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Proceedings of the 24th UK Conference of the
Association for Computational Mechanics in Engineering
31 March – 01 April 2016, Cardiff University, Cardiff

AN EVOLUTIONARY APPROACH TO MODELLING EFFECTS OF CHEMCALS ON SOILS

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ABSTRACT

As part of a study undertaken to assess the impact of high-pH fluid circulation on the shear strength behaviour of a compacted soil with different additives and due to the complexity of the existing constitutive theories, a new approach was used, based on an evolutionary polynomial regression, for modelling the processes. EPR is an evolutionary-based data mining technique with the capability of generating transparent and structured representation of behaviour of materials and systems from measured data without any need for the data to be processed. EPR model developed and assessed using data from a set of triaxial tests. The outcome from developed model was compared to the experimental results expressing good consistency.

Keywords: *mechanical behaviour of soils; chemicals; evolutionary data mining*

1. Introduction

Cuisinier et al [1, 2] conducted a study to investigate the influence of circulation of high-pH water on the hydromechanical behaviour of compacted materials to be used for backfilling. During the study the geomechanical behaviour and the microstructure of the considered materials were followed over a period of alkaline water circulation of 12 months. The influence of the alkaline fluid on the geomechanical characteristics of the materials as a result was seen to directly relate to the nature of the additives. The geomechanical behaviour of the sand – argillite mixture has, for instance, remained almost stable during the period of alkaline water circulation while, over the same period, dramatic modification of the lime – argillite mixture was observed. The next stage in the study was to identify the coupling parameter(s) between the chemical stress induced by the circulation of alkaline water and changes in the hydromechanical behaviour of the tested mixtures, however, the large number of tests on various mixes proved the process to be complex [3].
Therefore, a new approach was implemented, based on evolutionary polynomial regression (EPR) to model the complex hydromechanical behaviour of the soil during circulation of the alkaline fluid. EPR is a data mining technique, based on evolutionary computing, aimed to search for polynomial structures representing a system [our paper]. The key idea behind the EPR is to use evolutionary search for exponents of polynomial expressions by means of a genetic algorithm (GA) engine [4]. The main advantage of EPR over other data mining techniques such as neural networks is that it provides a transparent and structured representation of the behaviour of the system in the form of a clear mathematical expression that is readily accessible to the user. EPR has shown its potential in application in modelling of complex behaviour of soils [5-9].

2. Evolutionary Polynomial Regression (EPR)

EPR is a data-driven method based on evolutionary computing, aimed to search for polynomial structures representing a system. A general EPR expression can be presented as [4]:

$$y = \sum_{j=1}^{n} F(X, f(X), a_j) + a_0 \qquad (1)$$

where y is the estimated vector of output of the process; a_j is a constant; F is a function constructed by the process; X is the matrix of input variables; f is a function defined by the user; and n is the number of terms of the target expression. The general functional structure represented by F(X, f(X), a_i) is constructed from elementary functions by EPR using a Genetic Algorithm (GA) strategy. The GA is employed to select the useful input vectors from X to be combined. The building blocks (elements) of the structure of F are defined by the user based on understanding of the physical process. While the selection of feasible structures to be combined is done through an evolutionary process, the parameters a_j are estimated by the least square method. This technique uses a combination of the genetic algorithm to find feasible structures and the least square method to find the appropriate constants for those structures. In particular, the GA allows a global exploration of the error surface relevant to specifically defined objective functions. By using such objective (cost) functions some criteria can be selected to avoid the overfitting of models, push the models towards simpler structures and avoid unnecessary terms representative of the noise in the data. An interesting feature of EPR is in the possibility of getting more than one model for a complex phenomenon. A further feature of EPR is the high level of interactivity between the user and the methodology. The user physical insight can be used to make hypotheses on the elements of the target function and on its structure. Selecting an appropriate objective function, assuming pre-selected elements based on engineering judgment, and working with dimensional information enable refinement of final models. The level of accuracy at each stage is evaluated based on the coefficient of determination (COD) i.e., the fitness function as:

$$\mathbf{COD} = 1 - \frac{\sum_N (\mathbf{Y}_a - \mathbf{Y}_p)^2}{\sum_N \left(\mathbf{Y}_a - \frac{1}{N} \sum_N \mathbf{Y}_a \right)^2} \qquad (2)$$

where Y_a is the actual output value; Y_p is the EPR predicted value and N is the number of data on which COD is computed. If the model fitness is not acceptable or the other termination criteria (in terms of maximum number of generations and maximum number of terms) are not satisfied, the current model goes through another evolution in order to obtain a new model. Detailed explanation of the method can be found in [4, 5].

3. Database used in developing the EPR model and model outcomes

Results obtained from 33 consolidated undrained triaxial tests on samples of argillite (MA), lime-MA, sand-MA, bentonite-MA mixtures, subjected to different periods of circulation of alkaline water, were considered in developing and validating of the EPR model. Of the total of 33 cases, 29 cases related to different circulation times (i.e. 0, 3, 6, 12 months) were used for training of the EPR model. Of these 29 cases, 11, 5, 2 and 11 cases were related to no circulation, 3 months, 6 months and 12 months of circulation of the alkaline water through the samples, respectively. The remaining cases relating to different soil and circulation times were kept unseen during the model development process and were used in the validation stage of the developed model. Parameters involved in the model development which were used as input for the EPR model were dry density, alkaline water circulation time, axial strain, pore pressure, effective confining pressure, porosity of macro-pores, porosity of micro-pores, and the specific surface of the soil particles. The only output was considered to be the deviatoric stress [3].

Figures 1 shows typical prediction results from the EPR model for lime-argillite mixture at confining pressure of 141 kPa after 6 months of circulation for training data. The results are compared with actual measurements. It can be seen that the EPR model has been able to capture the behaviour of the mixtures with a good accuracy. Figure 2 also presents results predicted by the developed EPR model for a testing data series that was kept unseen to EPR in training stage for lime-argillite at confining pressure of 274kPa after 6 months of circulation of alkaline water.

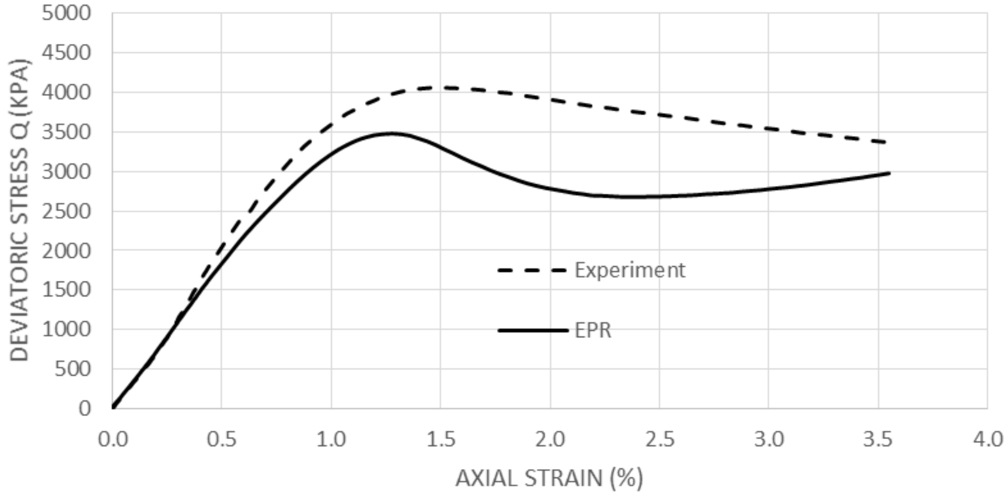

Figure 1: Results from the EPR model – lime-argillite, confining pressure =142kPa (training data)

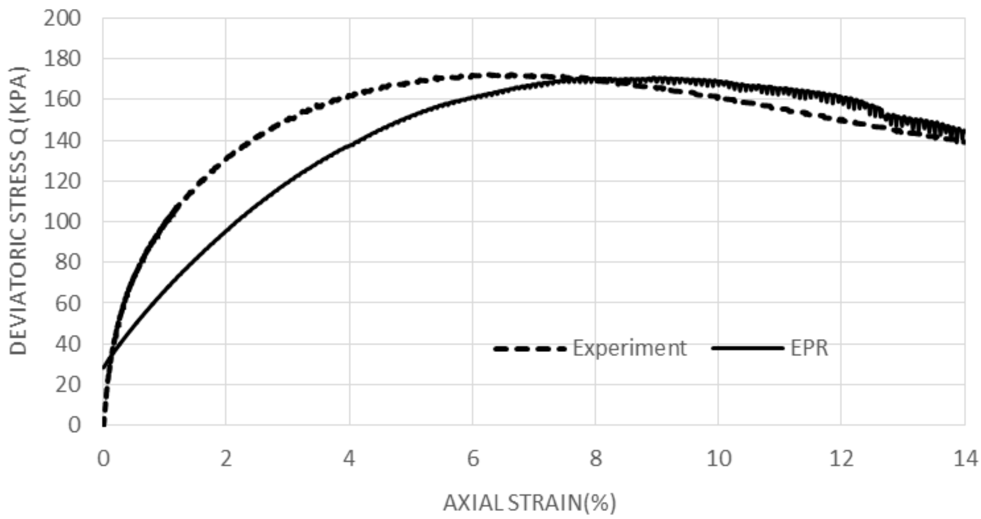

Figure 2: Results from the EPR model – lime-argillite, confining pressure =274kPa (testing data)

It can be seen that the developed model has presented high capabilities in generalising the training stage of the model development to conditions that were not introduced to the EPR during the stage that the training process took place.

4. Discussion and conclusions

The research was conducted to model the impact of alkaline fluid circulation on the mechanical behaviour of argillite mixes with different additives because of lack of sufficient constitutive relationships able to describe the behaviour of different mixtures in a unified framework. The work aimed at developing a model based on an evolutionary-based data mining technique, evolutionary polynomial regression (EPR), to represent and predict complex hydromechanical behaviour of soils during circulation of an alkaline fluid.

The presented predictions from the developed EPR model showed that the model, which was trained from pure experimental data (with no pre-processing), was capable of capturing and representing many physical characteristics of the behaviour of the different mixtures considered in the study and the effect of the alkaline fluid circulation correctly, and with a high accuracy for training data. In order to validate the generalization capabilities of the developed model, unseen cases of data which were not presented to the EPR at the training stage was presented to the model. The predicted outcomes showed strong capabilities of the model in providing predictions for cases that were not previously known to the model.

An interesting feature of EPR is in the possibility of getting more than one model for complex phenomena. The best model is then chosen on the basis of its performances on a test set of unseen data. In general, EPR based modelling has several advantages including it provides a simple and straightforward framework for modelling of all materials. It does not require any arbitrary choice of the constitutive (mathematical) model, yield function, plastic potential function, flow rule etc. As EPR learns the material behaviour directly from raw experimental data, it is the shortest route from experimental research (data) to numerical modelling. Additional advantage of EPR model is that as more data becomes available, the material model can be improved by re-training the EPR.

References

[1] O. Cuisinier, F. Masrouri, M. Pelletier, F. Villieras and R. Mosser-Ruck. Microstructure of a compacted soil submitted to an alkaline plume. *Appl Clay Sci*, 40, 159–70, 2008a.

[2] O. Cuisinier, D. Deneele and F. Masrouri. Shear strength behaviour of compacted clayey soils submitted to an alkaline plume. *Eng Geol,*108, 177–88, 2008b.

[3] O. Cuisinier, A. A. Javadi, A. Ahangar-Asr and F. Masrouri. Identification of coupling parameters between shear strength behaviour of compacted soils and chemical's effects with an evolutionary-based data mining technique. *Computers and Geotechnics*, 48, 107-116, 2013.

[4] O. Giustolisi, D. A. Savic. A symbolic data-driven technique based on evolutionary polynomial regression. *J Hydroinform*, 8, 207-22, 2006.

[5] A. A. Javadi and M. Rezania. Applications of artificial intelligence and data mining techniques in soil modelling. *Geomech Eng*,1, 53-74, 2009.

[6] M. Rezania, A. A. Javadi and O. Giustolisi. An evolutionary-based data mining technique for assessment of civil engineering systems. *J Eng Comput*, 25, 500-17, 2008.

[7] A. Ahangar-Asr, A. A. Javadi and N. Khalili. An evolutionary approach to modelling the thermo-mechanical behaviour of unsaturated soils. *International Journal for Numerical and Analytical Methods in Geomechanics*, 39, 539-557, 2015.

[8] A. A. Javadi, M. Hussain, A. Ahangar-Asr and R. Farmani. A surrogate model for simulation-optimization of aquifer systems subjected to seawater intrusion. *Journal of Hydrology*, 532, 542-554, 2015.

[9] A. Ahangar-Asr, A. A. Javadi, A. Johari and Y. Chen. Lateral load bearing capacity modelling of piles in cohesive soils in undrained conditions; an intelligent evolutionary approach. *Applied Soft Computing; an international journal*, 24, 822-828, 2014.