Computational Methods in Engineering - Recent Research and Future Perspective

A report submitted to

Korean Institute of Construction Technology (KICT)

submitted by

International Centre for Computational Engineering (IC2E)
Rhodes, Greece and Swansea, UK

January 2013

EXECUTIVE SUMMARY

This report has been prepared by the International Centre for Computational Engineering (IC2E), an educational charity based in Rhodes, Greece with a branch in Swansea, UK. It is being submitted to the Korean Institute of Construction Technology (KICT) who awarded a research contract to IC2E in February 2012 to report on emerging technologies and trends on the world scene.

This report describes research conducted in recent years by important geomechanics groups in UK and abroad. Four topics are highlighted. These are environmental geomechanics, issues related to petroleum engineering, mechanics of partially saturated soils and development of constitutive model for soils. Suggestions for future research based on the emerging technologies are also indicated.

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INTRODUCTION

International collaboration is one the most important aspects of modern day research in any field of science and technology. More and more engineering research is becoming globally collaborative. The main reason for this trend is rapid developments in communication and information technology. Though there are still some unavoidable barriers such as language and time zones, they can be overcome given the will to harness existing knowledge pools rather than everyone develop their own. Setting up of International Centre for Computational Engineering (IC2E) is a modest attempt to facilitate international co-operation.

In late 2011, a contract was awarded by KICT to IC2E with the following remit:

(1) Conduct a survey of research trends on a number of world leading research groups and periodic reporting in the field of convergence technologies in combination with Geotechnical Engineering & IT/CE (Computational Engineering).

(2) Searching for key technologies to make a breakthrough in inherent difficulties in geotechnical engineering and detailed research plans for the found items are made by coordination of key algorithms and resources.

(3) Developing a number of new research items with the industrial X-ray CT facility available in KICT and establishing detailed research plan for each item. Some feasibility studies are made for chosen items if needed.

This report deals with items 1 and 2 above. The report has two main sections. The first deals with recent advances in geomechanics and the second points out future directions emerging due to changes taking place on the world scene. A section on recommendations for future work concludes the report.

Recent advances in computational geomechanics

Here, we present a short survey of developments that have taken place during the past 5 years. There are four main areas under which research has progressed globally.

1. Environmental Geomechanics

Research in environmental related issues affecting design, construction and maintenance of engineering structures has been on the forefronts during recent years. Change in global climate is being experienced by the world population as severe cold and hot weather becomes routine. This in turn leads to higher demand for energy which is further accelerated by phenomenal growth in so called 'developing countries'. Many countries have adopted policies for generation of electricity using nuclear material and requirement of their safe disposal will have to be met globally. The disposal of nuclear waste and storage of CO_2 in deep underground repositories seems to be only viable solution. Although many Governments and research bodies have been working on the topic of nuclear waste disposal for decades, sequestration of CO_2 is fairly new concept (Selvadurai, 2011).

A realistic design of waste disposal facility will require extensive computer simulation using *coupled hydro-mechanical-thermal analysis* since physical experiments will be almost impossible to conduct and they will never be able to simulate 'time' properly. In the past, geotechnical engineers have often used uncoupled hydro mechanical analyses effectively. However, it will not be possible to use these approaches in complex situations.

French, Belgian and Swiss engineers have been working on the underground waste disposal problems for over 25 years and all three have underground laboratories in their countries.

Accurate solution of coupled equations involves a number of material parameters which are strain, gradient (hydraulic and thermal) and temperature dependant. Determination of these is not likely to be easy and simple. Here 'inverse analysis' using Artificial Intelligence which has been developed (Shin and Pande, 2000) will be of great use, if developed further and packaged in usable commercial environment.

2. Petroleum Geomechanics

Geomechanics in petroleum engineering has evolved over a period of ten years. In the past most studies of reservoir models involved fluid flow without any considerations of stresses and deformations in the porous medium.

However coupled analyses are being routinely used by most oil companies. The results of these analyses are as realistic as the parameters used in them. One important issue in all coupled problems is that of 'permeability tensor'. For example, permeability of an oil reservoir may be crucial in establishing its viability for exploitation whilst prevention of leakage from underground storage facilities for oils and gas, nuclear waste as well as CO2 crucially depends on its long term values. Permeability is an illusive parameter which is difficult to obtain not only in field situations but also in controlled laboratory environment. Its determination is further complicated by the fact that values are needed for low permeability porous media such as clays/rocks at various degrees of saturation and at elevated temperatures which makes physical experiments not only expensive but also difficult and time-consuming. Permeability is indirectly related to the porosity, pore-size distribution and pore-architecture. A well-known way to obtain this information is through mercury porosimetery but this procedure has safety issues associated with it as well as it is not an easy experiment to conduct. Attention is currently being focussed by many researchers on determining permeability tensor through indirect means such as flow models and pore network models (Pearce & Pande, 2007; Shin & Pande, 2013).

3. Mechanics of partially saturated porous media

The writer of this report and his co-workers have been skeptical of the research on partially saturated soils which has become fashionable over the past 15 -20 years. Books and a large number of papers have been written by researchers in soil mechanics who seem to have a poor understanding of the principles of mechanics.

This has led to a plethora of empirical equations, hypotheses claimed to be applicable to partially saturated soils. Vast amounts of money have been spent worldwide on this fruitless research. Reasons for this are pointed out by Pande and Pietruszczak (2011).

The followers of traditional point of view introduce an additional state parameter such as ‘suction pressure’, being defined as the difference of the pore air pressure (u_a) with reference to the pore water pressure (u_w). They argue that suction is required as a 'state parameter' to capture the behaviour of partially saturated soils. Following the paper by Alonso et al. (1990), the Basic Barcelona (BB) model has been extended and refined by many researchers, too numerous to mention here. However, the present authors have had a different view on the description of the problem that was expressed in a number of papers published in 1990’s (Pietruszczak & Pande; 1991, 1996). The basic assumption in these papers is that partially saturated soils can be viewed as a composite material with soil skeleton, pore water and pore air as three constituents. With this assumption, given the microstructure of saturation and the constitutive relations for the constituents (e.g. soil skeleton, water and air), the averaged behaviour of partially saturated soil at any degree of saturation can be defined following the well established procedures of homogenisation. Numerical experiments with the constitutive model based on this approach indicate that even a small reduction in the degree of saturation from the fully saturated state makes the soil significantly less susceptible to liquefaction (Pietruszczak et al., 2003). This hypothesis has been verified through numerical simulations as well as physical experiments (Pande & Pietruszczak, 2008). The additional parameter needed for the description of the behaviour of partially saturated soils is pore size distribution.

In the early stages, many researchers criticized work of Pietruszczak & Pande saying that it will be impossible to introduce pore size distribution characteristics in soil behaviour. However, recent developments in CT scanning technology indicate that it is perfectly feasible (Shin, Kim & Pande, 2012). In this paper, the authors demonstrate the use of micro X-ray CT scanning technique to obtain porosity and its variation in clays. Since the resolution of micro CT equipment is not high enough to be able to observe specific pores in clays, an experimental programme to correlate porosity with data from scanning was undertaken. It consisted of consolidating specimens made from a mixture of kaolinite and bentonite in an oedometer, unloading them and obtaining 32mm samples from various locations, scanning them as well as determining void ratio of these specimens using standard laboratory procedures. It is observed that the Average CT Number (ACTN) for the specimens correlated well with the porosity (void ratio) whilst spatial variation of CT numbers seems to indicate the capability of scanners to capture pore size distribution. This indicates the possibility of computing porosity and pore size distribution of even fine grained soils.

4. Constitutive models for soils

This topic has been researched for over three decades and still seems to attract many new researchers. Pande & Pietruszczak (2011) presented a commentary on this topic and brought to attention vital points which are still missing from constitutive models. These will be highlighted here. In the eighties a number of models based on nonlinear elasticity, simple elasto-plastic models and critical state based models (isotropic, volumetric hardening) were proposed. For simulating cyclic loading two, multi- and infinite surface models (Pietruszczak & Mroz, 2001; Dafalias, 1986) were proposed. These were largely extensions of metal plasticity models extended and adapted for geomaterials. A new class of models termed as later termed as multi-mechanism framework models were proposed. These included spatially mobilised plane (SMP) concept (Nakai & Matsuoka, 1986), multilaminate framework (Pietruszczak & Pande, 1988; Sharma & Pande, 1988; Schweiger & Pande, 1986) and micro-plane framework (Bazant & Pratt, 1988). Another line of work called endochronic theory (Bazant, 1978) was promoted by some researchers as panacea of all problems. In addition a number of adhoc models such as the 'Brick model' (Simpson, 1992), MIT Model (Whittle & Kavvadas, 1996), 'Hardening soil model' (Schanz et al. 1999), 'Soft soil model (Schanz et al. 1999) have been proposed. Some of these are not correct but have been made available in software in an obscure way. In addition there are also 'Damage theory' based models.

In spite of this there are two pending issues.

1. Modelling of anisotropy - Inherent due to deposition history, fabric structure, joints and discontinuities and induced due to plastic flow is captured correctly by only a few models. Both are equally important.
2. Influence of Rotation of Principal Stress Axes is modelled by the multi-laminate framework based models

There are three possible ways of modelling this: (a) Incorporation of microstructure/fabric tensor (b) Critical plane approach (c) Casting the constitutive model in the multilaminate framework

Only a few aspects of plastic flow induced anisotropy (e.g. Bauschinger effect) in initially isotropic materials can be modelled by kinematic hardening models. Directional dependence of mechanical behaviour cannot be achieved by manipulating yield surfaces. Of the three approaches mentioned above, casting the constitutive model in the multi-laminate framework is the simplest and a practical approach.

Future Perspective

It seems to the writer of this report that there are some notions in the mechanics of soils need to be revived or emphasised. These are:

Pore-size, particle size characterisation:

Particle size distribution is well embedded in geotechnical engineering practice. Practicing engineers always look at the gradation curve which indicates whether the soil is well-graded or poorly graded. Gradation curve must also play an important role in the constitutive behaviour of soils. Constitutive models are usually tied to the type of soil, i.e. clay, sand etc. They may also be governed by the history of consolidation, i.e. normally consolidated, over-consolidated etc. The influence of an 'average' particle size, coefficient of variation of the particle size, coefficient of conformity etc. are the parameters that need to be introduced in constitutive models.

Moreover, all soils for engineering practice are not pure sands, silts and clay.

Pore size distribution is the dual of particle size distribution. The two are intuitively inter-related. There seems to be not enough research conducted on this topic in the past. However, advanced techniques like X-ray CT scanning should be used to establish a correlation between the two. Transport properties are more likely to be influenced by porosity and certainly pore-size distribution than any other factors.

Rotation of principal stress axes

The phenomenon of plastic flow induced anisotropy, plastic flow due to pure rotation are real and need to be accounted for in geotechnical modelling. The problem of construction of tunnels involves rotation of principal stress axes by 45 degrees. A soil element under undrained conditions can liquefy without change of stress under pure rotation. We cannot analyse liquefaction potential of a sand layer under earthquake conditions if our model does not take into account the influence of rotation of principal stress axes.

Inverse analysis and Artificial Intelligence

The pioneering research conducted by Dr Shin (Shin & Pande, 2000) indicated that there is a potential for developing a mechanical testing machine which would enable determination of multiple material parameters from a single mechanical test. This will also have the advantage that the specimen preparation effort will be greatly reduced or eliminated.

Unfortunately no progress has been made in this area in the UK or USA due to lack of funding which needs support from industry. However, the writer of this report belives that it is an opportunity for a progressive organisation like KICT to seize this opportunity.

Partially saturated soils

Role of pore-size distribution cannot be over-emphasised here. Researchers are simply mis-guided and continue to work in the well-established wrong lines. In recent years determination of soil-water retention curves (SWRC) has been undertaken by a number of researchers. A well known researcher believes that we should use this to describe behaviour of partially saturated soils. Little do people realise that a SWRC is indeed a reflection of pore-size distribution curve. Indeed, SWRC can be used to study pore-size distribution of a soil. However some experiments and validation will have to be carried out. Models proposed by Pietruszczak & Pande (1996) need to be re-visited and with some experimental work can form the basis of a ground-breaking paper.

<u>X-ray CT technology</u>

The writer of this report believes that KICT with their CT capabilities is in a unique position to lead industrial research of practical importance. This opinion is based on rapid progress being made on the following issues:

- Determination of Porosity from CT scans- this has already been demonstrated by (Shin & Kim, 2011)
- Determination of spatial variation of porosity (Shin, Kim & Pande, 2012)
- Determination of pore-size distribution
- Determination of degree of saturation and its spatial distribution from CT scanning

The KICT facility will have to be calibrated under controlled conditions. Effectiveness of filtering techniques and interpretation of CT data is the key factor. Two feasibility studies (Swansea University, UK & NAGRA, Switzerland) are being proposed for taking this research forward. These should be completed expeditiously.

A 'round robin' test programme with organisations world-wide having X-ray CT facilities participating in it can be organised by IC2E.

Conclusions

This report represents the writers personal views. It emphasises how many aspects of behaviour of geomaterials in dry, partially saturated and fully saturated states can be understood, modelled and applied to the analysis of geotechnical structures. A single factor which is required to be determined relates to the materials pore/particle size distribution. This can be determined from X ray CT technology after additional research.

Many other suggestions are also included in the report.

Acknowledgement

The writer thankfully acknowledges the financial support given by KICT to IC2E. It also gave an opportunity to the writer to interact and work with Dr Hyu Shin of KICT who spent a year in Swansea.

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