ELSEVIER

Engineering Geology 53 (1999) 235–241

ENGINEERING GEOLOGY

Discrete element modelling of fragmentable geomaterials with size dependent strength

A.P.S. Selvadurai *, K. Sepehr

Department of Civil Engineering and Applied Mechanics, McGill University, 817 Sherbrooke Street West, Montreal, QC, Canada, H3A 2K6

Abstract

This paper presents the application of a discrete element technique to the analysis of the dynamic indentation of either a purely brittle or a brittle viscoplastic geomaterial which can experience fragmentation resulting in fragments with size dependent strength characteristics. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Discrete element modelling; Fragmentable geomaterials; Dynamic indentation; Viscoplasticity

1. Introduction

Brittle geomaterials are characterized by their susceptibility to fragmentation during loading. With such geomaterials, an initially continuum region can transform to a discontinuum. The extent to which the fragmentation process can materialize in an initially continuum region will depend on the internal structure of the geomaterial and the magnitude and nature of the application of the loads. In geomaterials with a dominant coarse internal structure, a fragmentation process can result in the transformation of an initially continuum region to essentially a granular medium. In geomaterials with a finer internal structure, the fragmentation process can be restricted to specified planes where splitting can occur under the action of either tensile or compressive stresses. The application of discrete element techniques represents the most convenient method for examining this class of transition processes involving an initially continuum region. In the past, discrete element techniques have been applied to examine this transformation process (Hocking et al., 1985; Mustoe et al., 1987). In these early developments, there is the provision for the fragments themselves to experience continued fragmentation; while this reflects accurately the behaviour of the fragmentation process, it does restrict the efficiency of the computational scheme. Moreover, experience with geomaterials indicates that the strength characteristics of brittle geomaterials can be influenced by the size of the fragment being considered. Experimental investigations conducted by Bieniawski (1968) indicate that the compressive strength of coal is significantly influenced by the size of the specimen being tested. Experiments conducted by Jahns (1966) on calcareous iron ore and experiments conducted by Pratt et al. (1972) on quartz diorite indicate that the compressive strength of these materials is also influenced by the size of the sample being tested.

In this paper we develop a discrete element

* Corresponding author. Tel.: +1 514 398 6672; fax: +1 514 398 7361.
E-mail address: apss@civil.Ian.mcgill.ca (A.P.S. Selvadurai)

PII: S0013-7952(99)00039-3

approach to the study of fragmentation in certain two-dimensional plane strain problems of interest to geomechanics. The basic "shell" used in the investigation is a discrete element code DECICE (INTERA Technologies, 1986). The code is capable of examining the mechanics of multiple interacting deformable bodies undergoing finite motions. These fragments can undergo progressive fragmentation which can result in the generation of progressively smaller distinct material fragments. In this research effort, the discrete element code has been modified to account for strain softening phenomena and size dependent strength criteria. The contact between fragments is characterized by Coulomb frictional effects. The generalized treatment of the discrete element procedure can also account for viscoplastic flow in the intact material, characterized by a yield criterion and a fluidity parameter-based flow rule. The yield criterion can also accommodate softening effects through a change in the constitutive parameters. The fragmentation process is defined in relation to either tensile or compressive action in elements.

The modified discrete element procedure is used to examine the problem of the indentation of a confined brittle elastic layer by a rigid indentor. The fragmentation is assumed to be induced by both tensile and compressive loadings. The analysis of the problem is extended to include viscoplastic effects and the consideration of situations where fragmentation is initiated only in elements which exhibit tensile stress states and viscoplastic flow takes place only when both principal stresses are compressive.

2. Constitutive modelling

The generalized constitutive response, for the intact geomaterial, adopted in the discrete element modelling is an isotropic elastic viscoplastic model. The rate form of the elastic constitutive model for the geomaterial is given by:

$$\mathring{\epsilon}_{ij}^{e} = \frac{\mathring{\sigma}'_{ij}}{2G} + \frac{\mathring{\sigma}_{kk}}{9K}\,\delta_{ij}, \tag{1}$$

where ($^\circ$) denotes the time derivative, $\mathring{\sigma}'_{ij}$ is the stress deviator tensor and G and K are, respectively, the linear elastic shear modulus and the bulk modulus.

The viscoplastic model proposed by Perzyna (1966) has been successfully applied by a number of investigators, including Zienkiewicz and Cormeau (1974), Cormeau (1975) and Selvadurai and Au (1992) for the computational modelling of a variety of geomaterials. The viscoplastic strain rate is given by:

$$\mathring{\epsilon}_{ij}^{vp} = \gamma\langle\Phi(F)\rangle\frac{\partial F}{\partial \sigma_{ij}}, \tag{2}$$

where γ is a fluidity parameter, F is the current yield function and $\Phi(F)$ is a flow function defined by:

$$\langle\Phi(F)\rangle = \Phi(F) \text{ if } F \geq 0; \quad \langle\Phi(F)\rangle = 0 \text{ if } F < 0. \tag{3}$$

The yield function F and the flow function $\Phi(F)$ are material properties which need to be determined through experiments. Two commonly used representations, however, are:

$$\Phi(F) = \exp\left\{\frac{M(F-F_0)}{F_0}\right\} - 1; \quad \Phi(F) = \left\{\frac{(F-F_0)}{F_0}\right\}^N, \tag{4}$$

where M and N are constants and F_0 is a uniaxial failure stress. The Mohr–Coulomb yield function is utilized to describe the failure behaviour of a wider class of geomaterials

$$F = \frac{I_1}{3}\sin\phi + \sqrt{J_2}\left\{\cos\Theta - \left(\frac{1}{\sqrt{3}}\right)\sin\Theta\sin\phi\right\} - c\cos\phi, \tag{5}$$

where c is the cohesion, ϕ is the angle of internal friction:

$$I_1 = \sigma_{kk}; \quad J_2 = \frac{1}{2}\,\sigma'_{ij}\sigma'_{ij}; \quad J_3 = \frac{1}{3}\,\sigma'_{ij}\sigma'_{jk}\sigma'_{ki} \tag{6}$$

$$\Theta = \frac{1}{3}\sin^{-1}\left\{-\frac{(3\sqrt{3}J_3)}{(2J_2^{3/2})}\right\}; \quad \left(\frac{-\pi}{6} \leq \Theta \leq \frac{\pi}{6}\right).$$

The yield behaviour in the tension range can also be truncated by incorporating a tension cut-off

σ_T. In this case the Mohr–Coulomb yield criterion is a three parameter model which is defined by c, ϕ and σ_T.

3. Initiation of fragmentation

In an intact region, processes which initiate fragment development are directly related to the strength parameters associated with the peak values. The principal stresses and their orientations within each element can be evaluated during the stress analysis procedure. The attainment of either a critical compressive strength or a tensile strength can be assumed for the initiation of fragment development.

The process of fragment development during *compressive* shear failure is prescribed by considering the Mohr–Coulomb criterion. This criterion can be written in terms of the principal stresses in the form:

$$\sigma_1 \geq \sigma_c + \sigma_3 \tan^2\left(\frac{\pi}{4} + \frac{\phi}{2}\right), \tag{7}$$

where σ_c is the unconfined strength in compression, ϕ is the angle of internal friction and σ_1 are σ_3, respectively, the maximum and minimum principal stresses. The unconfined compressive strength is related to the shear strength parameters c and ϕ associated with the Mohr–Coulomb failure criterion according to:

$$\sigma_c = 2c\{(\tan^2\phi + 1)^{1/2} + \tan\phi\}. \tag{8}$$

For the compression failure mode there are two possible conjugate orientations of fragmentation inclined at equal angles $(\pi/4 - \phi/2)$ to the direction of the stress on either side of it. In two dimensions, these are defined by:

$$\theta = \tan^{-1}\left\{\frac{(\sigma_1 - \sigma_{xx})}{\sigma_{xy}}\right\} \pm \frac{(\pi/2 - \phi)}{2}, \tag{9}$$

where θ is the angle between the fragmentation plane and the positive global axis, σ_{xx}, is the x-component of the stress tensor and σ_{xy} is the xy shear component of the stress tensor. In the computations, the sign of the second term on the right hand side of Eq. (9) is determined by using a random number generator. This allows for the development of a relatively random fragmentation pattern.

The *tensile* fragmentation criterion assumes that the material will fragment when the minimum principal stress σ_3 reaches the tensile strength of the material, σ_T. For two dimensions, the criterion can be written as:

$$\sigma_3 \geq \sigma_T. \tag{10}$$

The orientation of the fragmentation plane is given by:

$$\theta = \tan^{-1}\left\{\frac{(\sigma_1 - \sigma_{xx})}{\sigma_{xy}}\right\}, \tag{11}$$

where, in two dimensions, θ is the angle between the fragmentation plane and the positive global x-axis. In this case, the θ-direction is aligned with the maximum principal stress direction.

3.1. Viscoplastic flow versus fragmentation

Experimental observations tend to support the postulate that the processes of brittle fragmentation would occur in regions where the stress state is predominantly tensile and viscoplastic flow would occur in regions where the state of stress is predominantly compressive. Such an assumption would enable the utilization of the same failure criterion for describing both the initiation of viscoplastic flow in the compression range and fragmentation in the tensile range. The consideration of distinct stress states which will initiate either viscoplastic flow or fragment development can be ascertained only by appeal to experimentation. In the current study, fragment development and failure initiation for viscoplastic flow are described by the Mohr–Coulomb criterion specified in terms of c and ϕ.The following computational schemes are adopted:

1. The intact geomaterial will experience brittle fragmentation only for situations where any single stress component or both are in the tensile mode.
2. Viscoplastic flow will occur for only stress states involving pure compressive stress states for both principal stresses. In the case where viscoplastic

flow occurs first, there is provision for subsequent fragmentation in tension; this fragmentation will be governed by the prescribed post peak strength characteristics of the geomaterial, which can include softening.

3. The intact geomaterial will experience brittle fragmentation in *both* tensile and compressive modes for all choices of σ_1 and σ_3.

4. Fragment interaction responses

The interaction between fragments is characterized by responses which relate the normal (n) and shear (s) forces to their respective differential displacements at the contacting surfaces (see, Selvadurai and Boulon, 1995), for example:

$$\mathrm{d}F_i = k_i(\mathrm{d}u_i^1 - \mathrm{d}u_i^2);$$

$$\text{(no sum over repeated indices `}i\text{')}, \tag{12}$$

where $i = n, s$, $\mathrm{d}F_i$ are the incremental changes in the contact force unit length between the contacting planes, $(\mathrm{d}u_i^1)$ and $(\mathrm{d}u_i^2)$, are displacement increments at the contact plane between regions $(^1)$ and $(^2)$ and k_i are stiffness coefficients defined in the normal and shear directions of the average plane at the point of contact. The stiffnesses themselves could be a function of the differential displacements $((\mathrm{d}u_i^1 - \mathrm{d}u_i^2))$. In this study, the generated inter-fragment shear behaviour is characterized by a Coulomb friction (μ_f) and an adhesion (c_f) based limiting value in the shear behaviour.

For this response,

$$k_s = k_s^*; |\mathrm{d}\tau_s| < c_f + \mu_f \sigma_n;$$

and

$$k_s = 0; |\mathrm{d}\tau_s| = c_f + \mu_f \sigma_n, \tag{13}$$

where τ_s is the shear stress, σ_n is the normal stress at the inter-fragment contact plane, is the coefficient of inter-fragment friction and is the inter-fragment adhesion. For the interaction response in the normal direction, it is reasonable to assume elastic behaviour provided the contact force between fragments is compressive. The interactive stiffness will vanish when the fragments separate, that is:

$$k_n = k_n^*; \quad \mathrm{d}\sigma_n \le 0; \quad \text{and } k_n = k_s = 0; \quad \mathrm{d}\sigma_n > 0. \tag{14}$$

4.1. Size dependency of strength

Geomaterials are composed of crystals and grains in a fabric that can include random distributions of defects such as cracks and fissures. Thus, the geomaterial strength can be size-dependent. In particular, geomaterials such as coal, granitic rocks and shale exhibit the greatest degree of size dependency; the ratio of laboratory to field strengths sometimes attaining values in excess of 10. Some limited but definitive studies have been made to examine the influence of size effects on the strength over a broad range of specimen sizes. Bieniawski (1968) reported results of compression tests on prismatic in situ coal specimens measuring up to 1.6 m × 1.6 m × 1.0 m. The results of these experiments are shown in Fig.1. Results of similar tests conducted by Jahns (1966) on cubical specimens of calcareous iron ore and those obtained by Pratt et al. (1972) for fissured quartz diorite, are also shown in Fig. 1. Available data from these investigations are insufficient to provide a conclusive recommendation valid for a variety of geomaterials; however, these results generally indicate that there is a limiting size beyond which larger specimens exhibit no further decrease in the compressive strength.

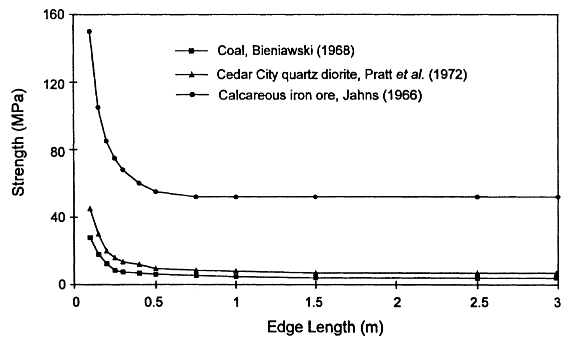

Fig. 1. Specimen size dependence of tensile strength.

5. Computational aspects

The principal computational aspects associated with the discrete element modelling of a fragmentable viscoplastic material basically involves two components. These are:

1. the procedures used to examine the nonlinear material phenomena such as viscoplasticity and nonlinear inter-fragment interactions; and
2. the procedures used in the solution of the dynamic equations of motion associated with the entire system of interacting fragments, intact continuum regions and structural components.

6. Computational procedures for viscoplasticity

The computational procedures for viscoplasticity are well documented in a number of articles including those by Zienkiewicz and Cormeau (1974) and Owen and Hinton (1980). Briefly, the viscoplastic strain increment at time interval $\Delta t_n = (t_{n+1} - t_n)$can be obtained via a scheme given by:

$$(\Delta\epsilon^{\mathrm{vp}})_n = \Delta t_n \{(1-\Omega)(\mathring{\epsilon}^{\mathrm{vp}})_n + \Omega(\mathring{\epsilon}^{\mathrm{vp}})_{n+1}\}, \tag{15}$$

where Ω takes the following value depending upon the integration scheme:

$\Omega = 0$, fully explicit. $\Omega = 1$, fully explicit.

$$\Omega = \frac{1}{2}, \text{ Crank–Nicholson.} \tag{16}$$

The incremental stress at the iteration n can be given in the form:

$$(\Delta\sigma)_n = [\boldsymbol{D}^{-1} + \Omega(\Delta t_n)(\boldsymbol{H})_n]^{-1}\{[\boldsymbol{B}]_n(\Delta \boldsymbol{d})_n - (\mathring{\epsilon}^{\mathrm{vp}})_n(\Delta t_n)\} \tag{17}$$

where

$$(\Delta\epsilon)_n = [\boldsymbol{B}]_n(\Delta \boldsymbol{d})_n;$$

$$(\Delta\epsilon^{\mathrm{vp}})_n = (\mathring{\epsilon}^{\mathrm{vp}})_n(\Delta t_n) - \{\Omega(\Delta t_n)(\boldsymbol{H})_n\}(\Delta\sigma)_n \tag{18}$$

$$(\boldsymbol{H})_n = \left(\frac{\partial \mathring{\epsilon}^{\mathrm{vp}}}{\partial\sigma}\right)_n, \tag{19}$$

and $\boldsymbol{D}$ is the elasticity matrix given by:

$$\mathring{\sigma} = \boldsymbol{D}\mathring{\epsilon}^{\mathrm{e}}. \tag{20}$$

The time integration scheme is unconditionally stable if $\Omega \geq 1/2$; that is, the procedure is numerically stable but does not ensure accuracy of the solution. Consequently, even for values of $\Omega \geq 1/2$, limits must be imposed on the selection of the time step to achieve a valid solution. For viscoplasticity problems which are based on an associative flow rule ($Q = F$), a linear flow function for $\Phi(F) = (F)$ and described by the Mohr–Coulomb yield criterion, the recommended limit for the time increment is:

$$\Delta t \leq \frac{[4(1+\nu)(1-2\nu)c\cos\phi]}{[\gamma(1-2\nu+\sin^2\phi)E]}. \tag{21}$$

6.1. Computational procedures for the discrete element method

The basic concept of the discrete element method involves the solution of the dynamic equations of equilibrium for the intact continuum and for all fragments in the system. For each discrete element, the dynamic equilibrium equations can be written in the form:

$$[\boldsymbol{M}]\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}[\boldsymbol{u}]\right\} + [\boldsymbol{C}]\left\{\frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{u}]\right\} + [\boldsymbol{K}]\{\boldsymbol{u}\} = \{\boldsymbol{f}\}, \tag{22}$$

where $\{\boldsymbol{u}\}$is the displacement; $\{\boldsymbol{f}\}$ is the force vector; $[\boldsymbol{M}]$, $[\boldsymbol{C}]$ and $[\boldsymbol{K}]$ are, respectively, mass, damping and stiffness matrices.

The solution of the dynamic equations of equilibrium is constrained by:

1. incrementally nonlinear material phenomena occurring within the nonlinear regions;
2. non-linear interactive phenomena at the boundaries of fragments;
3. non-linear constraints concerning contact/separation at fragment boundaries; and
4. non-linear constraints concerning fragment evolution.

The algorithms for the solution of the equations take advantage of a modal decomposition approach which presents certain advantages in the explicit formulation of the discretized forms of the governing equations, that is

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}[\boldsymbol{u}]\right\}_n = [\boldsymbol{M}]^{-1}\left[\{\boldsymbol{f}\}_n - [\boldsymbol{C}]\left\{\frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{u}]_{n-1/2} - [\boldsymbol{K}]\{\boldsymbol{u}\}_n\right\}\right], \quad (23)$$

and

$$\left\{\frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{u}]\right\}_{n+1/2} = \left\{\frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{u}]\right\}_{n-1/2} + \left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}[\boldsymbol{u}]\right\}_n (\Delta t), \quad (24)$$

$$\{\boldsymbol{u}\}_{n+1/2} = \{\boldsymbol{u}\}_n + \left\{\frac{\mathrm{d}}{\mathrm{d}t}[\boldsymbol{u}]\right\}_{n+1/2} (\Delta t), \quad (25)$$

where Δt is the time increment and the subscripts denote the time step number. In the explicit algorithm, the equations of motion are integrated separately using an explicit central technique. The stability condition for the time increment Δt, which employs an explicit–explicit partition (applicable to linear systems), takes the form:

$$\Delta t \leq \frac{2\{(1+\tilde{D}^2)^{1/2} - \tilde{D}\}}{\omega_{\max}} \quad (26)$$

where $\omega_{\max}$ is the maximum frequency of the combined system involving both rigid body motion and deformability of the system, and $\tilde{D}$ is the fraction of critical damping at $\omega_{\max}$. Other stability criteria have been proposed in the literature on computational methods for transient dynamic analysis; these include:

$$\Delta t \leq \frac{2}{\omega_{\max}} \text{ and } \Delta t \leq \eta L\left[\frac{\rho(1+v)(1-2v)}{E(1-v)}\right]^{1/2}, \quad (27)$$

where η is a coefficient which depends on the element type used and L is the smallest length between any two nodes. This constraint is found to be suitable for application to nonlinear systems.

7. A contact problem

In this section, we briefly discuss the application of the basic procedures described previously for the study of the dynamic indentation of a layer (thickness of layer = 2.0 m; length of layer = 12.0 m; width of indentor = 2.4 m). The layer is bonded to a rigid stratum. The indentor has a prescribed velocity of $v_0 = 0.1$ m s^{-1}. The material parameters and responses used in the computational simulations are as follows: elastic parameters: $E = 3500$ MPa; $v = 0.35$; failure parameters: $c = 1.5$ MPa; $\phi = 30°$; viscoplasticity parameters: $\gamma = 1.0 \times 10^{-3}$ s^{-1}; $N = 1$; interfragment responses: $k_n = k_s = 1.0 \times 10^{10}$ Pa m^{-1}; $c_f = 0$; $\mu_f = 0.577$. In this study, it is assumed that σ_T and σ_c vary according to the following empirical rules:

$$\sigma_T = \left(\frac{0.3125}{A}\right)\text{MPa}$$

if $0 \leq A \leq 0.625$ m^2; $\sigma_T = 0.5$ MPa

if $A > 0.625$ m^2,

where A is the 'area' of the two-dimensional fragment in m^2; the equivalent edge length is:

$$d = \sqrt{\frac{4A}{\pi}}$$

and

$$\sigma_c = \left(\frac{0.9375}{A}\right)\text{MPa}$$

if $0 \leq A \leq 0.625$ m^2; $\sigma_c = 1.5$ MPa

if $A > 0.625$ m^2.

Fig. 2 illustrates the initial finite element discretization used in the computations. Fig. 3 illustrates the extent of fragmentation that takes place after 0.12 s, for the simulation which accounts to the development of brittle fragmentation in *both* tensile and compressive stress states. Fig. 4 illustrates the extent of fragmentation that takes place after 0.12 s for the simulation where viscoplastic processes occur when both principal stresses are compressive and brittle fragmentation occurs for any other stress state.

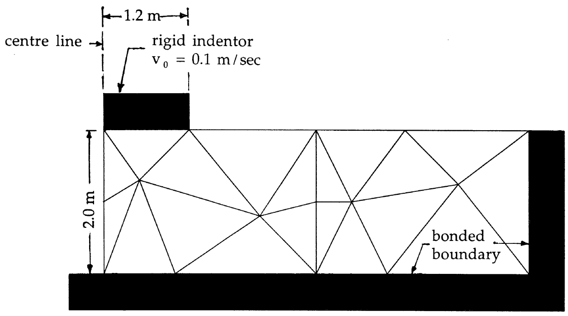

Fig. 2. Mesh discretization for the analysis of the dynamic indentation problem.

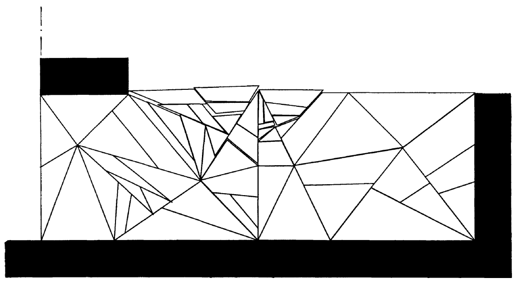

Fig. 3. Fragmentation pattern for a brittle geomaterial which exhibits fragmentation in both tension and compression.

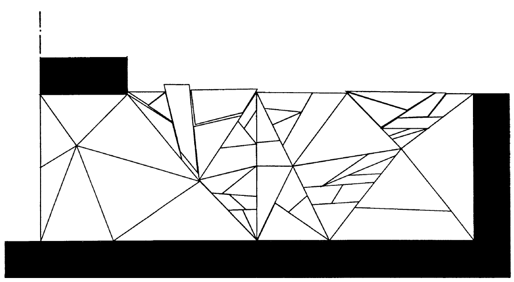

Fig. 4. Fragmentation pattern for brittle-viscoplastic geomaterial which exhibits viscoplastic flow in compression only and brittle fragmentation in all other states.

8. Concluding remarks

The development of fragmentation in brittle geomaterials is examined by employing a discrete element approach which accommodates, where appropriate, viscoplastic flow and brittle fragmentation in both tension and compression. In particular, the analysis is modified to accommodate size dependent fragmentation strengths, both in tension and compression. The results of the analysis indicate that the evolution of fragmentation within a constrained region subjected to dynamic indentation, can be influenced by the ability of the medium to undergo viscoplastic failure in regions where compressive stresses dominate.

References

Bieniawski, Z.T., 1968. The effect of specimen size on compressive strength of coal. Int. J. Rock Mech. Mining Sci. vol. 5, 325–335.

Cormeau, I.C., 1975. Numerical instability in quasi-static elasto/visco-plasticity. Int. J. Num. Meth. Engng vol. 9, 109–127.

Hocking, G., Williams, J.R., Mustoe, G.G.W., 1985. Dynamic global forces on an offshore structure from large ice floe impacts, Civil Engineering in the Arctic Offshore, ASCE Specialty Conference, San Francisco. ASCE, USA, pp. 202–219.

INTERA Technologies, 1986. DEC-ICE Theoretical Manual. INTERA Technologies, Lakewood, CO.

Jahns, H., 1966. Measuring the strength of rock in-situ at increasing scale, Proc. 1st Cong. ISRM (Lisbon) vol. 1. ISRM, pp. 477–482.

Mustoe, G.G.W., Williams, J.R., Hocking, G., Worgan, K., 1987. Penetration and fracturing of brittle plates under dynamic impact. NUMETA '87, Swansea, U.K. A.A. Balkema, The Netherlands.

Owen, D.R.J., Hinton, E., 1980. Finite Elements in Plasticity: Theory and Practice. Pineridge Press, Swansea.

Perzyna, P., 1966. Fundamental problems in viscoplasticity. Recent Advances in Applied Mechanics. Academic Press, New York.

Pratt, H.R., Black, A.D., Brown, W.D., Brace, W.F., 1972. The effect of specimen size on the mechanical properties of unjointed diorite. Int. J. Rock Mech. Mining Sci., vol. 9, 513–530.

Selvadurai, A.P.S., Au, M.C., 1992. Damage and viscoplasticity effects in the indentation of a polycrystalline solid. In: Boehler, J.P., Khan, A.S. (Eds.), Plasticity '91, Proceedings 3rd International Symposium on Plasticity and its Current Applications. Elsevier Science, The Netherlands, pp. 405–408.

Selvadurai, A.P.S., Boulon, M.J. (Eds.), 1995. Mechanics of Geomaterial Interfaces, Studies in Applied Mechanics vol. 42. Elsevier Science, The Netherlands.

Zienkiewicz, O.C., Cormeau, I.C., 1974. Viscoplasticity, plasticity and creep in elastic solids — a unified numerical solution approach. Int. J. Numerical Analyt. Methods Engng vol. 8, 821–845.