APPLICATION OF UPDATING METHODS IN THE DISCRETE ELEMENT METHOD

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Abstract. *This work show the application of modal assurance criterion (MAC) as a reference tool to help in improving the correlation degree between numerical models based on the Discrete Element Method (DEM) and experimental testing. The DEM has many advantages in the analysis of structures of non-homogeneous materials subjected to static or dynamic fracture. In cases where experimental data is available, the method can deliver more accurate results if a model updating procedure is carried out during pre-analysis estages. Since model updating methods are virtually unexplored within discrete element methods, this work presents a simple scheme to calibrate a DEM model with reliable experimental data avaliable from the literature. The improvements obtained in the results are compared with the ones obtained without the updating.*

Keywords*: Discrete elements, Numerical Analysis, Model Updating*

1. INTRODUCTION

In the Discrete Element Method (DEM), masses are concentrated in nodal points and connected by one-dimensional elements with arbitrary constitutive relations. Therefore, the DEM differs significantly from more popular numerical methods like the Finite Element Method (FEM) as it tries to discretely simulate a 3D continuum medium without the aid of 3D shape functions.

Figure 1 shows the cubic system adopted in this work. A basic cubic module includes 20 members and 9 nodes. Each node has three degrees of freedom, corresponding to the three components of displacement vector in a global reference system. Further information on the model adopted in this work can be found in Bergamini (2010).

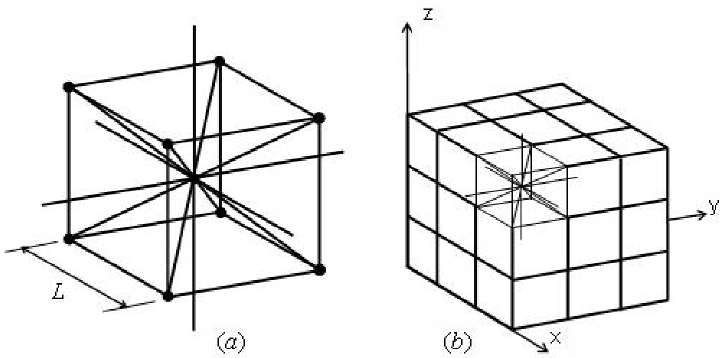


Figure 1 - Cubic model of the DEM: (a) basic cubic model, (b) generation of prismatic body

On the other hand, like any numerical method applied to engineering problems, it could benefit from experimental data by updating the model to deliver results closer to these data than the original model. Model updating procedures (Friswell and Mottershead, 1993) are a common tool in engineering models nowadays, but its application has been limited to the FEM. To the best of authors' knowledge, model updating has never been applied to DEM models.

The basic idea of any model updating procedure is to change the numerical model artificially in order to reproduce as well as possible a set of experimental or analytical results. If this goal is fulfilled, the confidence in the numerical model is naturally increased to simulate more complex situations, provided mesh/discretization aspects are not an issue.

The present work shows a simple methodology based on the use of a modified MAC index (Modal Assurance Criterion) to update a DEM model using laboratory tests carried elsewhere (Kupfer, 1973) as updating parameters. The improvements in the results are discussed and compared with the ones obtained previously without model updating.

2. SENSITIVITY ANALYSIS

Since model updating is based on the minimization of the error between two sets of results, it can be regarded as an optimization and, as such, sensitivity analysis can help the analyst to decide which ones are the best updating parameters (design variables). The objective of sensitivity analysis is to determine the gradients of the objective function and constraints with respect to a set of design variables. These gradients indicate the response sensitivity of the objective function to small changes in the variables of the problem. An analysis of these gradients also helps to accelerate the iterative updating procedures.

On the other hand, errors in the gradient accuracy inevitably lead to convergence problems in optimization algorithms. Therefore, the choice of the method to be used to calculate the gradients should consider accuracy and efficiency. Besides these, one should take into account numerical implementation aspects.

There are two basic forms of analysis to calculate the sensitivity: (1) direct or implicit differentiation, and (2) variational analysis. The first is a straightforward method to implicitly differentiate the equilibrium equations already in their discretized form, while the latter produces a continuous differentiation of the governing equations with respect to the design variables prior the discretization process. In this work, we adopted the finite difference method to evaluate the sensitivities.

2.1 Finite difference method

The simplest way to calculate the gradients needed in an optimization process is to use finite differences (FD). The FD starts by expanding the function $f(x)$ in Taylor series:

$$f\left(x+\Delta x\right)= f\left(x\right)+\frac{\partial f}{\partial x}\Delta x+\frac{\partial^2 f}{\partial x^2}\frac{\left(\Delta x\right)^2}{2!}+\cdots \tag{1}$$

Truncation of the higher order terms leads to the well known approximation for the derivative of f

$$f'\left(x\right)\approx\frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x} \tag{2}$$

Alternatively, central differences can be used:

$$f'\left(x\right)\approx\frac{f\left(x+\Delta x/2\right)-f\left(x-\Delta x/2\right)}{\Delta x} \tag{3}$$

The accuracy of FD is strongly linked to the magnitude of the perturbation Δx used, as well as nonlinearity of the function. Too small values for Δx can lead to stability and truncation problems, while excessively large values will produce wrong results. The confidence interval is a problem dependent aspect and will not be discussed here. The advantage of this method is its easy implementation - virtually no changes need be made in the numerical code. On the other hand, the use of FD with huge computational models or highly nonlinear problems will demand very high computational cost.

3. MODAL ASSURANCE CRITERION (MAC)

The MAC index is a very useful and effective way to quantify the deviation of an approximated vector from its reference value. It was developed initially for testing the accuracy of model shape vectors obtained in FEM, provided at least one experimental mode is available. Nowadays many variations exist (Allemang, 2003). In its original form, the MAC compares the experimentally obtained mode shapes with the analytical/numerical mode shapes, using arguments of orthogonality between them (Friswell and Mottershead, 1993):

$$MAC_{ij}=\frac{\left|\phi_{mj}^T\phi_{ak}\right|^2}{\left(\phi_{ak}^T\phi_{ak}\right)\left(\phi_{mj}^T\phi_{mj}\right)} \tag{4}$$

MAC values therefore range between 0 and 1. Ideally, MAC should equals 1 when $i = j$ and 0 otherwise. That is, perfectly matching results will produce an identity MAC matrix. Of course both modes must contain the same number of entries, which is not always possible. This may need condensation of the degrees of freedom in the numerical model or mode expansion for the experimental models.

4. EXPERIMENTAL MODEL

The material used for the experiment consisted of concrete with a density of 2400 kg/m³, with gravel aggregate with maximum size of 15 mm. Three types of concrete composition were prepared with water/cement ratio of 1.22, 0.90 and 0.425, and with the corresponding amount of concrete of 145 kg/m³ 190 kg/m³ and 445 kg/m³, respectively. The nominal results of compression tests until rupture - f_{cu}, for the three types were, respectively, 191 kgf/cm², 311 kgf/cm², 594 kgf/m². The specimens were stored for 7 days in an environment with 100% humidity, after this period were transferred to an ambient temperature of 20 °C and 65% humidity, and the time spanned from manufacturing until the test was 28 days.

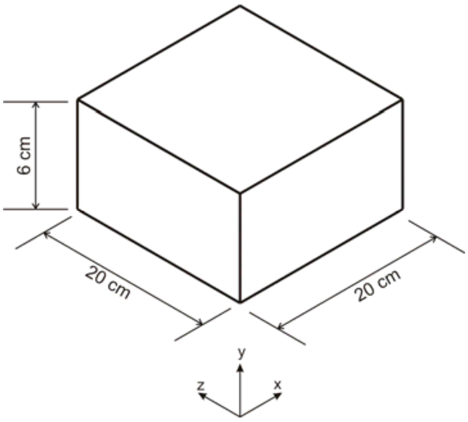


Figure 2 - Schematic model of the specimen used in the experiment.

The specimens tested have a prismatic geometry of 20 cm x 20 cm x 6 cm, as shown in Figure 2. They were subjected to different loading along the principal axes. The samples were tested σ_1/σ_2 ratios, for each quadrant of the $\sigma_1 \times \sigma_2$ diagram. The test specimens were subjected to various principal stress ratios σ_1/σ_2 in the compressive, tensile and compressive-tensile ranges for each stress-quadrant.

The equipment used in the test consisted a simple hydraulic system generating a constant principal stress ratio (Figure 3). Instrumentation of the test specimens consisted of load cells and strain gauges for the determination of the forces and strain applied in the principal directions, Figure 4. Graphs illustrating the failure criteria obtained for the specimen studied under biaxial stress states are shown in Figure 5.

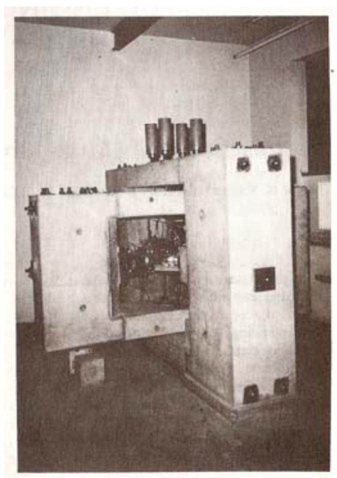


Figure 3 - Compression testing machine used by Kupfer (1973)

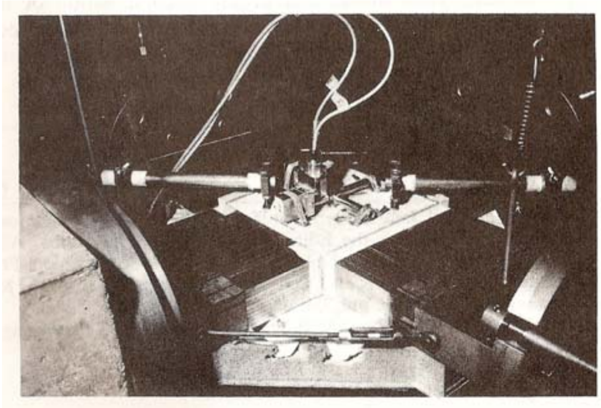


Figure 4 - Testing of the specimen (Kupfer, 1973).

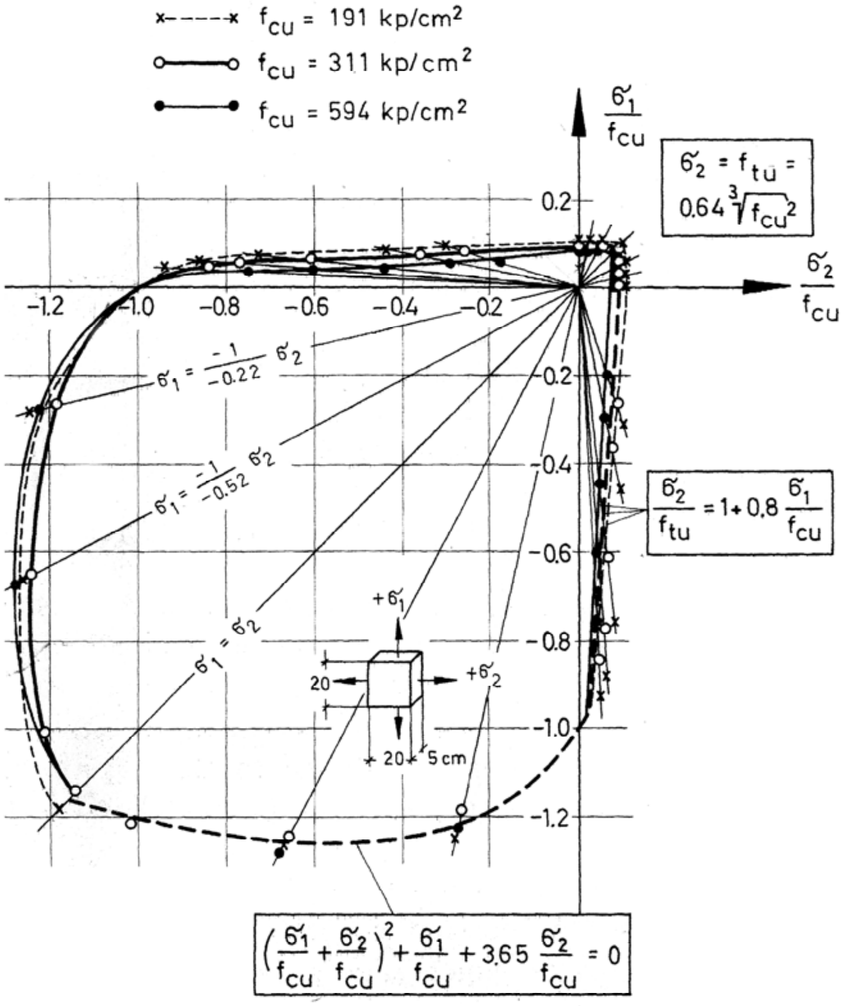


Figure 5 - Biaxial loading for three kinds of concrete (Kupfer, 1973).

5. IMPLEMENTATION OF NUMERICAL MODEL

Aiming its updating, the numerical model implemented has the same geometrical and mechanical properties of the experimental test specimen. Table 1 shows the mechanical properties of the specimen simulated. Since the length of each DEM cubic module used was 7.5E-3 m, the model used consists of 28 modules in the *X* and *Z* directions and 8 modules in the direction *Y*.

Table 1 - Properties of the test specimen simulated concrete

E	7.5e10	N/m^2
ε_p	1.087e-4	
Cube's sides	0.5	m
CV(G_F)	40%	
Poisson	0.25	
f_{cu}	191	kgf/cm²

Four cases of compression loading were simulated, with four samples for each case. The loadings applied on these benchmarks are on *XZ* plane, only (no loading was applied on *Y* direction to reproduce the Kupfer (1973) test).

No kinematic boundary conditions needed to be applied because the applied loading prevents any rigid body movement. Figure 6 shows loading cases used in the DEM simulations.

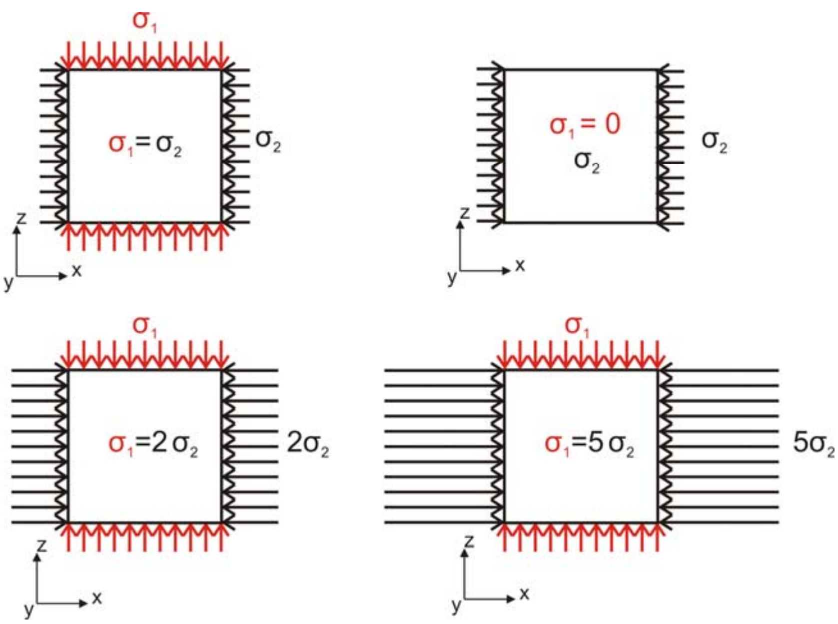


Figure 6 – Load cases used in the DEM.

6. DEFINITION OF THE OBJECTIVE FUNCTION AND DESIGN VARIABLES

The objective function to be minimized in the updating scheme was the critical strain ε_p. Since each bar in the DEM mesh has its parameters related to this variable, the following function was a natural choice:

$$\varepsilon_p = Rfc\sqrt{\frac{\frac{Gfr}{E}}{\left(1-\upsilon^2\right)}} \tag{5}$$

where *Rfc* [$\sqrt{m}$] is the factor of failure, *Gfr* [N/m] is the specific energy of fracture, *E* [N/m²] is the Young's modulus, and υ is the Poisson ratio . The design variables adopted in this first study were *Gfr* and *E*, both with a coefficient of variation of 40%.

Two variables were initially selected as design parameters: *Gfr* and *E*. In order to determine the sensitivities of the objective function with respect of these parameters, a random field of ε_p was generated around a typical value (Figure 7).

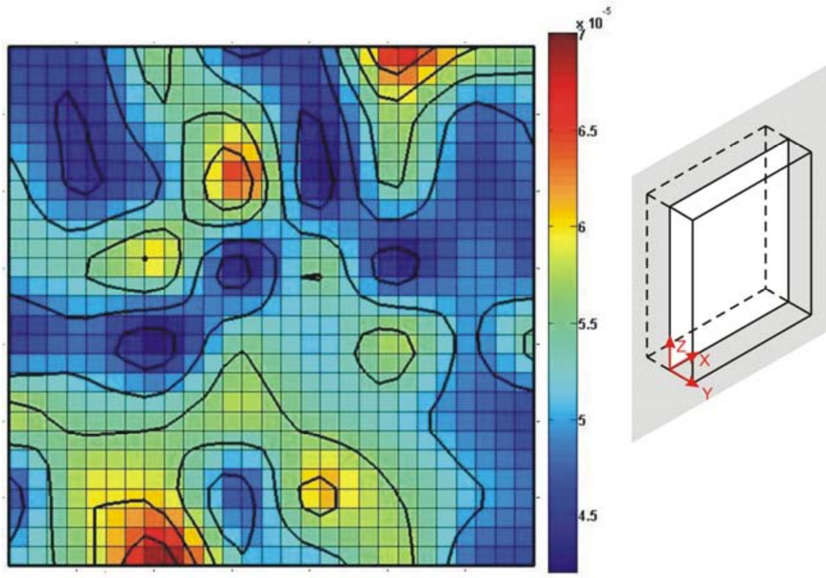


Figure 7 - ε_p map along the XZ section of the specimen simulated (Bergamini, 2010).

This random field was differentiated with respect to the design variables, Gfr and E, to provide the sensitivities of the objective function, i.e.:

$$\frac{\partial \varepsilon_p}{\partial Gfr} = \frac{\varepsilon_p\left(Gfr + \Delta Gfr\right) - \varepsilon_p\left(Gfr\right)}{\Delta Gfr} \tag{6}$$

$$\frac{\partial \varepsilon_p}{\partial E} = \frac{\varepsilon_p\left(E + \Delta E\right) - \varepsilon_p\left(E\right)}{\Delta E} \tag{7}$$

Figure 8 shows the converged values of the gradients obtained by equations (6) and (7). With these values defined, the most significant design variable was selected as the one producing the highest gradients. It is clear that the objective function is much more sensitive to changes in *Gfr*. Therefore, numerical model was then updated iteratively by changing the value of *Gfr*.

7. IMPLEMENTATION OF MAC INDEX IN DEM

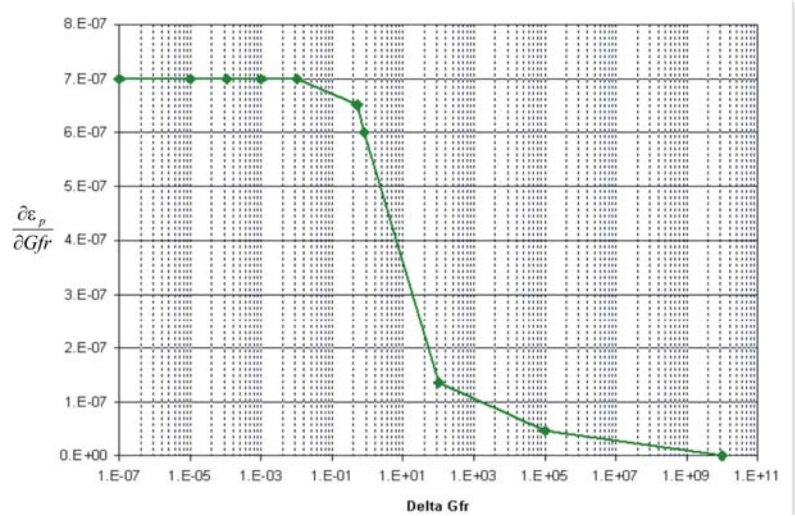
In order to use MAC index in the DEM, it was necessary to make adjustments to the method, since the present problem is not a modal one. Therefore, it was necessary to transform the ϕ_{ij} vectors in eq.(4) from mode shapes to rupture stress curves. The idea is that the polylines defining the failure criteria obtained experimentally in Figure 5 can be used as target values for the polylines obtained by DEM, updating the design variables chosen in section 6. The updating procedure becomes to iterate the numerical model until the following modified MAC index becomes as close as possible to the unity:

$$MAC_{\text{adapt}} = \frac{\left|\sigma_{mj}^{T}\sigma_{ak}\right|^{2}}{\left(\sigma_{ak}^{T}\sigma_{ak}\right)\left(\sigma_{mj}^{T}\sigma_{mj}\right)} \tag{8}$$

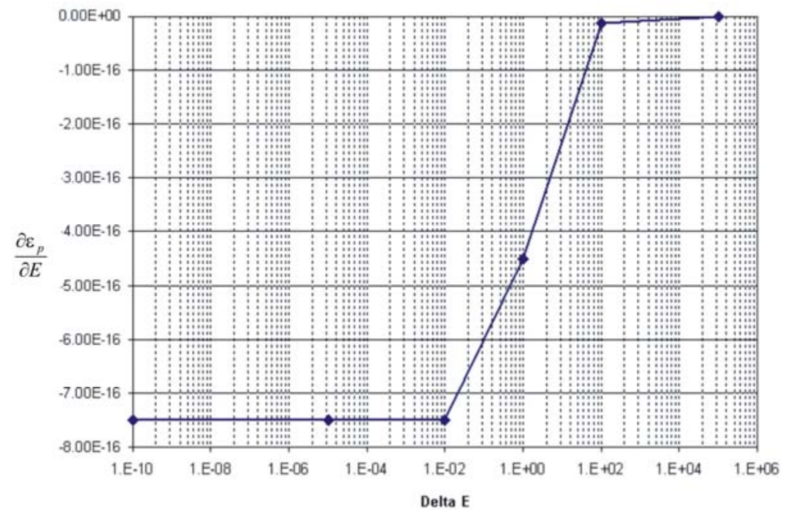
When the iteration ends, the final value of Gfr is the one which asserts the reproduction of the experimental results by the numerical DEM model.

Figure 10-a shows the rupture stress obtained for different values of MAC_{adapt}, the blue line corresponds to the perfect match between numerical and experimental values (MAC_{adapt} = 1). The red symbols show the values of

$\text{MAC}_{\text{adapt}}$ for different values of Gfr used in the numerical model during the updating. From the figure, it is clear that optimum value for Gfr is between 100 and 150 N/m, when the corresponding $\text{MAC}_{\text{adapt}}$ attained a value above 0.98.



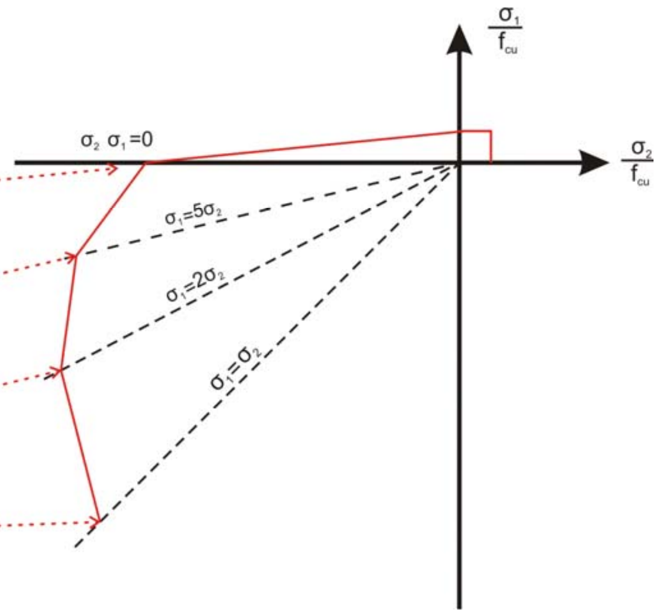
a)



b)

Figure 8 – Gradients of the objective functions with respect to the design variables. a) $\dfrac{\partial \varepsilon_p}{\partial Gfr}$; b) $\dfrac{\partial \varepsilon_p}{\partial E}$.

To further observe the effect of different $\text{MAC}_{\text{adapt}}$ indexes on the failure stress values, Figures 10-b to 10-d show the rupture stress results obtained for each loading in Figure 6, superposed to the experimental diagram of Figure 5. The symbols represent the simulated failure stress for each loading. Figure 10-b shows the results for Gfr = 60 N/m, clearly far from the experimental results. Figure 10-c shows that for Gfr = 200 N/m the results are still off. On Figure 10-d the value Gfr = 130 N/m, which was obtained from the best $\text{MAC}_{\text{adapt}}$ index of Figure 10-a, was used and the agreement with the experimental results of Kupfer (1973) is obvious.



$$\sigma_{ak} = \sigma_{mj} = \begin{Bmatrix} \sigma_2 \\ \sigma_1 \\ 5\sigma_2 \\ \sigma_1 \\ 2\sigma_2 \\ \sigma_1 \\ \sigma_2 \\ \sigma_1 \end{Bmatrix}$$

Figure 9 - Position of the stress values on their respective vectors

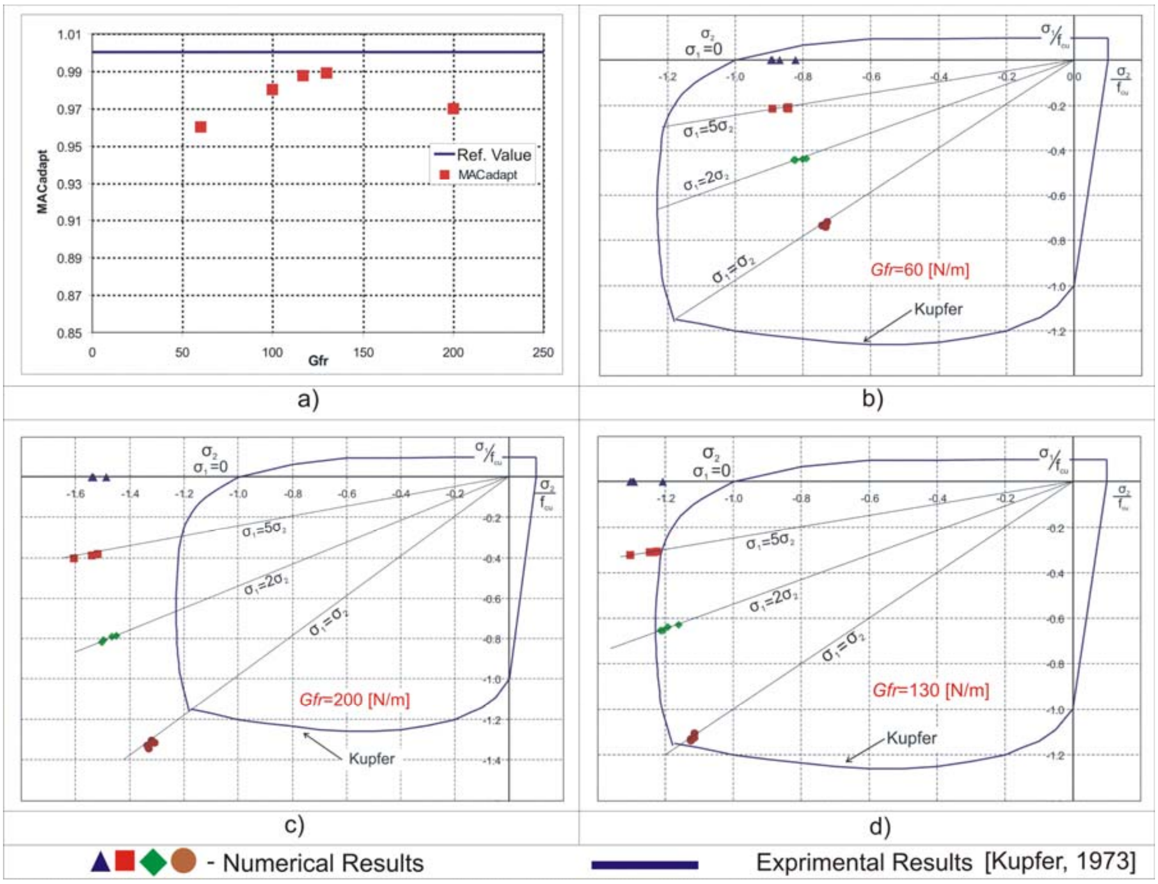


Figure 10 – Failure stress values obtained during the updating.

9. CONCLUSIONS

The use of Modal Assurance Criterion (MAC) as updating criteria in a DEM model was satisfactory. The values obtained with the updated numerical model are much closer to the experimental results than the original model, delivering a correlation of 0.99 obtained for a *Gfr* of 130 N/m.

The single design parameter *Gfr* was selected because it produced the highest sensitivity of the objective function. Its optimal value was obtained by replacing the original eigenvectors in the MAC definition by polygons defining the failure stress in the case studied, and updating the numerical model accordingly. The final *Gfr* values produced the best MAC value. Similar procedures can be developed for other loading cases and geometries. This work showed that DEM models can be updated with MAC (or similar) parameters, assuring good agreement between the numerical and experimental results, and increasing the confidence in the updated numerical model.

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