Performance of the discrete element method to represent the scale effect

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Abstract

The scale effect in materials is a well known phenomenon, responsible for the variation of the properties of the materials when the size of the bodies in analysis is changed or when different strain velocities during the tests are applied. The scale effect analysis with different numerical models allows us to have an important indication of their capacity to simulate the material behavior appropriately. The utilization of numerical models based exclusively on the Continuum Mechanics principles shows important limitations to explain this behavior because the material nature is not continuum. A more accurate explanation requires to consider that the material structure is defined by lengths, called *characteristic lengths*, that identify the material behavior. In the same way it is possible to observe that materials have dynamic properties which can be reduced to constants that depend dimensionally only on time, the so called *characteristic strain velocities*.

In the present work, the results obtained with DEM (Discrete Element Method) and some conclusions on the *material characteristics length MCL* and the material characteristics strains rate *MCSR* that the model used are shown.

Keywords: scale effect, strain velocity dependence, fracture mechanics, numeric simulation.

1 Introduction

For structural design, the knowledge about material properties in the real structure dimensions and the applied strain rate level are of fundamental importance. Generally the real structure material properties are different from those in a simple test specimen because exists an interaction between

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the material properties and the following factors: (i) structure size, (ii) strain rate applied on it. The material properties interaction with the size structure (size effect) has been studied since the modern science beginning - the Leonardo da Vinci and Galileo's works are evidence of that. Presently, the models created by [1] and [2] are examples of recent studies that have been generated in the size effect area.

The present paper is organized in the following way. In section 2, a brief description about the discrete element method (DEM) proposed by [3] is illustrated. In section 3 is shown the theoretical framework proposed by [4] to represent the scale law. The determination of non-dimensional parameters, the material characteristics length ***MCL*** and the material characteristics strains rate ***MCSR*** is briefly explained in sections 4 and 5. In section 6 the scale law verification is made in terms of characteristic lengths and strain rate. Finally, in section 7 the discussion of the physical significance of characteristic parameters and obtained results are pointed out.

2 The Discrete Element Method (DEM)

The DEM essentially consists in representing the continuum domain through, regular array of truss bars as shown in Fig. 1a,b, where group-working bar rigidity is equivalent to the mechanical behavior of the continuum domain in analysis. The elemental constitutive law represents the material non-linear behavior.

In [3] an elemental bilinear constitutive law is proposed. This law captures the material behavior until the rupture and is based on the original idea presented by [5]. The constitutive law is given in terms of force and strain.

In the Fig. 1(c), P_{cr} represents the maximum tensile force transmitted and ε_p the associate strain with P_{cr}; E_A is the cubic model bar rigidity and k_r is the factor that is related to ductility (this parameter permits to calculate the strain where the bar stop transmitting tensile force, $\varepsilon_r = k_r\ \varepsilon_p$). The limit strain ε_r must permit that the area in Fig. 1(c) multiplied by the bar length L_{ele} be equal to the available fracture energy *($Gf A_f$)* in the bar, where *Gf* is the specific fracture energy, and A_f is the fracture area that each bar represents.

As the material has a brittle behavior, the linear fracture mechanics can be applied. The toughness can be expressed in terms of the Irwin stress intensity factor (K_{Ic}) or in terms of the specific fracture energy (G_f), then it is possible to write

$$K_{IC} = \chi \cdot \sigma_t \cdot \sqrt{a} \text{ and } G_f = \frac{K_{IC}^2}{E}, \tag{1}$$

where χ is a parameter that depends on the problem geometry and a is the crack length. If the material behavior is linear up to rupture ($\sigma_t = \varepsilon_p E$), the critical strain is given by:

$$\varepsilon_p \ = \ R_f \cdot \left[\frac{G_f}{E\cdot}\right]^{1/2} \quad \text{where} \quad R_f = \frac{1}{(\chi \cdot \sqrt{a})} \tag{2}$$

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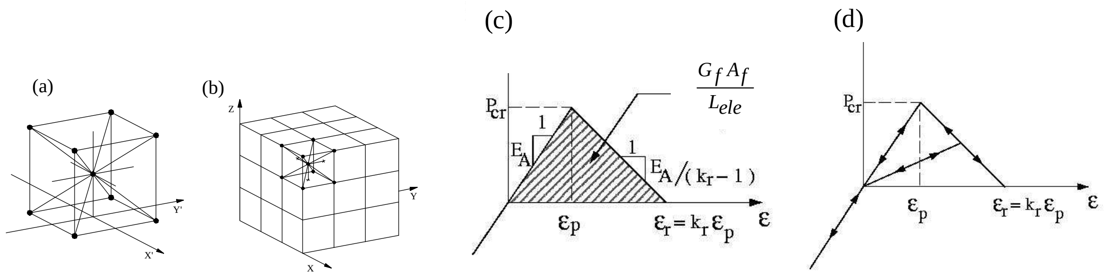

Figure 1: (a) Cubic Module. (b) Prism formed with several cubic Modules, (c) Uniaxial constitutive law, (d) Charge and discharge scheme.

and R_f is a fail factor. This factor permits to introduce information about the intrinsic form of material rupture. The motion equations for the spatial discretization can be written as:

$$M \cdot \ddot{u} + f(t) = q(t). \tag{3}$$

In the equation (3), M represents the diagonal mass matrix proportional to the density ρ,

u is the nodal displacement vector, $f(t)$ is the nodal internal force vector, $f(t)$ (that depends on previous and present displacements) and $q(t)$ is the nodal external applied force vector. As in elastic linear system, *f(t)=Ku(t)*, where K is the rigidity matrix. In systems with viscous forces, $f(t) = K \cdot u + C \cdot \dot{u}$. Considering the damping coefficient C proportional to the mass, ***C=MD***$_{f,}$, with D_f a constant that depends on the material. The motion Eq. (3) can be integrated numerically in the time domain with a explicit scheme (central difference methods). It is important to point out that P_{cr}, ε_P, ε_r,G_f ,R_f,,*E*sgρ and $D_{f,}$ are exclusively material properties while A_f and L_{ele} are exclusively related to the numerical model. Parameters E_A and k_r are function of both model and material. This method was successfully used in the modeling of concrete, soils and other composite materials such as is shown in [6]. All computational implementation and development of DEM was done that by research group of PPGEC/PROMEC/UFRGS.

3 Characteristic length and strain velocities

The scale effect is generally studied for a determined structure response, that here is generically named with the letter Y. This response can be, for example, the material nominal strength, the maximum elastic energy storage before fracture, etc. By comparing the results obtained in different size structures with geometric similarities, the scale effect can be verified.

Two structures (a and b) are considered geometrically similar when the quotients between dimensions ($\mathrm{d}_b/\mathrm{d}_a = \lambda$) are a constant, for any selected structural dimension. Obviously the obtained responses ($Y_a, Y_b, ...$) might be or not different for the different sizes of the structure. In the first case ($Y_b = Y_a = ... =$ constant), does not exist a scale effect, and the structural response is independent of the structure

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size. In the other case ($Y_b \neq$ g$_a \neq$ g..), the response is function of the structure size and consequently does exist a scale effect. An example of this scale effect is the microstructure size of grains in metals. It is known that the reduction of the grain size increases the metal hardness.

Consider that the response Y for a structure with a geometric dimension d is defined by a scale law function f as:

$$Y = Y_a f(\lambda), \tag{4}$$

where $\lambda = \mathrm{d}/\mathrm{d}_a$, Y_a is a response for the structure that has the reference size d$_a$ and f is a non-dimensional function that fulfill the condition $f(1) = 1$. If function f depends on the reference size d$_a$, it means that exists a material characteristic length (MCL). As stated by [1], when does not exist a MCL, it is possible verify that f has the following form:

$$f(\lambda) = \lambda^r. \tag{5}$$

The expression (5) represents the most generic form for the scale law, if there is not a MCL. In this equation r is a real number. If we consider that exists two MCL (dc_1 e dc_2) the response Y of the structure with geometric dimension d can be expressed as

$$Y = Y_a f(\lambda, \mu, \eta), \tag{6}$$

where the non-dimensional parameters are: λ=d/d$_a$, μ= d$_{c1}$/d$_a$ and η= d$_{c2}$/d$_a$. The function f must fulfill the condition: $f(1,\mu,\eta)$ =1, for any μ and η. Therefore, when exist two or more characteristic lengths (d$_{c1}$, d$_{c2}$, d$_{c3}$ ...), the function f must be independent of the selected reference dimension d_a, and will only depend on its characteristic lengths.

In a similar way, it is possible to define a material characteristic strain rate (MCSR) that arises when the structures responses due to loads applied with different strain rates are not the same. As an example, if the material has two MCL and two MCSR, the responses for two geometric dimensions Y_a and Y are defined as: Y_a => structural response with size d_a and strain rate $\dot{\varepsilon}_a$; Y => structural response with size $d$and strain rate $\dot{\varepsilon}$.

If we name d$_{c1}$ and d$_{c2}$ the MCLs and $\dot{\varepsilon}_{c1}$ and $\dot{\varepsilon}_{c2}$ the MCSRs, the non-dimensional parameters should be defined as:

$$\lambda = d/d_a, \mu = dc_1/d_a, \eta = dc_2/d_a, \theta = \dot{\varepsilon} \,/\, \dot{\varepsilon}_a, \pi = \dot{\varepsilon}_{c1}/\, \dot{\varepsilon}_a, \gamma = \dot{\varepsilon}_{c2} \,/\, \dot{\varepsilon}_a\,. \tag{7}$$

In this conditions, it is possible to write:

$$Y = Y_a f(\lambda, \mu, \eta, \theta, \pi, \gamma) \quad . \tag{8}$$

4 The scale law

In the present section, the methodology to identify the parameters of the scale law is shown. In all cases studied, the Poisson coefficient is maintained constant and in this manner the number of

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involved parameters is reduced. In the present analysis it will be considered that all input parameters are deterministic variables.

The following magnitude nomenclature will be utilized : **M:** Mass magnitude, **L**: Length magnitude, **T**: Time magnitude. The dimensional analysis by DEM is shown. In this case the following input parameters are used:

a) E = Elasticity Modulus,$[\mathbf{ML^{-1}\,T^{-2}}]$

b) ρ = Density, $[\mathbf{ML^{-3}}]$

c) G_f = Especific Fracture Energy, $[\mathbf{MT^{-2}}]$

d) R_f = fail factor, $[\mathbf{L^{-1/2}}]$

e) D_f = damping factor, $[\mathbf{T^{-1}}]$

The results Y_a and Y correspond to two structures composed with the same material and different sizes, but geometrically similar to each other and submitted to different strain rates. In addition to the material property parameters, the following variables will enter in the analysis:

f) d_a =size of the first structure, **[L]**

g) d= size of the second structure, **[L]**

h) $\dot{\varepsilon_a}$ = the strain rate applied to the first structure, $[\mathbf{T^{-1}}]$

i) $\dot{\varepsilon}$ = the strain rate applied to the second structure, $[\mathbf{T^{-1}}]$

In the DEM analysis, the bar length (L_{ele}) was maintained constant for all cases simulated. Then, L_{ele}does not entry as an input parameter. Consequently, it is possible to write:

$$\begin{aligned} Y &= F(E,\rho,G_f,R_f,D_f,d,\dot{\varepsilon}) \qquad \text{(a)} \\ Y_a &= F(E,\rho,G_f,R_f,D_f,d_a,\underset{a}{\dot{\varepsilon}}) \qquad \text{(b)} \end{aligned} \tag{9}$$

And the quotient of both responses will be:

$$\frac{Y}{Y_a} = F^*(E,\rho,G_f,R_f,D_f,d,d_a,\dot{\varepsilon},\underset{a}{\dot{\varepsilon}}) \quad . \tag{10}$$

The quotient of Eq. (10) can be expressed in terms of products of the power of input parameters as usual in dimensional analysis. It must be figured that:

$$E^{a1} \times \rho^{a2} \times G_f^{a3} \times R_f^{a4} \times D_f^{a5} \times d^{a6} \times d_a^{a7} \times \left(\dot{\varepsilon}\right)^{a8} \times \left(\dot{\varepsilon_a}\right)^{a9} = \text{non-dimensional} \tag{11}$$

and, consequently:

$$\begin{aligned} a_1 + a_2 + a_3 &= 0 \ \ \text{(for magnitude }\mathbf{M}) \\ a_1 + 3a_2 + a_4/2 - -a_6 - -a_7 &= 0 \ \ \text{(for magnitude }\mathbf{L}) \\ 2a_1 + 2a_3 + a_5 + a_8 + a_9 &= 0 \ \ \text{(for magnitude }\mathbf{T}) \end{aligned} \tag{12}$$

Using the Eqs. (12) it is possible to eliminate a_1, a_7 and a_9 to obtain that:

$$\left(\frac{\rho\left(\underset{a}{\dot{\varepsilon}}\right)^2 d_a^2}{E}\right)^{a2} \times \left(\frac{G_f}{Ed_a}\right)^{a3} \times \left(R_f d_a^{1/2}\right)^{a4} \times \left(\frac{D_f}{\underset{a}{\dot{\varepsilon}}}\right)^{a5} \times \left(\frac{d}{d_a}\right)^{a6} \times \left(\frac{\dot{\varepsilon}}{\underset{a}{\dot{\varepsilon}}}\right)^{a8} = \text{non-dimensional} \tag{13}$$

It is important to point out that other ways to make this simplification are possible.
Equation (10) can be then rewritten as:

$$\frac{Y}{Y_a} = f(\lambda, \mu, \eta, \theta, \pi, \gamma). \tag{14}$$

From nine variables illustrated in Eq. (10), five were material function (E,ρ,G_f, $R_f$and D_f), two were structure dimensions function (d and d_a) and two were function of the applied strain rate ($\dot{\varepsilon}$ and $\underset{a}{\dot{\varepsilon}}$). These input variables define the studied problem in DEM, as shown in table 1, and were reduced to six non-dimensional parameters, as illustrated in table 2. In this case, four parameters define the material properties (μsηsπsγp, one the structure dimensions (λpgnd one the applied strain rate oθ). The MCL and MCSR are shown in table 3.

Table 1: Input data for DEM

	Var$_1$**[ML**$^{-1}$**T**$^{-2}$**]**	**Var**$_2$ **[ML**$^{-3}$**]**	**Var**$_3$**[MT**$^{-2}$**]**	**Var**$_4$**[L**$^{-1/2}$**]**	**Var**$_5$[T^{-1}]
Input Data	E	ρ	G$_f$	R$_f$	D$_f$

Table 2: Non-dimensional parameters for DEM

Non-dimensional parameters	$\lambda = \frac{d}{d_a}$	$\mu = \frac{R_f^{-2}}{d_a} = \frac{dc_1}{d_a}$	$\eta = \frac{G_f}{Ed_a} = \frac{dc_2}{d_a}$	$\theta = \frac{\dot{\varepsilon}}{\underset{a}{\dot{\varepsilon}}}$	$\gamma = \frac{R_f^2}{\underset{a}{\dot{\varepsilon}}}\sqrt{\frac{E}{\rho}} = \frac{\underset{c1}{\dot{\varepsilon}}}{\underset{a}{\dot{\varepsilon}}}$	$\pi = \frac{D_f}{\underset{a}{\dot{\varepsilon}}} = \frac{\underset{c2}{\dot{\varepsilon}}}{\underset{a}{\dot{\varepsilon}}}$

Table 3: Characteristic parameter (MCL and MCSR) for DEM

	d$_{c1}$**[L]**	d$_{c2}$**[L]**	$\underset{c1}{\dot{\varepsilon}}$ **[T**$^{-1}$**]**	$\underset{c2}{\dot{\varepsilon}}$ **[T**$^{-1}$**]**
Characteristic Parameter	$\frac{1}{R_f^2}$	$\frac{G_f}{E}$	$R_f^2\sqrt{\frac{E}{\rho}}$	D$_f$

5 Verification methodology

Four simulations with responses Y_1, Y_{a1}, Y_2 and Y_{a2} were considered in order to verify the algorithm. The following conditions were considered:

1. The magnitudes that define the material properties are equal for the two first cases (1, $a1$) and for the last two cases (2, $a2$), although not necessarily equal between them.
2. The quotients between the sizes d_1/d_{a1} and d_2/d_{a2} are equal.
3. The quotients between the strain rates $\dot{\varepsilon_1} / \dot{\varepsilon_{a1}}$ and $\dot{\varepsilon_2} / \dot{\varepsilon_{a2}}$ are equal.
4. The non-dimensional parameter (including Poisson coefficient) are equal in all cases.

If the four conditions are fulfilled it is possible to say that:

$$\lambda_1 = \lambda_2, \mu_1 = \mu_2, \eta_1 = \eta_2, \theta_1 = \theta_2, \pi_1 = \pi_2, \gamma_1 = \gamma_2 \tag{15}$$

and consequently

$$\frac{Y_1}{Y_{a1}} = f(\lambda_1, \mu_1, \eta_1, \theta_1, \pi_1, \gamma_1, \nu) = \frac{Y_2}{Y_{a_2}} = f(\lambda_2, \mu_2, \eta_2, \theta_2, \pi_2, \gamma_2, \nu). \tag{16}$$

or

$$Y_1/Y_{a1} = Y_2/Y_{a2}. \tag{17}$$

These verifications were done in terms of characteristic strengths, strains, and energy values presented in the simulated processes. A bar in simple tension was considered for the scale law verification. The aspect ratio of all models is equal to 5 and the loading was imposed in terms of prescribed displacement at the ends of the bar as presented in Fig. 2. The bar had square section and a full 3D analysis was performed. In table 4, the bar properties as well as the discretization (l_c) are shown. In Tab. 5 the results in terms of ratio responses Y/Ya are shown, where σ_f is the yield stress, σ_r the peak stress, ε_r the corresponding strain to σ_r and the ε_{max} ultimate strain. $E_{elastic}$, $E_{kinematic}$, E_{damage} are the highest values of the elastic energy stored in the body, the kinematic and damaged (or dissipated) energy values that occurred during the simulations, respectively. In Figs. 3 and 4, the four tests are plotted in terms of the parameters mentioned above. Finally, the final configurations of the four tests are shown in Fig 5.

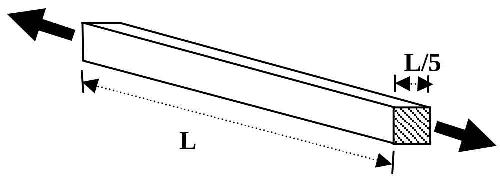

Figure 2: The tension bar tested by DEM.

In the Fig. 3, the stress versus strain curves for the four cases tested are shown.

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Table 4: The geometrical and material properties used in the DEM simulation.

	L (m)	**Dε/dt** (mm)	**lc** (m)	**E** (N/m^2)	ρ (Kg/m^3)	**G**$_f$ (N/m)	**R**$_f$ (m$^{1/2}$)	**D**$_f$ (1/s)
1	2	1	0.01	2.E11	1E+3	1E2	5	10
1a	3	10	0.01	2.E11	1E+3	1E2	5	10
2	0.5	100	2.5E-3	17500	6.4E4	1E6	10	1000
2a	0.75	1000	2.5E-3	17500	6.4E4	1E6	10	1000

Table 5: Results in terms of the ratio Y1/Y1a and Y2/Y2a

	σ_f **[N/m^2]**	σ_r **[N/m^2]**	ε_{max}	ε_r	**E** $_{elastic}$ **[Nm]**	**E**$_{kinematic}$ **[Nm]**	**E**$_{damage}$ **[Nm]**
$\frac{Y1}{Y1a}$	4,15	4,26	5,81E-2	3,97E-2	0.60	1.52	0.32
$\frac{Y2}{Y2a}$	4,18	4,25	5,89E-2	4,19E-2	0.61	1.52	0.33

6 Discussion and conclusions

In the present work the formulation carried out by Morquio and Riera (2004) was applied to formulate a scale law in terms of non-dimensional variables for the Discrete Element Method (DEM) . It can be concluded that:

a) The verification done for DEM showed very good correlation as the section 5 indicates.

b) With Eq.(16), and the responses for different scales for a material (1) (Y_{1a},Y_{1b},Y_{1c},Y_{1d},Y_{1e},..), it is possible to obtain the responses $Y_{2b}, Y_{2c}, Y_{2d}, Y_{2e}, \ldots$ (for another material (2) that can be analyzed in the same model), only knowing a response for one size (Y_{2a}). Hence, it is possible to write

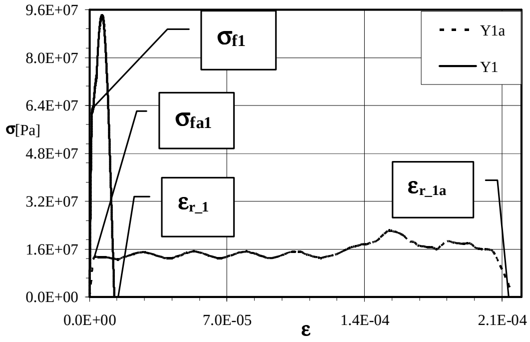
$$Y_{2i} = (Y_{1i}/Y_{1a})Y_{2a}, (\ i = b, c, d, e, ..). \tag{18}$$

The dimensions of the specimen that produce the responses $Y_{1a}, Y_{1b}, Y_{1c}, Y_{1d}, Y_{1e}$, must accomplish the relations below:

$$Y_{1i}/Y_{1a} = f(\lambda_{1ai}, \mu_{1a}, \eta_{1a}, \theta_{1ai}, \pi_{1a}, \gamma_{1a}) = Y_{2i}/Y_{2a} = f(\lambda_{2ai}, \mu_{2a}, \eta_{2a}, \theta_{2ai}, \pi_{2a}, \gamma_{2a}), \tag{19}$$

where $\lambda_{1ai} = \lambda_{2ai}, \mu_{1a} = \mu_{2a}, \eta_{1a} = \eta_{2a}, \theta_{1a} = \theta_{2a}, \pi_{1a} = \pi_{2a}$ *and* $\gamma_{1a} = \gamma_{2a}$ *(i = b, c, d, ...).*

(a)



(b)

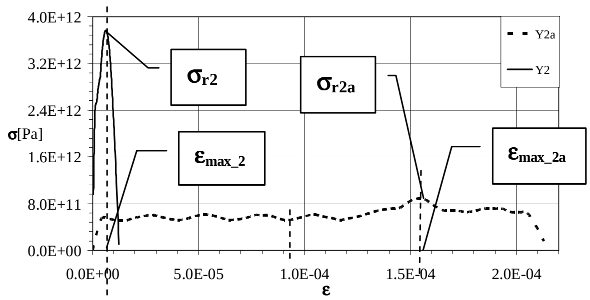


Figure 3: Results in terms of stress (σp versus overall strain εp. for the four tests.(a) Y1,Y1a, (b)Y2, Y2a).

c) Trying to understand the physical meaning of characteristic parameters shown in table 3, the following relations are defined:

$$K_{IC} = \frac{\sigma_t}{Rf}, \quad G_f = \frac{K_{IC}^2}{E}, \quad \sigma_t = E\varepsilon_p, \tag{20}$$

Where K_{Ic} and G_f are the toughness in terms of stress intensity factor and specific fracture energy, respectively. It can be observed that:

c1) Using Eq. (20), the length characteristic d_{c1}, shown in Tab. 3, can be expressed as:

$$d_{c_1} = \frac{1}{Rf^2} = \frac{G_f}{E\varepsilon_p^2}. \tag{21}$$

Trying to find a physical meaning for d_{c1}, the following transformation is done:

$$d_{c1} = \frac{G_f}{E\varepsilon_p^2} = \frac{G_f}{E\varepsilon_p^2}\frac{((1/2)l_1^3)}{((1/2)l_1^3)} = \frac{G_f l_1^2}{U\left(\varepsilon_p\right)}(\frac{l_1}{2}) \quad . \tag{22}$$

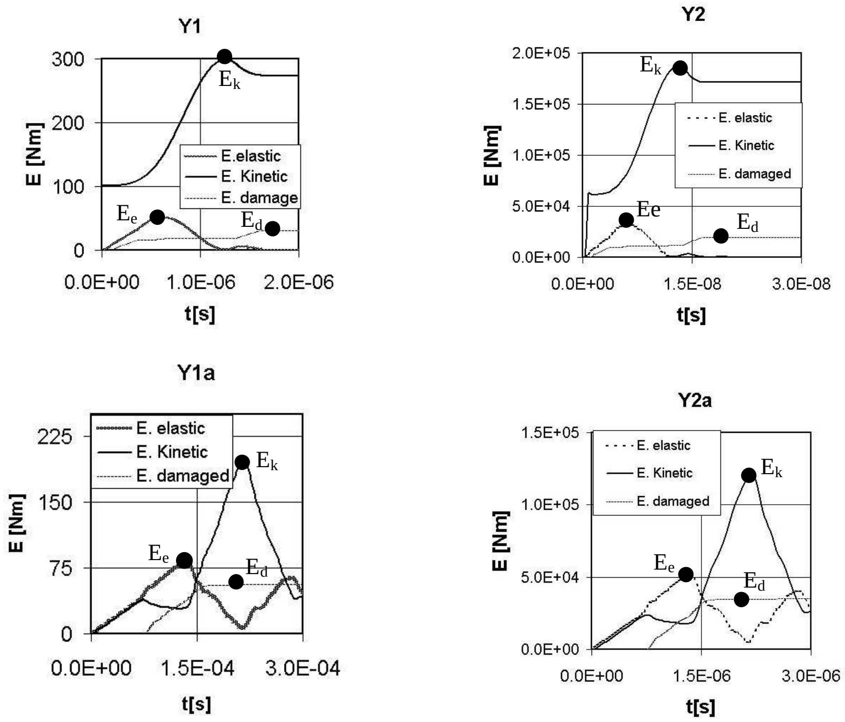


Figure 4: Results in terms of Elastic, Kinetic and Damaged Energies dissipated during the process for the four tests.

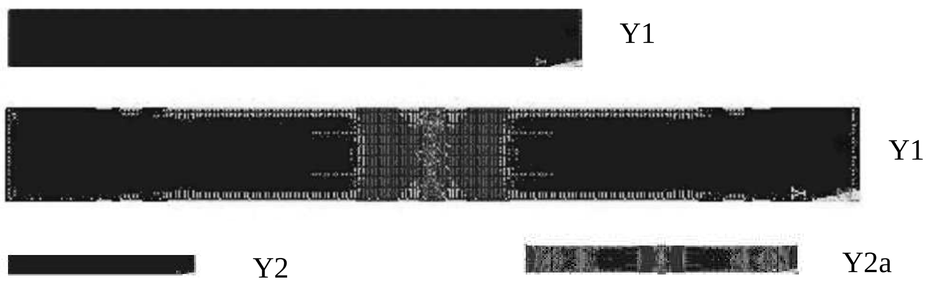


Figure 5: The final configuration of the four body tests. (gray color indicated damaged region. The bodies fractured at the end of the bar).

If we interpret l_1 as the length of the side of a cube that, for its critical strain ε_p, stores an elastic strain energy U equal to the necessary energy to break an area ($l_1)^2$, then it is possible to rewrite d_{c1} in terms of l_1 as:

$$d_{c_1} = \frac{G_f}{E\varepsilon_p^2} = \frac{l_1}{2}. \tag{23}$$

Consequently d_{c1} can be interpreted as the half of the l_1.

c2) The characteristic length d_{c2} in the table 3 can be eliminated if the critical strain ε_p is considered a non-dimensional parameter into the material analyzed scale law. In this way, the expression (17) can be replaced by

$$\frac{Y_1}{Y_{a1}} = f(\lambda_1, \mu_1, \theta_1, \pi_1, \gamma_1, \nu, \varepsilon_p) = \frac{Y_2}{Y_{a_2}} = f(\lambda_2, \mu_2, \theta_2, \pi_2, \gamma_2, \nu, \varepsilon_p). \tag{24}$$

In [7], a comparison of the results obtained from three different numerical methods was carried out. These different numerical methods allow to simulate fracture in solids. Two of these formulations are based on the Finite Element Method: the Cohesive Interface Method [8] and a Distributed Fissure Method proposed by [9]. The third method is the Discrete Element Method analyzed in the present work. The characteristic length d_{c2}=Gf/E appears in the three parameter sets of the scale laws of the models mentioned above.

c3) Regarding the characteristic strain rates,

$$\underset{c1}{\dot{\varepsilon}} = R_f^2\sqrt{\frac{E}{\rho}} = \frac{1}{d_{c1}}\sqrt{\frac{E}{\rho}}. \tag{25}$$

It is possible to define $\underset{c1}{\dot{\varepsilon}}$ as the wave elastic propagation speed when taking the characteristic length d_{c1}as the length unit.

c4) The other characteristic strain rate $(\underset{c2}{\dot{\varepsilon}})$ is linked to the viscous damping and to the structures mass (D_f).

d) The method could be generalized for non deterministic input data. In this case, if one of the input datum is a random field, its statistical distribution (Normal or Weibull, for example) remains defined by the following parameters: the mean value and the standard deviation that could also be incorporated to the correlation length of the random field.

When the problem is non deterministic, it is possible to obtain the response Y in terms of mean value and standard deviation. In this case, instead of the value of the input parameter used in the deterministic analysis, the mean value will appear and another input data, the standard deviation, will be incorporated. We could also consider the mean value and a non-dimensional parameter: the variation coefficient of the random input data. The correlation length of the random field appears as a characteristic length.

e)As a final conclusion, it is possible to say that the scale law analysis permits to infer fundamental information about the meaning of the parameters used by the DEM method. The comparison among different methods gives a new light in the interpretation of these parameters.

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