SELECTING ADVANCED CONSTITUTIVE MODELS: AN OVERVIEW

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ABSTRACT

Numerical modelling is becoming universal in rock engineering practice. Most applications focus on the prediction of failure loads of 2D problems, where the numerical models are useful extensions to analytical methods and experience-based design criteria. For 3D problems and problems where the assessment of serviceability indicators – displacements, ground-structure response, etc. – are of importance, the selection of the constitutive models themselves and the implications of the selection of material parameters may have a very heavy impact on the reliability of the model outcome and its predictive capability.

This paper overviews basic common aspects of constitutive equations used in practical rock engineering and summarizes some challenges that are frequently observed when reviewing numerical models performed for routine problems in rock engineering.

KEYWORDS

Continuum mechanics, constitutive models, material parameters, strength, deformation, plasticity.

INTRODUCTION

Numerical methods

From a philosophical perspective models, either analytical or numerical, are idealizations of a perceived reality. For us engineers, models are just tools we use to guide our judgement and understanding of the problem in hand. When dealing with problems in rock engineering, we resort to a wide range of techniques:

- 1. Closed form solutions like confinement-convergence methods for circular tunnels: these methods satisfy equilibrium and compatibility requirements at the cost of a crude simplification of the material behavior and geometry;
- 2. Limit analysis methods, like bearing capacity formulas: lower bound methods satisfy equilibrium but sacrifice compatibility, and upper bound methods do the opposite. Material behavior must be simple, geometry admits limited freedom;
- 3. Limit equilibrium methods, like method of slices for slope stability: they satisfy restricted forms of equilibrium, do not satisfy compatibility requirements, require simple material behavior but have a much greater flexibility on geometry;
- 4. Numerical methods, where a mesh is employed to discretize the problem geometry: when properly formulated, these methods satisfy equilibrium and compatibility requirements and give reasonable approximations to the behavior of very complex geometries and construction sequences. Very little restrictions remain on geometry and material behavior, but the cost of calibrating the material parameters can be very high.

All these techniques can be used to compute ultimate loads, probability of failure and factors of safety. Methods 1 and 4, the only ones fully friendly with physics, may be also used to estimate displacements and other serviceability requirements.

In a numerical model, the behavior of the material is idealized by a constitutive equation (conceptually, a stress-strain curve), the geometry is idealized by a mesh and the construction/production process is idealized by a sequence of loads and changes in the mesh geometry and/or the input data for the

constitutive equations. Poor definition of any of these three ingredients yields unusable results, and that is why numerical models are tricky and prone to error, and should be used only when at lest one of these statements applies (Potts et al 2002):

- 1. Complex geometry and geological conditions are addressed;
- 2. Deformation of interacting structures should be predicted;
- 3. The effect of complex material behaviour, including non-linearity, plasticity and creep, should be considered;
- 4. The solution is considerably influenced by the in situ stress state;
- 5. The effect of construction techniques, construction sequence and construction speed should be estimated;
- 6. Monitoring is planned and limiting values of the expected displacements, pore pressures and other quantities are required;
- 7. Possible failure mechanisms and the corresponding deformation criteria should be determined;
- 8. Back analysis of measurement results is performed and the material properties (constitutive models and parameters) are to be identified.

Numerical models are now routinely used for solving problems in the various fields of rock engineering, mainly to assess the risk of failure of a given problem. We pay close attention to stress, strength, probability of failure and "satety factors"; any outcome of the model dealing with deformations is regarded with caution. Only statements 1, 7 and 8 of the above list are frequent; other statements rarely apply.

Standard vs advanced modelling

More value from numerical models in rock engineering can be obtained if we improve the consistency of our estimates for risk of failure – the current main use of numerical models – and the reliability of our estimates for deformation, displacement and other serviceability indicators. For the first objective, the community effort is enormous and ongoing, led by the academia but now widely used in practice. For serviceability, the huge efforts of the academia permeate more slowly into practice: serviceability forecasts are most frequently based on the calibration of past behavior of the same operation, green-field predictions are used with less confidence.

In this paper, standard models are defined as such numerical models which mainly intend to obtain a stress field, an estimate of risk of failure or a safety factor. For instance, models addressing slope stability problems and using rock-mass characterization tools for estimating strength parameters fall in this category.

Advanced models intend to go beyond that point, either addressing ground-structure interaction problems – like deformation of supported underground openings – or by dealing with very dissimilar materials – like the modelling of tailings infilling of abandoned labours. For such advanced models, the risk of badly erring in the outcome is heavily dependent on the choice of the constitutive equations themselves, not just the calibration of its material parameters.

Continuum vs discontinuum models

Rock masses are discontinuous media, and therefore discontinuum media methods – UDEC and 3DEC, for instance – offer a fundamentally sound approach to rock modelling despite the many challenges they must still address (Bobet et al 2009). These models are involved and expensive because their predictive capability depends on the accurate description of the geometry, spacing and mechanical behavior of the controlling structures, features that must be included in the model with the required level of detail.

For routine analyses, tools based on the theory of continuous media are by far the most widely used. FLAC, Phase², Plaxis, Abaqus are examples of such tools. Here, the discontinuous nature of rocks is blurred into "anisotropy" and "rock-mass". Discontinuous behavior, rock-mass and anisotropy are yet fundametally different. In "engineering" words, anisotropy means different behavior in different directions, rock-mass means different behavior at different scales, while discontinuous behavior means blocks moving at their interfaces.

When using continuous media tools, scaling of properties is mandatory and well accepted in practice. Contributions from academia on procedures for scaling material properties have been enormous and most promising: we may expect that over-mature empirical formulas be complemented by Synthetic Rock Mass (SRM) procedures (Ivars et al 2011, Pierce et al 2007) to compute rock-mass material properties using a more fundamentally correct approach (Hoek 2009). If this is the case, the popular use of numerical models for advanced problems may be closer in time for the industry of rock engineering, and – maybe – will allow us to predict deformations of rock masses with a level of confidence similar to what we enjoy in soils engineering today.

The focus of this paper

This paper focuses on the challenges identified during years of review of numerical models in the practice of soil and rock engineering and the opportunities that they give beyond solving strength problems. Only models based on continuum mechanics are discussed, discontinuous techniques like UDEC, 3DEC or PFC models or similar are beyond the scope of the paper. It aims to overview the basics behind the constitutive equations available in codes like FLAC, Abaqus, Plaxis, Phase², etcetera and to highlight where there is hidden value for practitioners. The scope is limited to practical aspects of the constitutive methods themselves and the meaning of their input parameters. Data collection, procedures for calibration, methods of analysis and the interpretation of any outcome of models are beyond the scope of this paper.

MATHEMATICAL STRUCTURE OF A CONSTITUTIVE MODEL, AND IMPLICATIONS

Definition

A constitutive model – or constitutive equation – is a set of equations, expressions and formulas that fully determines the state of the material for any known state and after any change in its configuration. Restricted to practical aspects of rock engineering, a constitutive model is a set of equations that can be seen as a box: the input is the current value of the stress tensor $\boldsymbol{\sigma}$ at a given step *n* (boldface indicates a tensorial quantity), the current value of some state variables, denoted as ρ , and a strain increment $\Delta \epsilon$, and the output is the updated stress and the updated value for the state variables. In formulas

$$\boldsymbol{\sigma}_{n+1} = f(\boldsymbol{\sigma}_n, \rho_n, \Delta \boldsymbol{\epsilon}) \tag{1}$$

$$\rho_{n+1} = f(\boldsymbol{\sigma}_n, \rho_n, \Delta \boldsymbol{\epsilon}) \tag{2}$$

Material parameters and state variables

Material parameters are input constants that do not change during the calculations. Bulk modulus is a typical example of a material parameter in many models.

State variables describe the actual state of a material and change during the calculation over a wide (physically allowable) range. It should be possible to measure state variables directly – at least theoretically – at any moment in time. Stress and temperature are examples of state variables. Material parameters and state variables combine to form functions of state variables.

The separation between material parameters and state variables is model dependent. For instance, the bulk modulus may be a material parameter in one model, and a state variable in a different model. In linear elasticity, the pressure is a state variable. Its increment p is computed using the simple expression

$$\dot{p} = K \dot{\epsilon}_{v} \tag{3}$$

where $\dot{\epsilon}_v$ is the volumetric strain increment and *K* is the bulk modulus (a material parameter). In a more advanced model we can have a pressure-dependent bulk modulus K(p) and therefore

$$\dot{p} = K(p) \,\dot{\epsilon_v} \tag{4}$$

A common expression used in soils engineering is

$$K(p) = K_{ref} \left(\frac{p}{p_{ref}}\right)^m \tag{5}$$

In this case, K(p) is a function of the state variable p, and the material parameters of the model are K_{ref} , m and p_{ref} .

To reproduce the behavior of a nonlinear elastic material, one may use a model like the one described by eqns. (4) and (5). One should not use eqn. (3) and change K by hand, because the bulk modulus is an outcome of the model and not an input value. The distinction is not just of "academic value". In the elementary example of eqns. (4) and (5), the exact solution for p is

$$p = \left(\frac{\kappa_{ref}}{p_{ref}} \cdot \epsilon_{v}\right)^{\frac{1}{1-m}} p_{ref} \tag{6}$$

Table 1 compares the results obtained by updating K by hand in five steps and the exact solution given by eqn. (6) for an initial pressure $p_0 = 100kPa$ and various values of m. $K_{ref} = 100MPa$ and $p_{ref} = 100kPa$ were adopted in this example. The computed error in the range 43% - 98% is self explanatory and is the proof supporting *Recommendation 1*:

<u>Recommendation 1</u>: Choose the simplest constitutive model that will reproduce the material behavior of your particular problem, provided you do not change its material parameters during the execution of the model.

	$\Delta \epsilon_v = 2\%$	$\Delta \epsilon_v = 4\%$	$\Delta \epsilon_v = 6\%$	$\Delta \epsilon_v = 8\%$	$\Delta \epsilon_v = 10\%$	Eqn. (6)	Error
m = 0.30	300	578	916	1,305	1,738	3,074	43%
m = 0.50	300	646	1,155	1,835	2,691	12,100	78%
m = 0.70	300	732	1,537	2,891	4,999	296,012	98%

Table 1. "By hand" prediction of final pressure after five equal strain increments, exact value, and % error.

For instance, infill materials should not be modelled using the standard Mohr-Coulomb model because this model uses a constant bulk modulus, and changing it by hand would violate the recommendation. Modelling of strain-softening behavior by just adjusting the cohesion by hand would be a second example of improper use of numerical models. From this perspective, advanced modelling would mean taking full advantage of what numerical methods can give, yet considering physics a non-negotiable.

Kinematics

For the vast majority of applications, constitutive models in rock engineering are based on local, inifinitesimal strain, time-independent elastoplasticity. Standard additive decomposition of the infinitesimal strain tensor ϵ into the elastic strain tensor ϵ^{e} and the plastic strain tensor ϵ^{p} is adopted in most codes. It holds

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^p \tag{7}$$

In the one dimensional case, the axial strain reduces to

$$a = \frac{\Delta h}{h_0} \tag{8}$$

This definition is far from trivial. The axial stress computed in standard triaxial compression tests takes into account the change in volume and cross section of the sample

F

$$\sigma_d = \frac{P}{A} \tag{9}$$

where

$$A = \frac{1 + \epsilon_{\nu}}{1 - \epsilon_a} A_0 \tag{10}$$

and A_0 is the initial cross section of the sample. Eqn. (7) and eqn. (10) are not compatible, because one use an infinitesimal strain definition an the other one is a form of finite strain. The ultimate meaning of this is that the stress-strain curve that comes out of a model may be – and usually is – different to the expected value based on the input data, see Figure 1.



Figure 1. Implication of the definition of strain. Solid line: experimental result used to calibrate parameters. Dashed line: actual model outcome.

This issue is circumvented by adopting *Recommendation 2*:

<u>Recommendation 2</u>: Always perform a numerical simulation of the in situ and lab tests you use to calibrate your model, and confirm that the model correctly reproduces the material behavior in the test. Adjust parameters if required.

Stress-strain equation

A stress-strain equation relates the increment of stress to that of elastic strain

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}: \dot{\boldsymbol{\epsilon}}^e \tag{11}$$

where \mathbf{D}^e is an elastic operator which can be constant – in the case of linear elasticity – or dependent on any state variables including stress. Linear elasticity – either isotropic or anisotropic – is commonly assumed in rock engineering. Empirical formulas that relate stiffness values like the Young's modulus to some indicator of rock quality like GSI do not add nonlinearity, because GSI does not change during the calculation process and is therefore just a material parameter, not a state variable. Many models in soils engineering include pressure-dependent stiffness. These models are available in the numerical codes employed in rock engineering as well and should be the default choice when stress-dependent stiffness is of interest. For an interesting example on a continuous and a discontinuous model for the Ok Tedi mine see Mylvaganam et al (2011). In that contribution, the nonlinear rebound of the rock mass upon excavation of a cutback was modelled using a Phase² elastoplastic model with constant elasticity and an UDEC model. The UDEC model succeeded in predicting – at least qualitatively – the rebound displacement of the pit face because it could reproduce the effect of joint decompression and dilatant sliding. The Phase² model yielded much lower displacements than those recorded in the field. The rebound – but not all other features of the UDEC model – might have been captured more realistically if a pressure-dependent bulk modulus – like that of eqn. (5) – were employed in the Phase² model. This statement supports *Recommendation 3*:

<u>Recommendation 3</u>: When significant for your problem, address the nonlinearity of the elastic response by using a proper elastic formulation. Do not expect to match all displacements by just playing around with the Young's modulus of the Mohr- Coulomb model. Prefer hyperelastic models when available.

Yield function and strength

A yield function is a function of stress and state variables indicating yielding, i.e. the appearance of plastic strain. Yield functions are of the general form

$$F(\boldsymbol{\sigma}, \rho) = 0 \tag{12}$$

and define a so-called yield surface in stress space. The standard switching condition states that if F < 0 only elastic strain develop, and that plastic strain only occurs when F = 0 and $\dot{F} = 0$, i.e. when the stress state reaches the yield surfaces and remains there.

Many yield functions are available in the literature and in research codes. In practical applications of rock engineering, however, only the Mohr-Coulomb and Hoek-Brown yield functions are employed routinely. In principal stress space, the Mohr-Coulomb criterion reads

$$F = \sigma_1 - \sigma_3 - (\sigma_1 + \sigma_3)\sin(\phi) + 2c\cos(\phi) = 0$$
(13)

where c and ϕ are material parameters and σ_1 and σ_3 are the major and minor principal stresses, respectively. The Hoek-Brown criterion (Hoek et al 2002) reads

$$F = \sigma_1 - \sigma_3 - \sigma_c \left(m \frac{\sigma_3}{\sigma_c} + s \right)^a = 0$$
(14)

where the material parameters are m, s, and a. For a discussion on the Hoek-Brown criterion, see Eberhardt (2012). Mohr-Coulomb parameters dependent on stress have been derived to match the Hoek-Brown criterion. For instance, the conversion for the mean friction angle reads (Hoek et al 2002)

$$\sin(\phi) = \frac{6 a(s+m \sigma_3)^{a-1}}{2 (1+a)(2+a)+6 a m (s+m \sigma_3)^{a-1}}$$
(15)

The Hoek-Brown criterion effectively reproduces the curvature of the failure surface observed in many rocks. The same result may however be obtained by employing eqn. (13) with a stress-dependent friction angle. One of the most frequently used formulas for rockfill is (Leps 1970)

$$\phi(p) = \phi_0 - \Delta \phi \cdot \log\left(\frac{\sigma_3}{p_{atm}}\right) \tag{16}$$

where ϕ_0 and $\Delta \phi$ are parameters and p_{atm} is atmospheric pressure. Note that eqn. (15) and eqn. (16) are fundamentally different. Eqn. (15) gives an average value for a constant friction angle to be used over a wide range of stress and is only useful for conversion purposes. On the other hand, eqn. (16) effectively yields a curved yield surface, $\phi(p)$ being the function of states variables controlling this feature and can be directly used in a proper numerical model.

Both the Mohr-Coulomb model (eqn. (13)) and the Hoek-Brown model (eqn. (14)) ignore the effect of the intermediate principal stress σ_2 , which plays a role for rocks (see discussion in Mogi 2006). Two very well-known yield functions that take σ_2 into account are the Lade-Duncan criterion (Lade and Duncan 1973) and the Matsuoka-Nakai criterion (1974) which read respectively

$$F_{MN} = q + \sqrt{\frac{3\,\mu}{6+\mu} - \frac{2}{9}\,\frac{9+\mu}{6+\mu}\,\left(\frac{q}{p}\right)^3\sin(3\theta)} \cdot p \tag{17}$$

$$F_{LD} = q + \sqrt{\frac{3L}{27+L} - \frac{2}{9}} \left(\frac{q}{p}\right)^3 \sin(3\theta) \cdot p$$
(18)

where $q = \sqrt{3 J_2}$, J_2 is the second deviatoric invariant of the stress tensor, θ is the Lode angle, while μ and L are material parameters, calibrated using conventional triaxial compression tests. Lade (1997) demonstrated the applicability of the Lade-Duncan criterion to rocks, and managed to reproduce the curvature of the yield surface – the main reason for using the Hoek-Brown model – by replacing the material parameter L by a function of pressure L(p). Experimental and desktop studies incorporating σ_2 are not uncommon in the literature and are being an active area of research, see for instance (Descamps et al 2012, Lee et al 2012, Lee and Bobet 2013, Liu et al 2012, Meyer and Labuz 2013, Sriapai et al 2013, Yu et al 2002, Zhang et al 2013). For an interesting comparison among some of them see for instance (Benz and Schwab 2009). Figure 2 shows the Mohr-Coulomb, Lade-Duncan and Matsuoka-Nakai criteria in the deviatoric stress plane.



Figure 2. Mohr-Coulomb, Lade-Duncan and Matsuoka-Nakai criteria in the deviatoric stress plane.

It is shown in Figure 2 that if the four yield functions are calibrated to match their strength in triaxial compression (TC), the more realistic Lade-Duncan and Matsuoka-Nakai criteria predict higher strengths in plane strain compression (PSC), a feature that has been proved valid for clays, sands and intact rocks, and that is assumed for rock masses. Parameters based on correlations are cited together with experimental results in many publications (see Zhang 2009 for an interesting review) showing that the subject is not raising enough attention by the practice.

In engineering words, the above sentence means that the wall of a tunnel is in a safer condition that a square pillar because a given rock resists more in plane strain that in triaxial stress state. Despite being addressed by ISRM suggested methods (Chang and Haimson 2012, Fontoura 2012, Haimson and Bobet 2012), this particular feature of the behavior of geomaterials is largely overlooked in practical applications in rock engineering, and probably on the unsafe side. Most estimations of rock-mass strength are based on back-analysis of observed behavior, where plane strain conditions outnumber triaxial conditions by a large amount – slopes, tunnels and stopes against pillars and the like – and therefore we must assume that correlations used in practice might better apply to plane strain strength parameters.

If the above statement holds true, 3D numerical models using the Mohr-Coulomb or the Hoek-Brown criteria, calibrated using GSI correlations, may over-estimate strength in portions of the model where triaxial conditions prevail, for instance, on corners, isolated pillars or crossings. Table 2 shows the ratio between the compression strength at the triaxial corner divided by the maximum compression strength predicted by the Mohr-Coulomb, Hoek-Brown, Matsuoka-Nakai and Lade-Duncan criteria.

compression strength predicted by various yield criteria.						
	Mohr-Coulomb	Matsuoka-	Lade-			
	Hoek-Brown	Nakai	Duncan			
$\phi = 35^{\circ}$	100%	82%	71%			
$\phi = 45^{\circ}$	100%	76%	58%			
$\phi = 55^{\circ}$	100%	71%	42%			

Table 2. Triaxial compression strength as a percentage of the maximum compression strength predicted by various yield criteria

This table supports *Recommendation 4*:

<u>Recommendation 4</u>: When employing correlations for estimating strength parameters, be aware of the background data supporting such correlations and the constitutive models they are intended for. Correlations intended for being employed in 2D constitutive models – remarkably, GSI-based correlations intended for the Hoek-Brown model – should be carefully reviewed when employed in 3D models.

When resourcing to SRM technology for calibrating rock masses exhibiting isotropic behavior, realizations of triaxial and plane strain conditions and other stress-paths can be employed to calibrate 3D yield functions (e.g. Estrada and Taboada 2013, Zhao and Evans 2009). Ubiquitous Joint models (e.g. Clark 2006, Wan and Huang 2009), available in commercial software – e.g. Plaxis, Phase², FLAC – are the most practical way of dealing with rock strength anisotropy within the framework of continuous mechanics. Sainsbury et al (2008a) present a procedure for the calibration of a ubiquitous joint model calibrated using SRM, and employed with in a very complex problem (Sainsbury et al 2008b).

Flow rule

The flow rule indicates the direction of plastic strain. Most models employed in practice adopt deviatoric associativity and volumetric non-associativity, which, in engineering words, means that some parameters are given to the user to control plastic dilatancy.

It has long been established in soil mechanics that dilatancy – volumetric strain that occurs in shearing – is not a material property but an observed behavior that is strongly dependent on stress and density, see Sfriso and Weber (2010) for a discussion on the subject. For soils, the peak friction angle can be splitted in two components

$$\phi(p) = \phi_c + \psi(p) \tag{19}$$

where ϕ_c is the friction angle when no dilatancy is observed and ψ is a density and pressure-dependent dilatancy term. In rock engineering, pressure-sensitivity is also observed, while density dependence is replaced by post-failure fracturing and fragmentation (see Alejano and Alonso 2005 for a review). This was acknoledged by Barton's expression for the shear strength in joints (see recent reference and discussion of the Barton-Bandis model in Barton 2013)

$$\phi(\sigma_n) = \phi_r + JRC \cdot \log\left(\frac{JCS}{\sigma_n}\right) \tag{20}$$

where ϕ_r , JRC and JCS are material parameters. Note the similitude between eqn. (16) and eqn. (20), they share the mathematical form of eqn. (19).

Various definitions for the dilatancy term are available. The simplest is a constant dilatancy angle ψ defining the volumetric plastic strain $\dot{\epsilon}_{v}^{p}$ as a function of the plastic distortion $\dot{\gamma}^{p}$

$$\dot{\varepsilon}_{v}^{p} = \sin(\psi) \cdot \dot{\gamma}^{p} \tag{21}$$

Vermeer and De Borst (1984) introduced a dilatancy angle dependent on strength mobilization

$$\sin(\psi) = \frac{\sin(\phi_{mob}) - \sin(\phi_c)}{1 - \sin(\phi_{mob}) \sin(\phi_c)}$$
(22)

where ϕ_{mob} is the mobilized friction angle. Zhao and Caic (2010) discussed the implications of using a constant dilation angle associated and concluded that it cannot reasonably simulate the displacement distribution around tunnels and showed the better predictions obtained a mobilized dilation angle model that depends on both confining stress and plastic shear strain is employed.

Few dilatancy models fully address real 3D stress-paths. Guo and Stolle (2004) and Sfriso and Weber (2010) introduced numerical implemmentations of Rowe's equation. Tsegaye and Benz (2014) also introduced a general stress-dilatancy formulation and applied it to the Hoek–Brown criterion. Sfriso et al (2011) further discussed the numerical implications of the use of a 3D dilatancy formulation.

The combination of basic Ubiquitous Joint models – elastic rock and elastoplastic joints – and dilatancy can yield unrealistic results, because plastic dilatancy may lock the very few kinematic mechanisms of UJMs, leading to very high yield stresses. Adhikary (2010) presented a review of the behavior of the standard UJM in FLAC2D and addressed some of the challenges. Dilatancy also affects significantly the ultimate load computation in many other standard boundary value problems in plasticity (e.g. Manzari and Nour 2000, Zhao and Caig 2010). Recommendation 5 is:

<u>Recommendation 5</u>: When specifying parameters that impose dilatant behavior to 3D models, check the model response for various stress-paths using simple numerical tests. Avoid using elastic rock plus dilatant ubiquitous joints in all but trivial configurations. Always run a version of the model with no dilatancy and check that the differences are reasonable. If not, carefully check whether your combination of yield function and flow rule allows for the development of realistic plastic deformations.

Evolution equations, hardening and softening

Evolution equations are expressions that account for the evolution of state variables. In general terms, evolution equations are of the rate form

$$\dot{\rho} = f(\dot{\epsilon}^p) \tag{23}$$

where $\dot{\rho}$ stands for the increment of a generic state variable. Evolution equations are required if an experimental nonlinear stress-strain curve is to be reproduced in the pre-peak hardening regime, and also

for softening in the post-peak regime. In this latter case, strain softening evolution equations must be used together with regularization techniques to guarentee mesh independence.

Cohesion softening and friction hardening models are becoming more popular to assess brittle behaviour (e.g. Barton 2013, Zea and Celestino 2011). While very significative from both theoretical and practical perspectives, any form of softening poses extreme challenges for continuum mechanics based numerical models. Figure 3 (Sfriso 2010) shows the displacement plot for a plane strain compression simulation of a post-peak strain-softening constitutive model. This type of displacement plots are nice, yet mesh dependent – i.e. unusable – for most commercial codes available. Figure 4 (Sfriso 2010) illustrates the high nonlinearity of the stress-strain curves for various points in an triaxial compression simulation of such model and the (apparently nice, but useless) average result.



Figure 3. Simulation of a plane compression test of a softening material exhibiting strain-localization (Sfriso 2010).



Figure 4. Simulation of a triaxial compression test in a strain-softening material showing a highly non-uniform displacement field (Sfriso 2010).

3DEC, PFC3D and other software packages based on discontinuum mechanics are available for modelling strain-softening behaviour, FLAC, Plaxis and Phase² are not suitable tools for this purpose. If the implications of damage and softening must be accounted for in these codes a conservative, yet acceptable alternative is to run the model using two sets of parameters, one for the peak strength and a second one for residual or otherwise damaged strength.

Mesh dependence is simply a fatal flaw, and a most probable issue when strain-softening constitutive models are employed. This statement triggers Recommendation 6:

<u>Recommendation 6</u>: Mesh dependence is a fatal flaw for numerical models. Unless absolute certain of the implications, avoid modelling strain softening because it may lead to uncontrolled localization of purely numerical nature. When applying Recommendation 2 (reproducing tests using models) to strain softening models use at least two meshes of widely different element sizes, and go ahead with the modelling only if you get similar parameters using the two meshes. Run the full model using two meshes, noticeably different in the localization, strain softening zones.

Need of adequate experimental data

Material parameters are those constants that define the material behavior. As such, they require a systematic procedure for determination that includes field and laboratory testing and a deep comprehension of the objectives of the model and the limitations of the available tools. The subject has been extensively discussed in the literature (for a comprehensive approach see Feng and Hudson 2004, 2010, Hudson and Feng 2007, 2010). A proper balance between the effort of producing an advanced numerical model and the value obtained from it should preclude the use of numerical models based on parameter estimations only. This statement supports Recommendation 7:

<u>Recommendation 7</u>: Perform 3D models and models intended for estimation of displacements and other serviceability indicators only when you have adequate in situ or lab test results. Do not build an "advanced" model based on parameter estimates.

From the modelling perspective, it is mandatory to sharply distinguish what will go to the rockmass parameters – i.e. into the smeared equivalent continuum – and what will be considered "structure" – i.e. included in the finite element mesh as a particular feature. This distinction has little to do with that of "intact rock" and "joints" and even to the rock-mass characterization approach. For large models, all but the most relevant joints shall be smeared into rock-mass properties. In sub-models of such large model, some of the features can be explicitly included in the mesh and must be therefore removed from the rockmass, a process that will change the material parameters of the latter. It is desirable that similar outcomes be obtained from both the large model and the detailed sub-model.

The rock-mass characterization approach for calibrating material parameters

Rock-mass characterization techniques were not intended for feeding parameters to numerical models. Citing AFTES (2003): The most important goal in the characterisation of rock masses is to provide the engineer with qualitative and quantitative data to describe their structure and assess their mechanical and hydraulic properties at a scale commensurate with the volume of rock affected by the structures. AFTES (2003) also has a clear statement: Correlations must be used with great caution, especially for strength parameters: avoid correlations 'in cascade' of the type $Q \Rightarrow RMR \Rightarrow (n,s) \Rightarrow (c, \phi)$.

The development of rock-mass characterization tools for determining material parameters has reached to an end. Citing Evert Hoek (2009): Hoek and Marinos have described the efforts that have been made, over a period of about 30 years, to refine the Hoek-Brown criterion and the GSI classification system to cover a wide range of rock masses and to improve its accuracy... In retrospect, and bearing in mind that the rock masses considered are limited by the assumptions of homogeneity and isotropy, it is apparent that these efforts have reached the point of vanishing returns... it is now time to see whether developments in computer technology and numerical methods can help us calibrate or move on from the empirical methods, such as the Hoek-Brown criterion, that have been used for so long.

The huge amount of experience hidden behind the rock-mass characterization tools cannot be, however, overlooked. Parameter estimators based on rock-mass characterization give reasonable bounds that help in identyfying when a test result is unreliable or wrong (e.g. Gibson 2005). Rock-mass characterization certainly helps in determining relevant geotechnical units and sub-units. Combined with preliminary modelling, it can also help in identifying which testing is required, either lab or in situ. From a

modelling perspective, rock-mass characterization cannot be completed before deciding which features of the massif will be modelled explicitly and which will be dumped in the rock-mass box.

Reporting

Potts et al (2002) is an excellent guideline on the planning, building, using and reporting of advanced numerical models in geotechnics. The reader is adviced to use it as a checklist of sound procedures. When reporting the results of a numerical model, a good practice is to include: i) the purpose, objective ans scope of the numerical model; ii) a short description of the constitutive models employed; iii) the list of input parameters, the procedure use for their determination, and the comparison between the experimental data and the model of the test; iv) any hand calculations or forecast of the output employed to check the validity of the results; v) results from sensitivity analyses (and proof of mesh independence, specially when dealing with strain-softening materials).

CONCLUSIONS

Numerical modelling is becoming universal in rock engineering practice and is the only tool available that addressesses complex geometries and the nonlinear behaviour of rock masses and yet is respectful with physics. Advanced constitutive models may be used for estimation of serviceability indicators, ground-stucture interaction and 3D problems. The academia has a large stock of continuum-mechanics based models that can be employed with confidence in practical applications.

The mathematical structure and ingredients of such constitutive models was briefly reviewed. For each ingredient, the implications of selecting models for practical applications were discussed and a few recommendations were given. These recommendations are:

- 1. Choose the simplest constitutive model provided you do not change parameters;
- 2. Always perform a numerical simulation of tests you use to calibrate your model;
- 3. Address elastic nonlinearity by using a proper nonlinear formulation. Refrain from changing elastic parameters by hand;
- 4. Be aware of the background data supporting correlations for strength parameters and the constitutive models they are intended for. Avoid using correlations in cascade;
- 5. When specifying dilatancy check the model response for various stress-paths using simple numerical tests. Run a version of the model with no dilatancy and check that the differences are reasonable;
- 6. Mesh dependency is a fatal flaw. Unless absolute certain of the implications, avoid modelling strain softening. If you must use strain-softening, run the full model using two meshes, noticeably different in the strain softening zones;
- 7. Perform models intended for estimation of serviceability indicators only when you have adequate test results. Do not build an "advanced" model based on parameter estimates.

These seven recommendations are based on many years of experience building, using, interpreting and reviewing numerical models for geotechnical applications, and might be useful for the practitioner that ocassionaly uses numerical models in rock engineering practice.

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