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3D DISCRETE ELEMENT MODELING OF CONCRETE: STUDY OF THE ROLLING RESISTANCE EFFECTS ON THE MACROSCOPIC CONSTITUTIVE BEHAVIOR

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Abstract. The Discrete Element Method (DEM) is appropriate for modeling granular materials [14] but also cohesive materials as concrete when submitted to a severe loading such an impact leading to fractures or fragmentation in the continuum [1, 5, 6, 8]. Contrarily to granular materials, the macroscopic constitutive behavior of a cohesive material is not directly linked to contact interactions between the rigid Discrete Elements (DE) and interaction laws are then defined between DE surrounding each DE. Spherical DE are used because the contact detection is easy to implement and the computation time is reduced in comparison with the use of 3D DE with a more complex shape. The element size is variable and the assembly is disordered to prevent preferential cleavage planes. The purpose of this paper is to highlight the influence of DE rotations on the macroscopic non-linear quasi-static behavior of concrete. Classically, the interactions between DE are modeled by spring-like interactions based on displacements and rotation velocities of DE are only controlled by tangential forces perpendicular to the line linking the two sphere centroids. The disadvantage of this modeling with only spring-like interactions based on displacements is that excessive rolling occurs under shear, therefore the macroscopic behavior of concrete is too brittle. To overcome this problem a non linear Moment Transfer Law (MTL) is introduced to add a rolling resistance to elements. This solution has no influence on the calculation cost and allows a more accurate macroscopic representation of concrete behavior. The identification process of material parameters is given and simulations of tests performed on concrete samples are shown.

1 INTRODUCTION

Designing large scale structures is a real challenge for engineers nowadays. Concrete is widely used in all sort of buildings which can be submitted to severe loadings due to material or anthropogenic hazards such as rock falls, explosions or missile impacts. Then it's very important to make an efficient design of these structures under such loadings leading to locally discontinuous behaviour.

The Discrete Element Method (DEM), based on the distinct element model [14] is appropriate for modeling a granular material, when a discrete element represents a grain, but also cohesive materials as concrete. Contact and cohesive interactions are used, and each rigid DE has an interaction range around it. Interactions laws are then defined between DE surrounding each element.

Using spherical geometry for discrete element is well suitable to keep the computational time as low as possible especially when large structures are considered. In this case, the contact detection algorithm is easier to implement than for ellipsoidal and polyhedral elements. Despite this advantage, an excessive rolling occurs under shear where the rotation velocities of DE are only controlled by tangential forces. Then the macroscopic behaviour of concrete is too brittle. Therefore to overcome this drawback, a non linear Moment Transfer Law (MTL) is introduced to add rolling resistance to discrete elements. By using the MTL, the calculation is kept low and the behaviour of concrete at the macroscopic scale is well represented.

In this paper, the discrete element model will be firstly presented. Then the identification process of DE parameters will be described. The second part illustrates the Moment Transfer Law (MTL) used, and local parameters calibration is presented in order to reproduce experimental macroscopic behaviour.

2 DISCRETE ELEMENT MODEL

2.1 Model description

The present numerical model has been described in [11]. Each element is a rigid sphere with an individual mass and radius. To provide a polydisperse assembly with a particular size distribution, a geometrical algorithm using disorder technique generates a random distribution of centroids of spheres [4]. Then pairs of initially interacting discrete elements are identified by mean of two types of interactions: contact and cohesive links. These ones are defined by two stiffnesses, normal K_N and tangential K_S characterizing the elastic behavior of concrete. Then "Micro-macro" relations [11], which give these local stiffnesses, come from homogenized models [13] used for regular assemblies, but they have been modified to be adapted for disordered assemblies. Equation (1) shows these relations between two spheres a and b, where $D_{init}^{a,b}$ represents the initial distance between two elements and S_{int} is the interaction surface. Also α, β, γ parameters will be identified by quasi-static tests.

$$\begin{cases} E = \dfrac{D_{init}^{a,b}}{S_{int}} K_N \dfrac{\beta + \gamma \frac{K_S}{K_N}}{\alpha + \frac{K_S}{K_N}} \\ \nu = \dfrac{1 - \frac{K_S}{K_N}}{\alpha + \frac{K_S}{K_N}} \end{cases} \quad \text{or} \quad \begin{cases} K_N = E \dfrac{S_{int}}{D_{init}^{a,b}} \dfrac{1 + \alpha}{\beta(1+\nu) + \gamma(1 - \alpha\nu)} \\ K_S = K_N \dfrac{1 - \alpha\nu}{1 + \nu} \end{cases} \qquad (1)$$

Then to model the non-linear behavior of concrete, two local criteria for rupture are used ((2) and (3)).

$$\begin{cases} f_1(F_n, F_s) = F_s - \tan(\Phi_i)\, F_n - S_{int} C_o & \text{(Sliding criterion)} \quad (2) \\ f_2(F_n, F_s) = S_{int} T - F_n & \text{(Tensile rupture criterion)} \quad (3) \end{cases}$$

Where C_o is the cohesion factor, Φ_i the frictionnal angle, T the local tensile limit and ξ the softening factor that needs to be identified from global parameters such as compressive and tensile strengths σ_c and σ_t and fracture energy G_f. Between elements in contact a classical Coulomb friction is used (Figure 1).

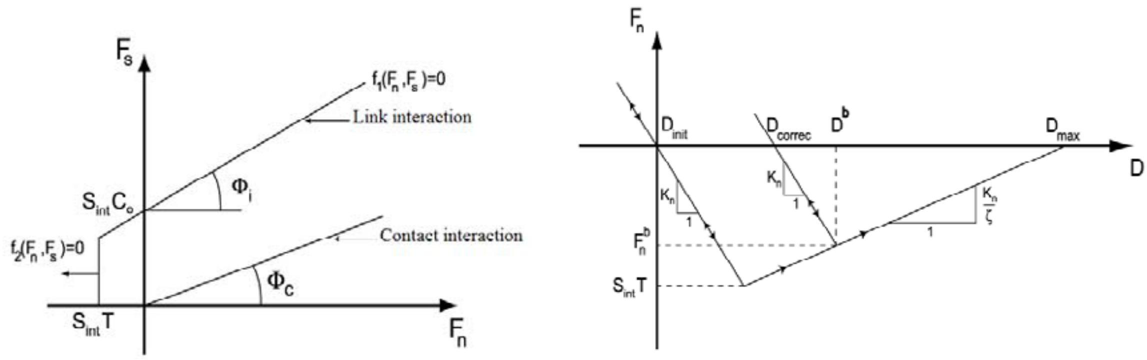


Figure 1: Interactions law

2.2 Identification procedure of parameters relative to the behavior

A procedure for identifying all material parameters based on simulations of quasi-static compression and tension tests has been defined [11]. The number of discrete elements must be as small as possible to maintain a reasonable computation time. The specimen must be representative of the real behavior, so it should contain enough elements to guarantee a minimum number of links along with a correct distribution. The radius of interaction is chosen such that the average number of interactions per DE equals 12. This value is the average number of links present in a regular Face-Centered-Cubic assembly of elements, and by using this value privileged directions of interactions are prevented, then an isotropic distribution is ensured.

After carrying out tests using the α, β, γ parameters for some values of K_S/K_N, the ratio E/E_0 and the Poisson's ratio were computed (a $K_S/K_N = 1$ yields the E_0 value). We should find the α, β, γ values that give the best-fit approximation (Figure 2).

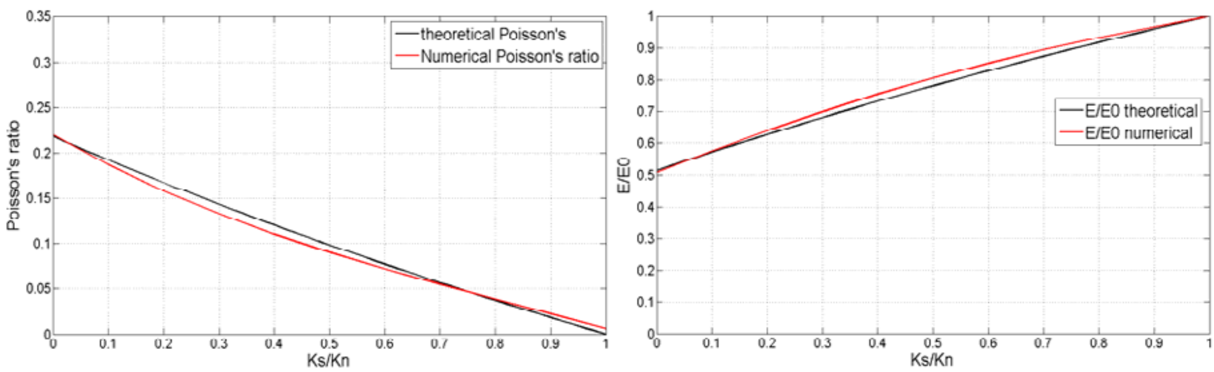


Figure 2: Comparison of theoretical and numerical values of Poisson's ratio and Young's modulus

After identifying the linear parameters, is applied the process to determine actual concrete parameters. Figure 3 shows the flowchart of the identification procedure in order to obtain local parameters. Quasi-static tensile tests allow identifying the local tensile strength T and the softening parameter ξ. During a subsequent approach, compressive tests provide the appropriate cohesion parameter Co. All these tests are simulated and compared with respect to an experimental behavior of concrete, and then the parameters are calibrated in order to reproduce it. Notice that after carrying out several tests, it has been found that the two local parameters Φ_i and Φ_c have almost no influence on the macroscopic behavior of concrete.

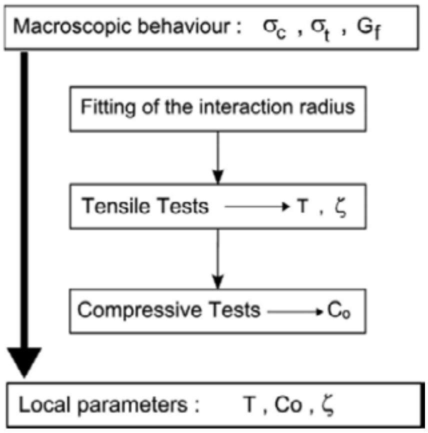


Figure 3: The identification process

3 MOMENT TRANSFER LAW

3.1 Drawback of DE model

A quasi-static compression test has been simulated by mean of the DE model described before. Once we have calibrated the interaction range, the parameters relative to the linear behavior has been established, then a quasi-static compression simulation has been done. The behavior obtained numerically is too brittle as shown in Figure 4.

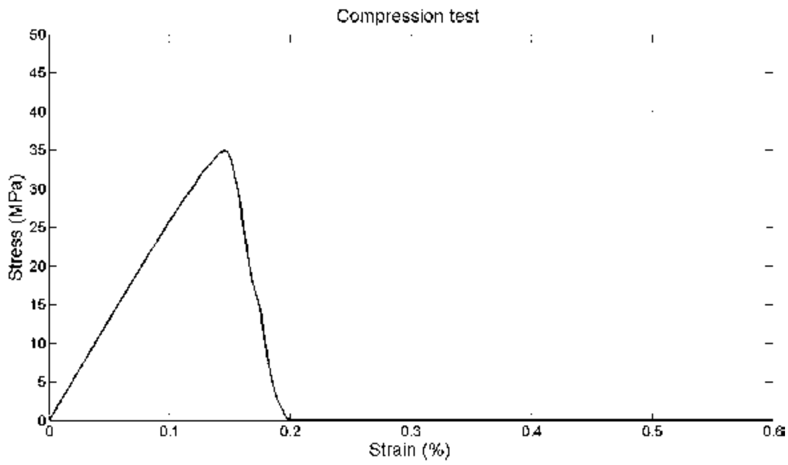


Figure 4: Compression test with DE model

This can be explained by the excessive rolling happening under shear due to the circular shape of discrete elements despite its advantage of keeping low cost of calculation. Therefore two solutions can be introduced to ensure a sufficient ductile behavior of concrete. The first one is to increase the interaction range for each element, so the interaction radius should be increased. By this way the numerical specimen has a higher strength and the behavior is more ductile. Figure 5 shows the results of quasi-static compression with two values of the average of interactions per DE: 12 and 24.

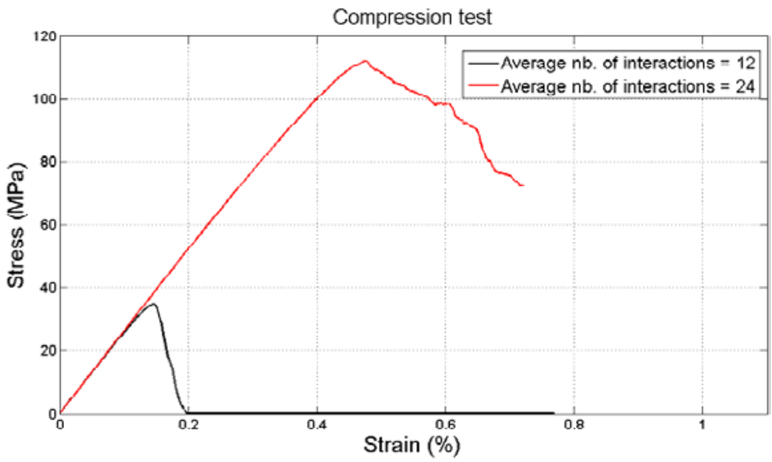


Figure 5: Influence of the interaction range on the numerical quasi-static compressive behavior of concrete

By increasing the value of the mean number of interactions from 12 to 24, we found that the compressive strength increases three times (from 35 MPa to 112 MPa), even the behavior becomes more ductile. We should notice that before simulating the non linear behavior for each case, the elastic parameters should be calibrated. The main disadvantage of this solution is the big computational cost when we increase the interaction range from 12 to 24 i.e. for a sample of 4850 DE it increases 5 times. Therefore we cannot adopt this choice because when simulating the behavior of full structure by mean of 3D DE, the computational time will be very huge especially it is considered as a main challenge at the scale of structure.

An alternative solution is to act upon the rotations of elements by adding certain rolling resistance between them. In the next, we will detail the description of the Moment Transfer Law (MTL) which defines the model of rolling resistance of DE.

3.2 Description of the MTL

Several previous researches have introduced the MTL between elements in contact for granular medium [3, 10], and they showed its capability to well estimate the shear resistance of the granular material by reproducing an appropriate value of friction angle [2]. Otherwise in our case of cohesive material, The rolling resistance model used is similar to that proposed in [7, 12], but also adapted to the concrete behavior in order to take into account the MTL for links between two remote elements. The MTL introduced later has been implemented within the Europlexus code which is a code being jointly developed since 1999 by CEA (CEN Saclay, DMT) and EC (JRC Ispra, IPSC) under a collaboration contact. The code uses an explicit algorithm and it is best adapted to rapid dynamic phenomena such as explosions, impacts, crashes etc.

Relative rotation between two DE controls the phenomenon of rolling. In the case of identical elements, it is obtained by the differential rotation between the two elements. But it is not the case for a polydisperse distribution mesh where the size of elements should be taken into account. Then we consider two spheres A and B having radius respectively r_A and r_B at two instants t and t+dt in the global reference G (Figure 6).

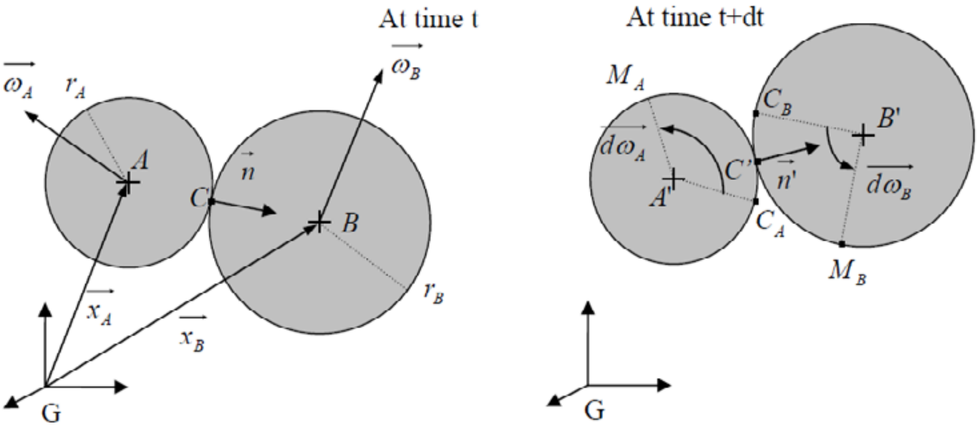


Figure 6: Contact evolution between two DE for two time steps t and t+dt

The positions of material points M_A and M_B, with respect to the new contact point C' are given by the sum of translation and rotation vectors:

$$\begin{cases} \overrightarrow{C'M_A} = \overrightarrow{C'C_A} + \overrightarrow{C_AM_A} = r_A\left((\vec{n}-\vec{n'}) + dt\,\overrightarrow{\dot{\omega}_A} \wedge \vec{n}\right) \\ \overrightarrow{C'M_B} = \overrightarrow{C'C_B} + \overrightarrow{C_BM_B} = r_B\left((\vec{n}-\vec{n'}) + dt\,\overrightarrow{\dot{\omega}_B} \wedge \vec{n}\right) \end{cases} \tag{4}$$

By supposing that the dispersion of radius is not so big, we can express the incremental displacement vector $\overrightarrow{dU_r}$, caused by the rolling process as following:

$$\overrightarrow{dU_r} = \frac{\overrightarrow{C'M_A} + \overrightarrow{C'M_B}}{2} \tag{5}$$

The rolling phenomenon is due to the relative rotation of elements and is defined by the incremental rolling vector $\overrightarrow{d\theta_r}$. We define first the unitary vector $\overrightarrow{n_{d\theta_r}}$ oriented along $\overrightarrow{d\theta_r}$:

$$\overrightarrow{n_{d\theta_r}} = \frac{\vec{n'} \wedge \overrightarrow{dU_r}}{\left\|\vec{n'} \wedge \overrightarrow{dU_r}\right\|} \tag{6}$$

The incremental rolling angular vector is given by:

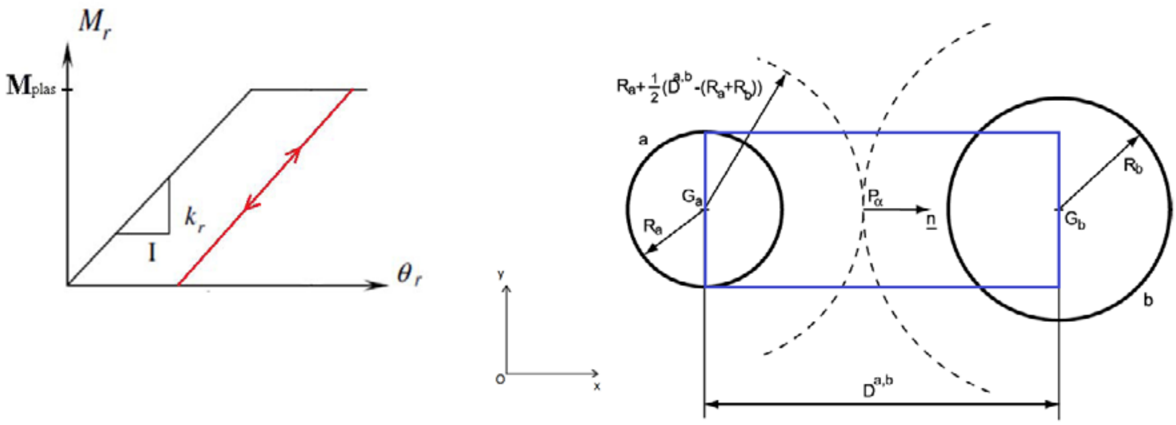
$$\overrightarrow{d\theta_r} = \frac{\left\|\overrightarrow{dU_r}\right\|}{r}\overrightarrow{n_{d\theta_r}} \tag{7}$$

Where r = min(r_A, r_B)

We define the angular vector of rolling by summing up the increments $\overrightarrow{d\theta_r}$. Using this vector we express later the resistant moment to reduce the rolling:

$$\overrightarrow{\theta_r} = \sum \overrightarrow{d\theta_r} \quad (8)$$

Then a constitutive law associated to the MTL should be defined and able to reproduce elastic and plastic behaviors. An elasto-plastic model is introduced for rolling moment (Figure 7a) where the elastic part is linear and described by the rolling stiffness K_r and the plastic one is defined by the plastic limit M_{plas}. In the plastic domain, an elastic recovery happens under unloading along a linear part with the same intial rolling stiffness K_r.



(a) **(b)**

Figure 7: (a) Elasto-plastic model for rolling moment (b) Beam model for cohesive link resistant moment

Then was considered the general case of two remote DE where D_{ab} is the distance between the centroids of 2 DE. The link is considered equivalent to a beam having circular section with a radius r = min (r_A, r_B). We define a contact point at the middle of the net distance between the two spheres (Figure 7b), and then each one has an updated radius as following:

$$\begin{cases} r'_A = r_A + \frac{1}{2}\left(D_{ab} - (r_A + r_B)\right) \\ r'_B = r_B + \frac{1}{2}\left(D_{ab} - (r_A + r_B)\right) \end{cases} \quad (9)$$

By using the strength of materials rules, the bending moment around the z-axis is provided by:

$$M_f = E\, I_{zz}\, y'' = E\, I_{zz} \frac{dy'}{dx} = \frac{y'_A - y'_B}{x_A - x_B} \quad (10)$$

Where I_{zz} is the quadratic inertia corresponding to the z-axis, and E the Young's modulus. By analogy with the case of rolling, we can simply replace $x_A - x_B$ by D_{ab} and $y'_A - y'_B$ by the relative rolling between the two spheres $d\theta = \theta_A - \theta_B$. Then the rolling stiffness is proportional to the term EI_{zz}/D_{ab}. A factor β_r can be introduced here to control the rolling resistance added as in reality with different types of constituent materials a concrete has different shear resistance, therefore numerically different rolling resistance can be added. Then the rolling stiffness can be expressed as (11):

$$K_r = \beta_r \frac{EI_{zz}}{r} \tag{11}$$

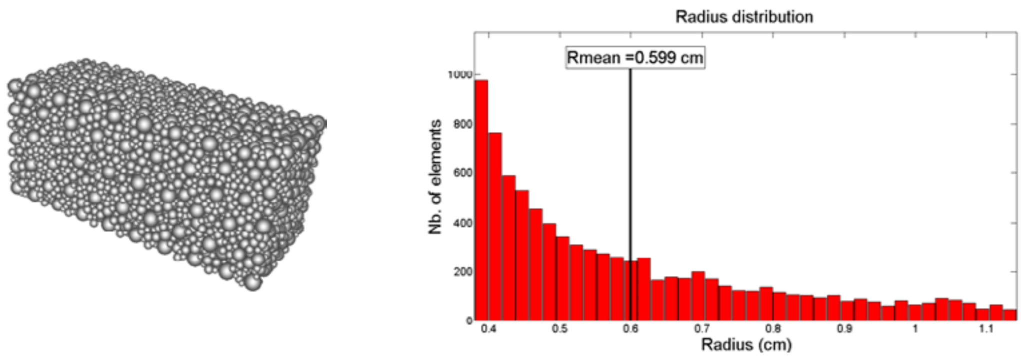
Also the plastic limit of rolling moment is proportional to the factor $\sigma I_{zz}/v$ where σ can be replaced by the local tensile strength T, and v by the radius r of the section. Therefore by adding a factor η to control the plastic limit, this one can be defined as (12):

$$M_{plas} = \eta \frac{TI_{zz}}{r} \tag{12}$$

Notice that the torque effect on the beam link is not taken into account.

3.3 Study of the identification of linear behavior with MTL

First of all, a sufficiently refined mesh has been chosen for the identification process, and later a verification of the obtained parameter values has been carried out for finer meshes. A 0.4m×0.2m×0.2m specimen has been used for simulating quasi-static compression tests. It contains 8630 DE with a mean radius of 0.6 cm and a compactness of 0.604.



(a) **(b)**

Figure 8: (a) DE mesh of the sample (b) Radius distribution of the DE mesh

Figure 8b shows that the most of the DE are of small size providing a higher compacity. After applying the linear identification process for different values of rolling resistance factor β_r, we obtained the results shown in Table 1:

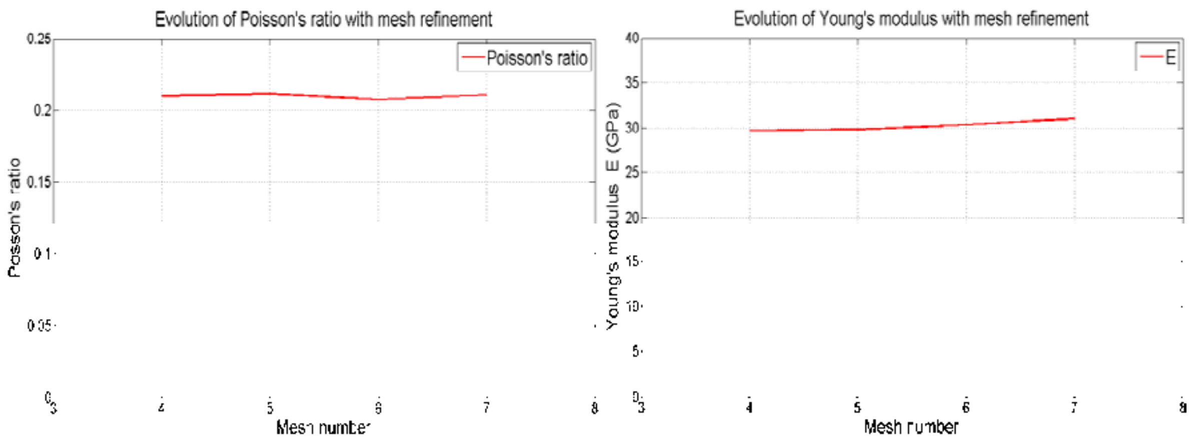
Table 1: Linear identification sensibility to the rolling resistance factor β_r

β_r	α	β	γ
1 to 40	4.4	3.3361	4.57

Table 1 shows that the same values of linear parameters α,β et γ are valid for a wide range of values rolling resistance factor β_r (1 to 40). We didn't make verification for a larger range as the linear identification is expensive to be carried out. But in all cases we will show in the following that we don't need for a value of β_r higher than 40 to reproduce the real behavior of concrete. Thus a verification of these values obtained for different mesh refinements (Table 2) has been performed in order to reproduce the chosen characteristics: Young's modulus E=30 GPa and Poisson's ratio ν=0.21.

Table 2: Different mesh refinements

Mesh number	Compactness	Number of DE	Rmean (cm)
4	0.604	8630	0.6
5	0.612	15890	0.49
6	0.613	23334	0.43
7	0.619	47140	0.34



(a) **(b)**

Figure 9: Reproduction of ν (a) and E (b) for different mesh refinements

Figure 9 shows an appropriate reproduction of linear characteristics of concrete for different mesh refinements. The maximum error of estimation of E is about 4.3% and 1.05% for ν. Otherwise, several meshes with different specimen shapes has been carried out, and the reproduction of linear characteristics has been verified (Table 3).

Table 3: Different specimens used for the study of reproducibility

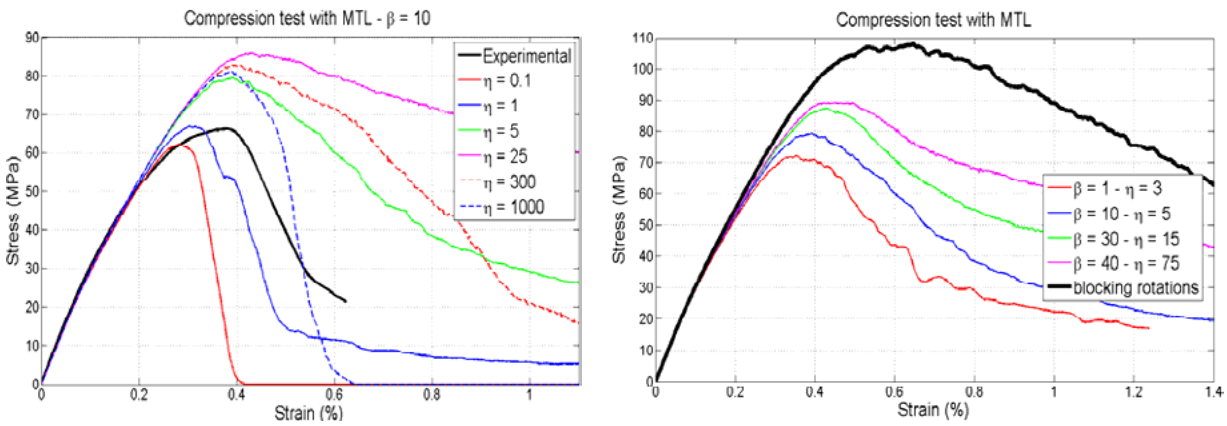
Specimen Nb	Height (m)	Width (m)	Larger (m)	E (GPa)	ν
1	0.6	0.3	0.3	31.1	0.2077
2	0.4	0.4	0.4	31.3	0.2105
3	0.25	0.25	0.25	29.1	0.2134
4	0.32	0.5	0.5	30.8	0.198

According to Table 3, the maximum error for estimating E is about 3.6% and 5.7% for ν. Thus we can say that the reproducibility is acceptable.

3.4 Identification of the non linear behavior with MTL

This procedure has been applied in order to identify local parameters of a regular concrete [9]. Numerous triaxial tests were performed on it, and here an unconfined compression test is presented for the identification of the DE model. The concrete has a Young's modulus of 30 GPa and Poisson's ratio of 0.21.

Before carrying out the identification process, the effect of LTM parameters on the macroscopic behavior of concrete should be investigated.



(a) (b)

Figure 10: Influence of MTL parameters on the compressive behavior of concrete

By reading the curves in Figure 10a, it is clear that for each value of rolling resistance there is a certain plastic limit factor η giving the maximum compressive strength and ductility for the macroscopic behavior. Also by increasing the rolling stiffness, the compressive strength becomes higher and the behavior converges to the limit state where the rotations of the DE are blocked (Figure 10b).

On the other side, the MTL has no big influence in traction. As shown in Figure 11, by using the MTL the tensile strength increases little bit and the behavior becomes more britlle.

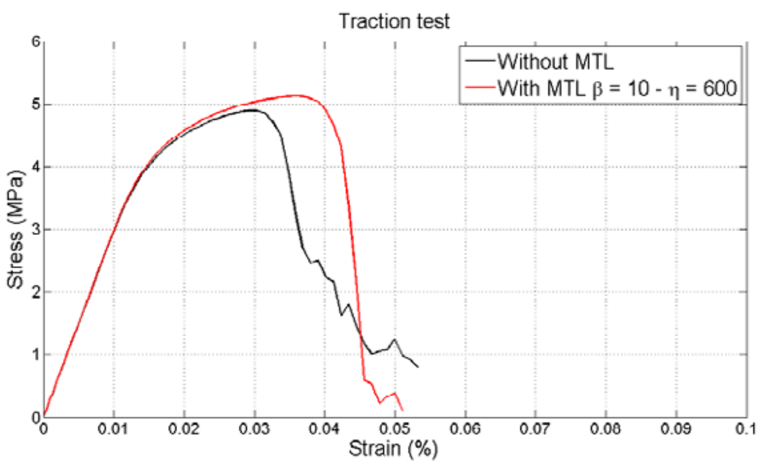


Figure 11: Influence of MTL on the tensile behavior

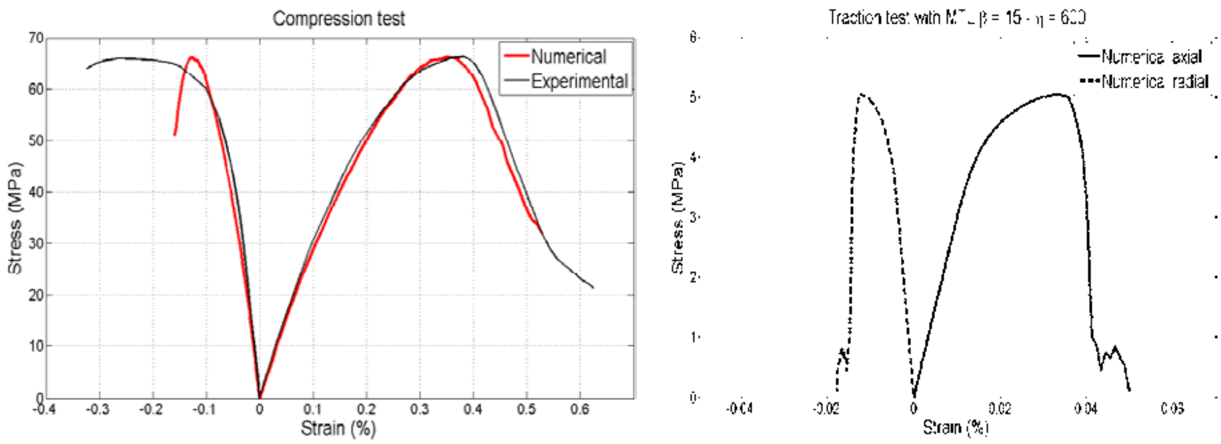
The compression strength of concrete is $\sigma_c = 66$ MPa obtained by an unconfined compression test. The tensile strength is $\sigma_t = 5$ MPa given by a Brazilian test, then the ratio σ_c/σ_t is about 13. This big value is mainly due to the high Poisson's ratio. Therefore reproducing the experimental behavior in this case is not possible by mean of the initial DE model without MTL. Indeed, the value of the softening factor ξ must be increased, so the maximum tensile strain at rupture becomes high.

The strategy of identification starts by fixing a value of the rolling stiffness factor β_r. For a high ratio σ_c/σ_t, $\beta_r = 15$ is an appropriate value for the identification process because it ensures the required ductility and at the same time it increases well the numerical compressive strength. Regarding the plastic limit factor of rolling, an introductory value $\eta = 600$ can be adopted according to Figure 10a. Moreover, the identification process of the non linear behavior has been carried out by using MTL parameters $\beta = 15$ and $\eta = 600$. The local parameters found are shown in Table 4:

Table 4: Local non linear parameters identified

T (MPa)	C (MPa)	ξ	Φi	Φc
3.8	15	14	5°	30°

The results of tensile and compression tests are shown in Figure 12.



(a) (b)

Figure 12: (a) Compressive test (b) tensile test

4 CONCLUSION

The MTL introduced is a gainful tool that can be used to well reproduce the macroscopic behavior of a cohesive material like concrete. It overcomes the britlle behavior that appears due to the spherical shape of DE, but also maintains the computational cost low which is useful for the challenge of time cost at the full structure scale modelisation. Also for a concrete with a high Poisson's ratio where the ratio of compressive over tensile strengths is high, then using MTL reproduce well the high value of compressive strength while keeping the tensile strength without a big change. This model has been used for the quasi static macroscopic behavior, but also dynamic tests at the structure scale will be further presented.

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