters have their distribution close to the normal distribution. The figure also indicates that the high sensitive parameters have narrow ranges of their probability density functions (i.e. P_0, λ, $\boldsymbol{k}_0$). Less sensitive parameters have wider ranges of their probability density distributions (i.e. λ_{sat}, κ_{s0}, n_D). For the non-sensitive model parameters, the probability distributions show no pattern and significantly deviate from the normal distribution. From this, we derive that the confidence intervals for these parameters may not be reliably estimated. The confidence intervals are estimated considering typical confidence coefficients ($\gamma_c = 95\%$), which means that the expected value of each of the identified model parameters is with 0.95 probability within to the confidence interval. Table 2 presents the mean value, the upper (CI_U) and the lower (CI_L) bound of the confidence interval. The result in Fig. 3 shows that in general the parameters, which are highly sensitive (e.g. $\boldsymbol{k}_0$, λ, P_0), have a more pronounced peakedness. In contrast, the low sensitivity parameters (e.g. λ_{sat}, κ_{s0}, n_D) have less pronounced peakedness.

Table 2: Confidence intervals of the optimal parameters

	P_0	λ	$\mathbf{k}_0$	λ_{sat}	κ_{s0}	n_D
Mean	1.51	0.339	2.03E-16	1.33	0.0071	0.79
CI_L	1.45	0.328	1.55E-16	1.28	0.0012	0.73
CI_U	1.58	0.349	2.50E-16	1.38	0.013	0.86

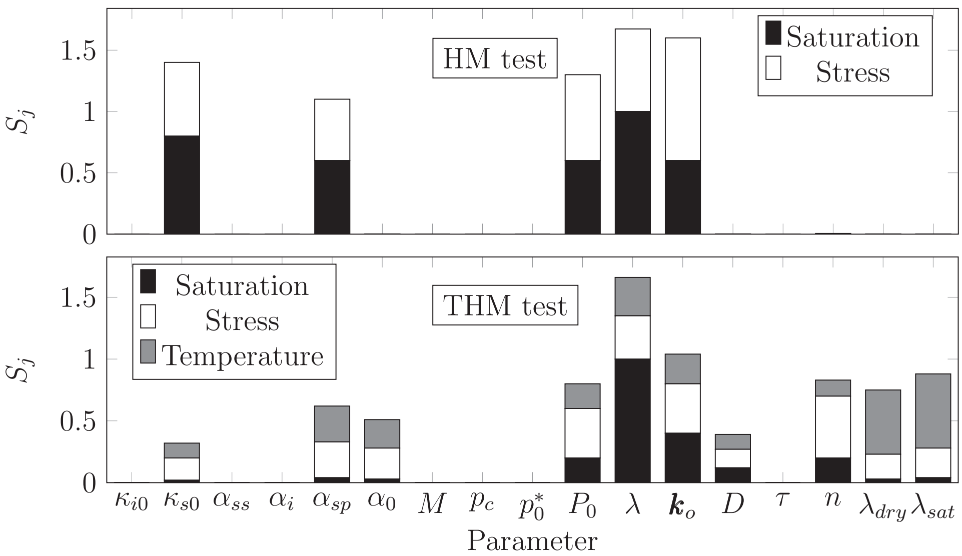

Figure 2: Sensitivity indices S_j.

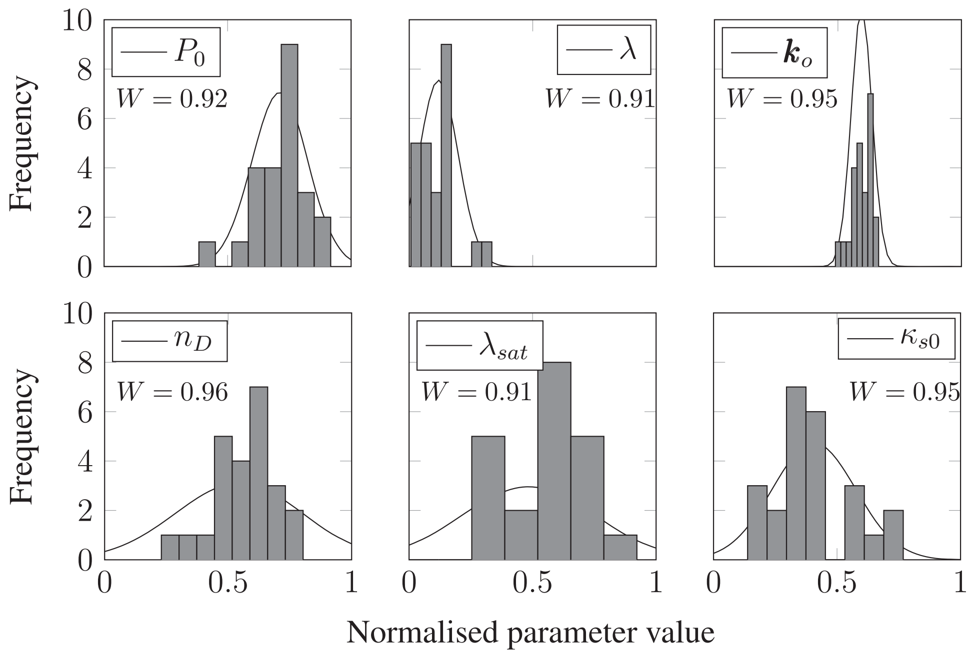

Figure 3: Histogram and PDF of the parameter samplings

4 CONCLUSIONS

We propose a back analysis approach combining model parameter identification and the assessment of the reliability of identified model parameters. The obtained results show that it is a promising method for model parameter identification, especially in coupled multi-physical process simulations involving complex non-linear constitutive laws. The reliability of an identified parameter depends on its sensitivity revealed under the particular boundary conditions taking place in the forward problem. The approach can be applied for back analysing a variety of geotechnical problems, especially, it is designed for parameter identifications of problems having a large set of constitutive model parameters and a large set of model responses.

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