Application of the Discrete Elements Method to Frequency Analysis and Use of the "Bond" Method for Fracture Modeling

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Abstract

Nowadays more and more complex mechanical behaviors have to be modelled. In order to do so, the generally used numerical methods, like finite elements, show some limitations. Particularly, finite elements' ability to model granular media is reduced, partly because of the contact handling complexity between each grain.

One of the alternatives is to use meshless methods. Within the software LS-DYNA®, there notably exists a meshless method named "Discrete Element Method" (DEM). This method was initially implemented in the software to model granular media, and especially granular flows, where the displacements of each particle are deduced from Newton's equation [1]. An extension of the method consisting in bonding particles together with smooth heterogeneous bonds essentially permits to model fracture (DEM-HBOND), which is a significant issue in many fields.

Our studies consist in two disconnected projects presented below:

As part of the Midi-Pyrénée project "TANKYOU", we are trying to find a granular material that would have the same vibratory behavior as a fluid. In order to do that, we have especially been seeking the mode shapes of a cylinder fully filled with Discrete Element Spheres (DES). The issue here is to vibrate DES with explicit calculations.
As part of an internship, a tensile test on a DES steel specimen has been performed to test fracture modeling. The impact of particles' organizations (meshes) in the specimen has been studied, and results have been compared with finite elements results.

Keywords:
Granular Flows, Discrete Element Method, Modeling Techniques, Aerospace, Fracture Modeling

1. Introduction

Considering that the finite elements method is not well appropriate to model granular media, an alternative way consists in using meshless methods. Within the software LS-DYNA, there notably exists a meshless method named "Discrete Element Method" (DEM). This method was initially implemented in the software to model granular media, and especially granular flows. It was then extended for bonding particles together, with smooth heterogeneous bonds permitting to model fracture. This extension is called DES-HBOND method.

Our studies present one application for these two numerical meshless methods:

i. First, as part of the project TANKYOU[1], our goal is to find a granular material that would have the same vibratory behavior as a specific fluid contained in a vibrating tank. In order to do so, we have been seeking the mode shapes of a cylindrical tank filled with Discrete Element Spheres (DES) using LS-DYNA explicit solver.
ii. Second, as part of an internship, a tensile test on a steel specimen has been performed to test fracture modeling with DES-HBOND, and to evaluate the particles organization impact on the tensile results.

2. Cylinder filled with Discrete Element Spheres modal analysis

Liquid hydrogen is at the center of space propulsion and new launcher generation issues. Nowadays, liquid hydrogen (LH2) dynamic vibratory behavior experiments and modellings in deformable launcher tanks cause some scientific and technical problems. Indeed the security, transport and conditioning problematics still remain critical.

The TANKYOU project aim is to offer the French space domain a metamaterial replacing LH2 during dynamic experiment test. This specified metamaterial will represent the LH2 dynamic behavior within a tank, without presenting the same flammability, explosiveness and fugacity risks. This new material developed by combining a numerical and an experimental methodology should permit to simplify and secure cryotechnical launcher tanks qualification. This approach aims to qualify analytical models, numerical and experimental representative of the filled with cryogenic fluid tank dynamic behavior. The referred representativeness considers the global modes and the impact strength.

Only the numerical approach of the project is described in this paper. A tank simplified model, in form of cylinder filled with DES, is studied in order to replicate the fully filled cryogenic tank mode shapes. The particular studied mode shapes are the bending one, the second one and the third one (Figure 1).
To achieve this objective, two types of simulation were conducted:

- The first one, to identify the appropriate boundary conditions and loads enabling to excite the expected modes;
- The other one, to establish a numerical sensitivity analysis in order to reproduce and optimize experimental configuration.

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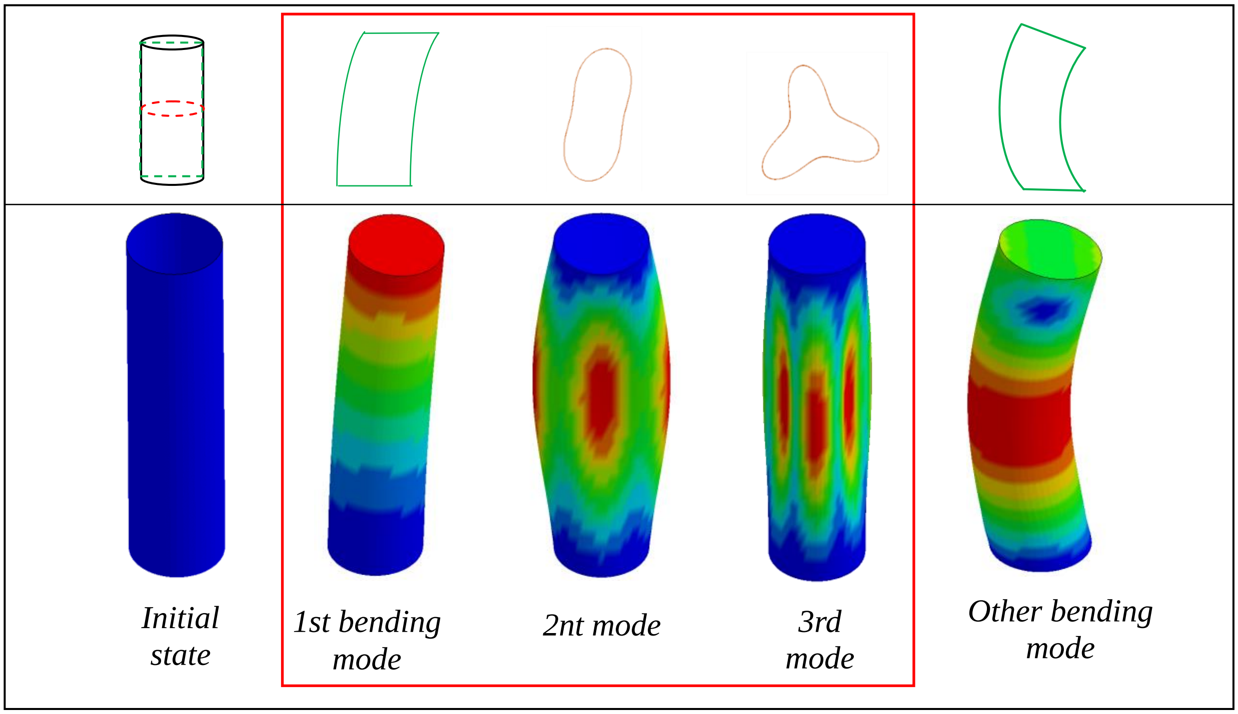


Figure 1 : Mode shapes illustration and specification of the three researched ones (red frame) obtained by an implicit calculation

2.1. Case presentation

2.1.1. Geometry, boundary conditions and loads

The simplified model geometry (Figure 2) comes from the experimental constraints (L=700mm and r=100mm). It is composed of a closed cylinder which dimensions permit to model the same slenderness as the tank one. The cylinder material is a translucent plastic, which thickness is 5mm. The top of the cylinder, made of aluminum, is free whereas the bottom is clamped.

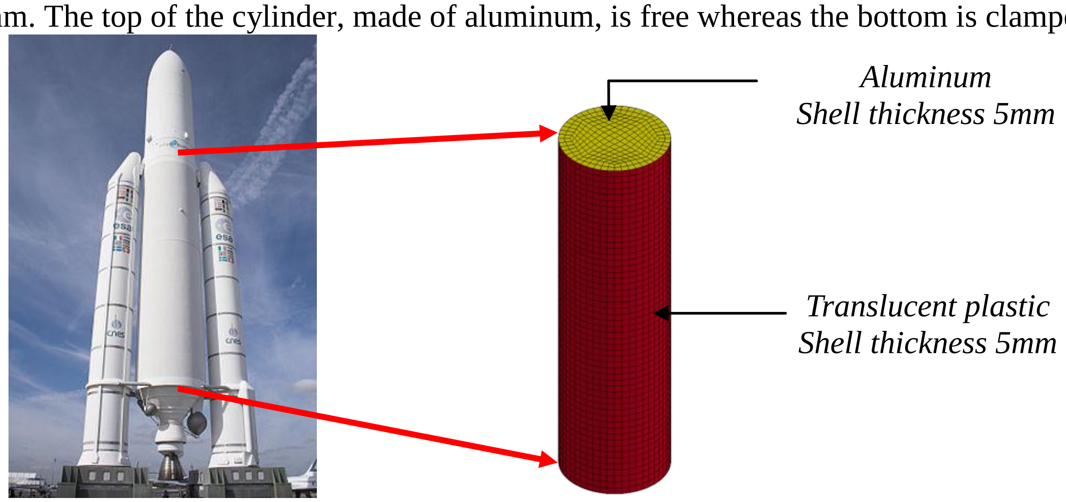


Figure 2 : Cryogenic tank simplified model

Three types of configurations are tested (Figure 3):

i. The first one is a purely numerical method using the LS-DYNA implicit solver to determine natural modes. This implicit method is not compatible with DES.

ii. The second one, called "vibrations method", corresponds to the experimental configuration and uses the explicit solver. The cylinder is clamped on a vibratory table by its bottom (Figure 3 (a)). It consists in vibrating the cylinder base via a table vibrating at a specific frequency. So, to obtain the cylinder behavior on a frequency range, multiple vibratory computations have to successively be performed (one frequency per computation). Even if this modelling method is efficient, it is really time consuming because of the computed simulations high number. So it cannot reasonably be used for sensitivity testing.

iii. The third one, called "pulse method", is also an explicit method and consists in applying a local and punctual pulse on the middle section area of the cylinder (Figure 3 (b)). The resultant displacements of the cylinder are extracted and a Fast Fourier Transform is applied, which permits to obtain the cylinder modal spectrum. This method does not take too much time and seems efficient. It is not an experimentally used method because of the noisy displacement response.

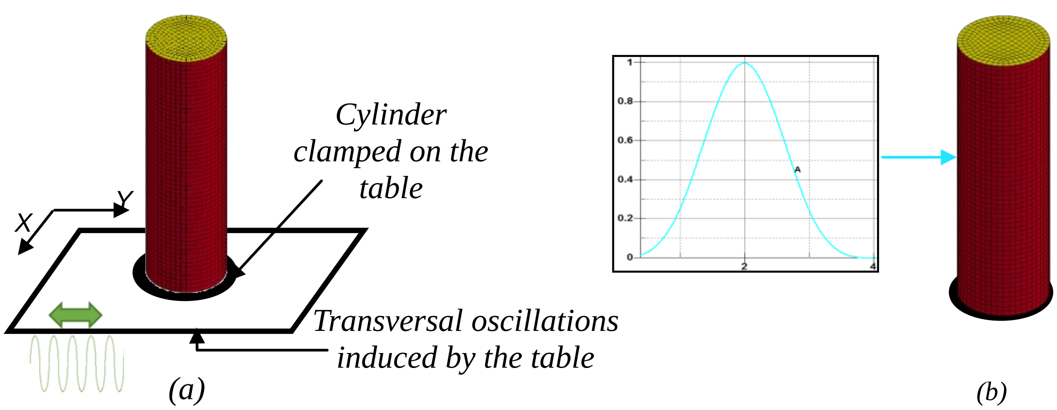


Figure 3: Load illustration for numerical mode detection: (a) transversal vibration, (b) pulse

Both explicit methods have been studied to bypass the DES incompatibility with the implicit solver. Both explicit methods have been compared to each other and validated thanks to the implicit one. The natural frequencies are similar for the three methods.

2.1.2. Mesh and computation time studies

Since the objective is to get, among others, the second and third mode shapes, the elements number over the cylinder circumference has to be divisible by two and three. This affirmation was verified thanks to implicit and explicit calculations.
The implicit calculations permit to quickly obtain the cylinder natural frequencies. The explicit calculations are vibratory calculations. Every vibration frequency corresponds to the natural ones obtained with the implicit approach (same explicit computation number as implicit natural frequency). A mesh sensitivity study and a performance one can then be done with explicit vibratory calculations (Figure 4).
As a result, the cylinder displacements are unchanged by the mesh variations, but for a four times refined mesh, the calculation duration is almost sixty times higher. So, when the cylinder is empty, a 24 elements on the circumference mesh is recommended.

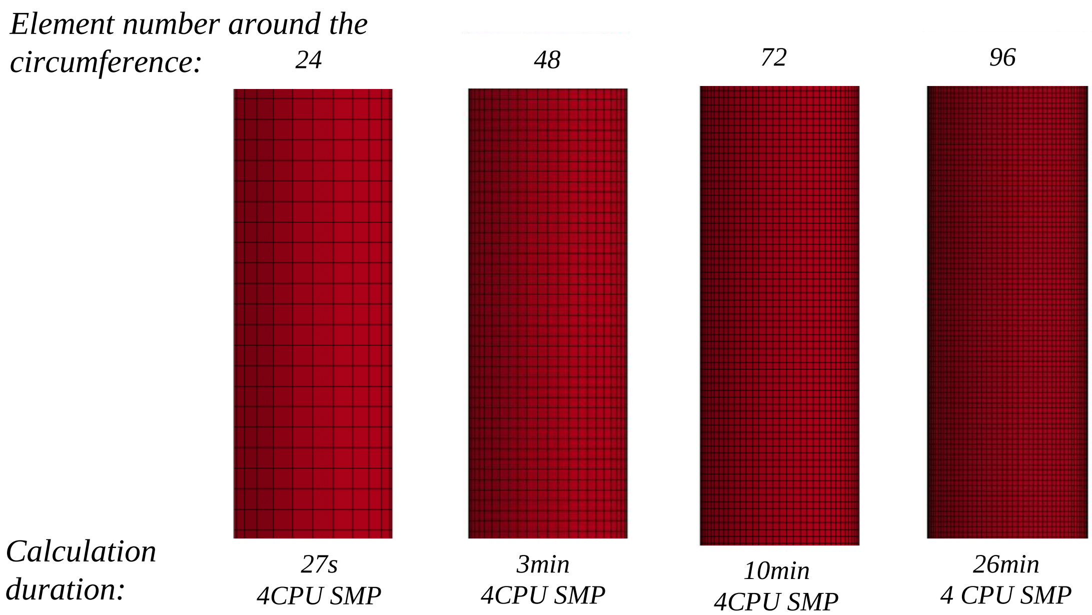


Figure 4: Mesh and performance studies with the vibratory explicit method

When the cylinder is filled with DES, a correlation study has to be made between the finite elements mesh size and the sphere radius.
As part of the TANKYOU project, spheres radius is a parameter that should be chosen to fit the researched fluid. Knowing that the manufacturing process imposes a radius range of [1mm, 10mm], the radius determination is then driven by numerical limits.
Many numerical tests were performed on various finite element mesh sizes (Figure 4) with fixed radius spheres to check the cylinder numerical behavior. When the shell element edge can only "contain" less than three entire DES, the contacts between the cylinder and the spheres are too much localized which causes numerical noise on finite elements displacements. To perform a first sensitivity study, the radius of the sphere was set to 3mm. To ensure the calculations accuracy, the cylinder elements number around the circumference is chosen to be 48.
Considering this mesh size, the Table 1 sums up the various computed simulations times for an empty cylinder and a fully filled one (around 800,000 spheres in a 30L volume after generation by LS-PrePost®).

	Implicit	Vibrations	Pulse
Empty cylinder	1 second (30 modes)	**20 minutes** for 6 frequencies (~3 minutes per frequency, 14 CPU SMP)	**14 min** (3 first modes, 14 CPU SMP)
Filled cylinder	/	**72 hours** for 6 frequencies (~11 hours per frequency, 28 CPU SMP)	**22 hours** (3 first modes, 28 CPU SMP)

Table 1: Computation time for an empty cylinder and a filled one with various computation methods

The DEM appears time-consuming due to the large number of necessary spheres (it is currently impossible to use the implicit solver with the DEM). The pulse explicit method permits to save time compared to the vibrations method. Also reducing the cylinder dimensions by two enables to decrease the sphere number and has been set up.

2.1.3. Spheres mechanical properties

The experimental granular media is composed of hollow spheres. Yet, the numerical DEM can not consider hollow spheres. Then, a numerical hollow sphere homogenization has to be performed and will be done thanks to an experimental sphere compression test. The aim of this study is first to find the shell Young's modulus corresponding to the experimental hollow sphere by rising a 2D-axisymetric finite elements modelling. Then, a DES model is made and the full sphere mechanical properties are adjusted to fit the experimental data and 2D-axisymetric hollow sphere model. Both models are presented on Figure 5.

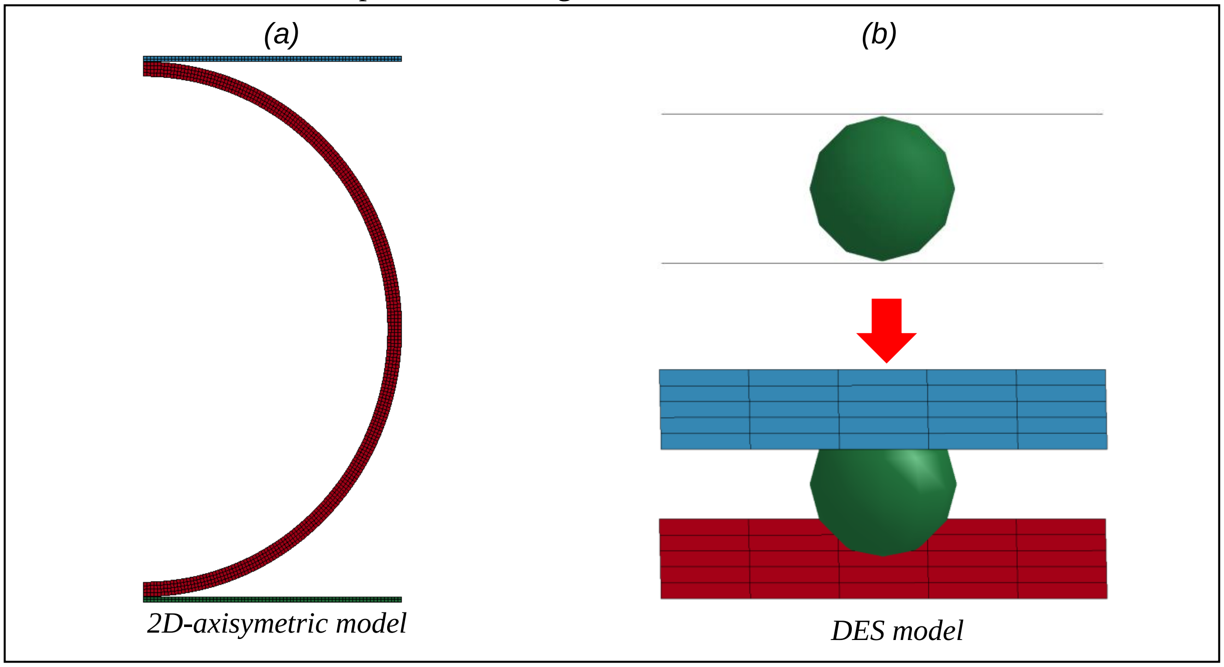


Figure 5: Compression test 2D-axisymetric model (a) and DES model (b)

The experimental tests gave some force-displacement curves until sphere failure. Only the elastic part, and especially small strains, are considered here. The numerical method used to find the experimental sphere Young's modulus was an iterative process which aimed at finding the same force-displacement curve stiffness.

The experimental sphere shell Young's modulus numerically found through the 2D test is around 4GPa. It corresponds to a full sphere Young's modulus around 30MPa. This last value seems to be in accordance with the Hertz theory [2] which was applied to the experimental force-displacement curve. The experimental, 2D-axisymetric and DES force-displacement curves are available on Figure 6 to illustrate the good results correlation, taking $E_{2D} = 4GPa$ and $E_{DES} = 30MPa$.

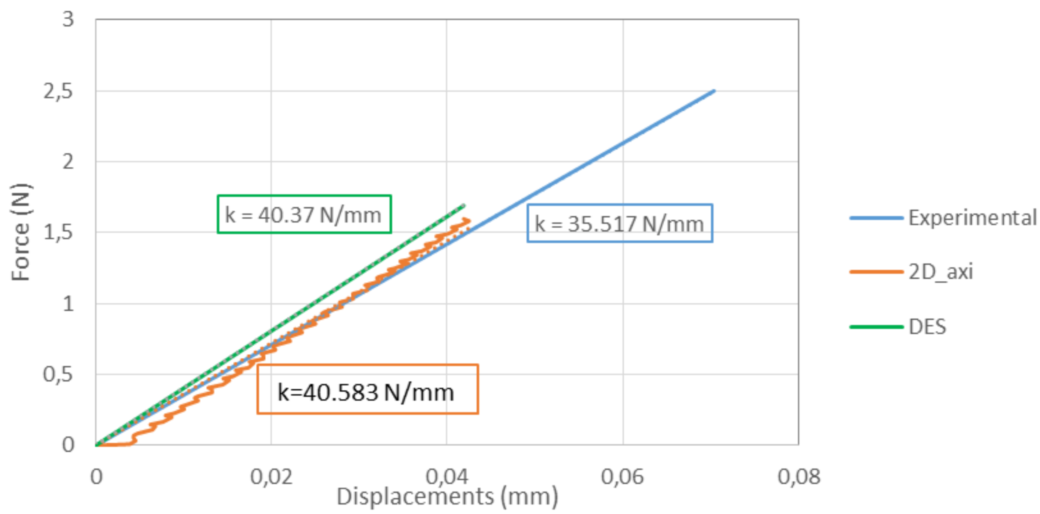


Figure 6: Force-displacement curve of the experimental (blue), hollow 2D-axisymetric (red) and full DE (green) spheres for small strains

The Table 2 sums up the sphere properties that have to be introduced to LS-DYNA®:

Young's modulus (MPa)	Poisson's ratio	Density (g/mm3)	Radius (mm)
30	0.3	$6e^{-4}$	3.33

Table 2: Spheres mechanical properties

2.2. Compactness study

After having found the spheres mechanical properties some sensitivity studies on the granular media compactness have to be made.

2.2.1. Compaction ratio

A granular media behavior is governed by the contacts between spheres. The number of contacts that a sphere has and the compaction ratio of the media determine if the media has a "fluid" or a "solid" behavior. Indeed, in the literature the compactness of a random spheres packing (fluid) should be in the range [56%, 64%], where 56% is a loose packing and 64% is a dense one [3]. Solid behaviors are better represented with compactness around 72%, which corresponds to lattice arrangements. In this framework, the studied compaction ratio range should be [56%, 64%], because high compaction rates reduce spheres movements during tank vibrations.
LS-PrePost software is able to generate DES in a closed domain from a closed shell shape. Then the compactness of the newly generated granular media is about 53%. Some post-generation solutions were explored to improve this compaction rate in order to meet the expected range, such as applying gravity, vibrating the media or generating it by "injection" [3]. This last solution is considered too much time-consuming, but the two other solutions are tested.
Applying gravity only permits to obtain a 57.5% compaction rate, which is not sufficient to prevent relative movements between vibrating spheres. So, after applying a first gravity cycle on the filled cylinder, some vibrations are applied on the cylinder base considering various magnitudes and frequencies. The Table 3 and Table 4 below show the compactness of the granular media vibrated by several magnitudes and frequencies.
Table 3 shows that the vibrations magnitude alone does not have a significant impact on the compaction ratio. However, when frequencies increase (table 4) the compactness seems to be

higher, especially when it is combined with a magnitude around one point five times the spheres diameter [3].

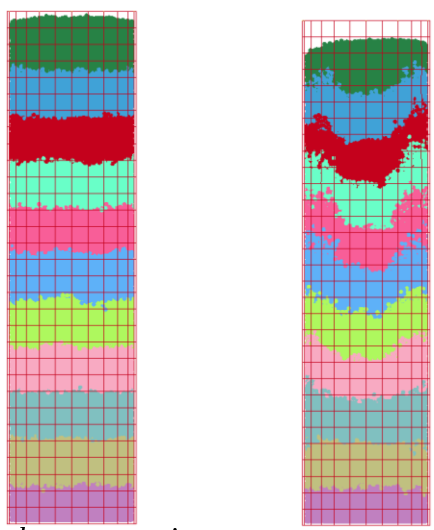
Amplitude A	A=1mm	A=3mm	A=4mm	A=6mm
Compaction ratio (Φ)	60.1%	59.8%	60.0%	60.0%

Table 3 : Compaction ratio depending on the vibrations magnitudes for a 50Hz frequency

A=1mm				A=4mm		
f=10Hz	f=50Hz	f=100Hz		f=10Hz	f=50Hz	f=100Hz
58.1%	60.1%	60.3%		59.0%	60.0%	60.4%

Table 4 : Compaction ratio depending on the vibrations frequencies for the magnitudes A=1mm (left) and A=4mm (right)

Figure 7 shows the vibrations influence on a cylinder filled with DES. The colors that have been assigned to each media parts are only present to show the spheres behavior. The picture obtained after applying vibrations shows a characteristic granular media rearrangement: spheres located near the cylinder walls are moving much more than the centered ones, which creates a kind of meniscus for middle layers. This result shows the method ability to represent granular media behaviors.



Initial state, gravity already applied *After vibrations*

Figure 7: Gravity compaction illustration

2.2.2. Compaction by compression

In order to solely reproduce internal fluid inertial effects with the metamaterial, only the fully filled cylinder is considered. Moreover, an outside stress is added to better limit spheres movements during vibrations, and so, noise on the cylinder displacements. The stress enables to preserve the cylinder from additional damping (coming from spheres friction for example). This stress is applied as a homogeneous pressure thanks to the mobile pushing cap (Figure 8). This stress has not to damage the DES spherical shape. Spheres must stay in a small strains configuration, which corresponds to a maximal contact force of 10N.

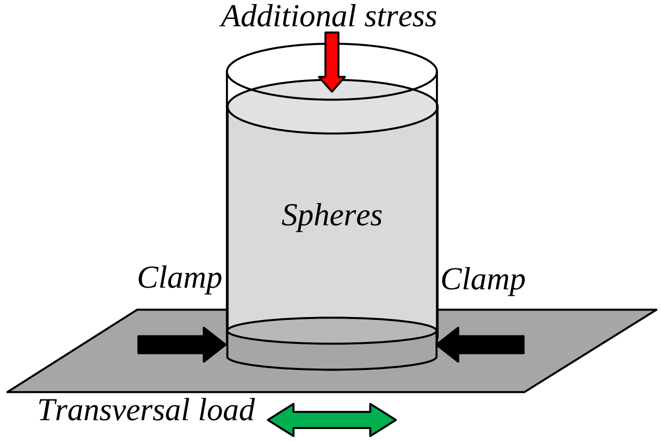


Figure 8: Illustration of the pressure used to constraint spheres and prevent their relative movements considering the vibration method

The following Table 5 summarizes the granular media compactness depending on the cylinder crushing distance, after applying gravity and vibrations:

Ratio between the distance travelled by the mobile cap and the cylinder length	1.7%	3.5%	5.2%	7.0%
Compactness (Φ)	60%	62%	63%	64%
Applied stress (Pa)	6.5	27	49	63
Average contact force in the media (N)	0.01	0.1	0.1	0.2

Table 5: Compaction ratio depending on the distance travelled by the cap

As expected, the more the spheres are compressed, the higher the compaction is. In order to increase the obtained compactness and reduce the damping coming from spheres movements in the vibrating cylinder, a pressure is applied to the granular media. This pressure has an impact on the cylinder vibrations (Figure 9 and Figure 10).

Figure 9 shows an example of a cylinder whose granular media is not compressed, and one of a cylinder whose cap displacement ratio is 7.0%. When the media is free, the cylinder movements separate the spheres from the cylinder walls, and consequently create sudden impacts between the spheres and the walls when the vibrations stop. This “sloshing” phenomenon damps the cylinder vibrations.

The cylinder displacements Fast Fourier Transform (FFT) is extracted from the pulse method and permits to obtain the cylinder frequency spectrum containing the modal frequencies (Figure 10). When spheres are free in the moving cylinder they significantly absorb its vibrations (high damping), which is not the case when they are compressed (vibrations magnitude is ten times higher with a compressed media). Moreover, the free spheres frequency spectrum is unreadable compared to the clean compressed spheres one, from which the three first natural frequencies can easily be extracted. Those natural frequencies are lower than the empty cylinder ones, which is an expected result.

The influence of the geometry change has also been studied and it has been established that its modal effects can be neglected on this model. So, a compressed granular media will be used in the project.

All these numerical tests permit to better understand the complex DEM and its limitations. Also, this work enables the experimental team to adapt the tests pattern and help the project to significantly progress. Finally, it extends the DEM applications.

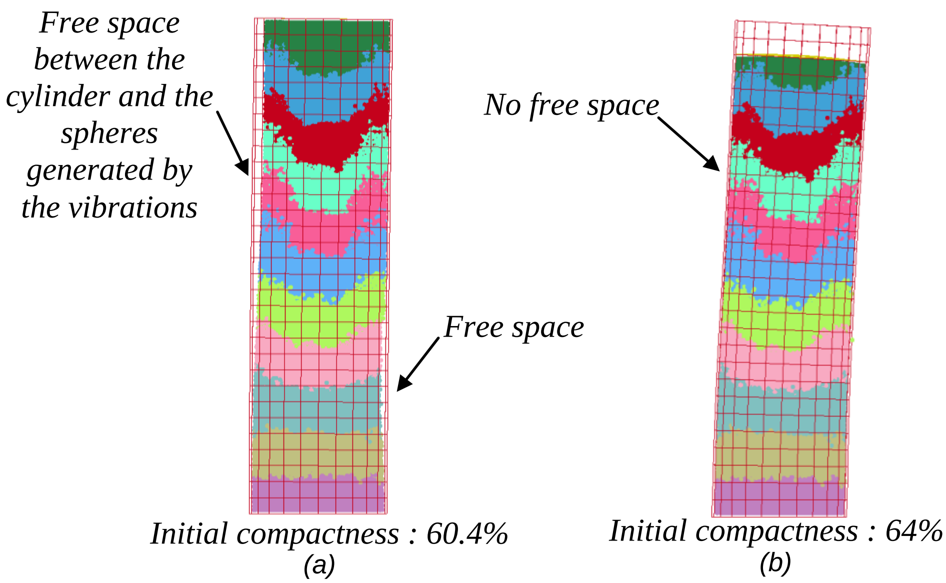


Figure 9: Comparison of the spheres behavior in the vibrating cylinder for unconstrained spheres (a) and constrained ones (b)

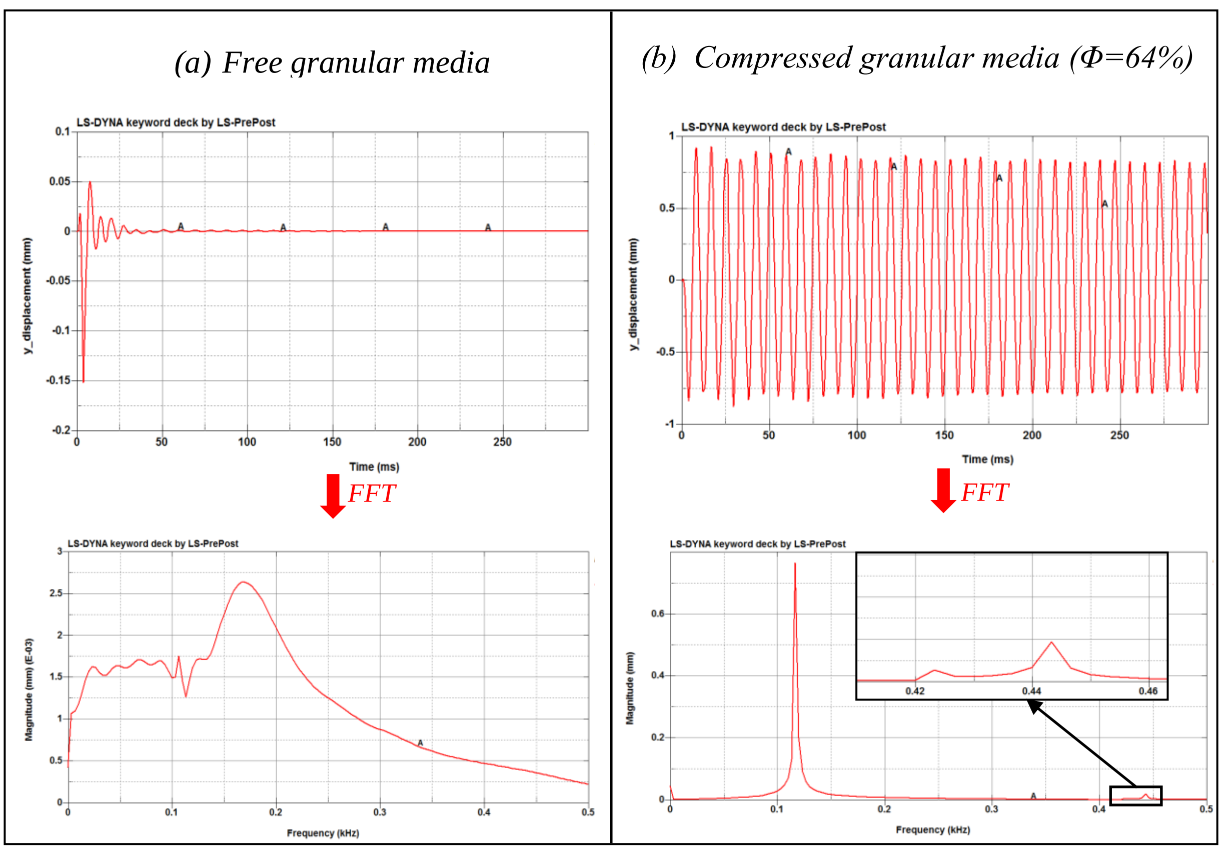


Figure 10: Time histories and associated spectrums of a cylinder filled with unconstrained (a) and compressed (b) spheres

3. Application of the Discrete Element "Bond" method to fracture modelling

The study aim is to quantify the ability of the Discrete Element Method to model a continuous medium behavior on a textbook case. It is based on the experimental tensile tests results of Cabezas and Celentano [4] which provide the stress/strain curve of a thin steel specimen. In order to evaluate the positioning of the DES-HBOND method against the Finite Element one, both DES and finite element specimens are studied.

A displacement is imposed on one end of the steel sample (through a rigid shell plate), whereas the other end is embedded (through another rigid shell plate), as represented on Figure 11:

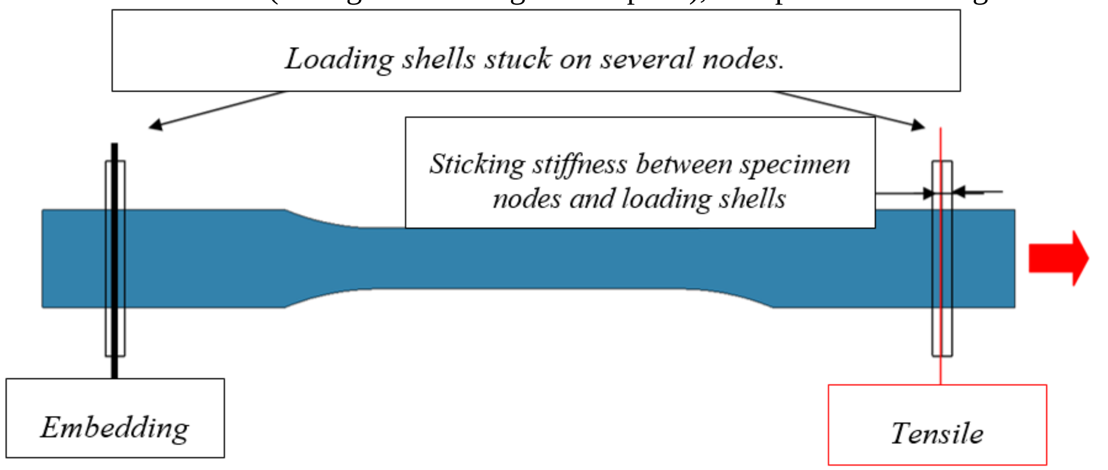


Figure 11: Boundary conditions and loads applied on every samples

The second aim of this study is to compare the results coming from two different DES arrangements in the specimen geometry: random packing and compact stacking (Figure 12).

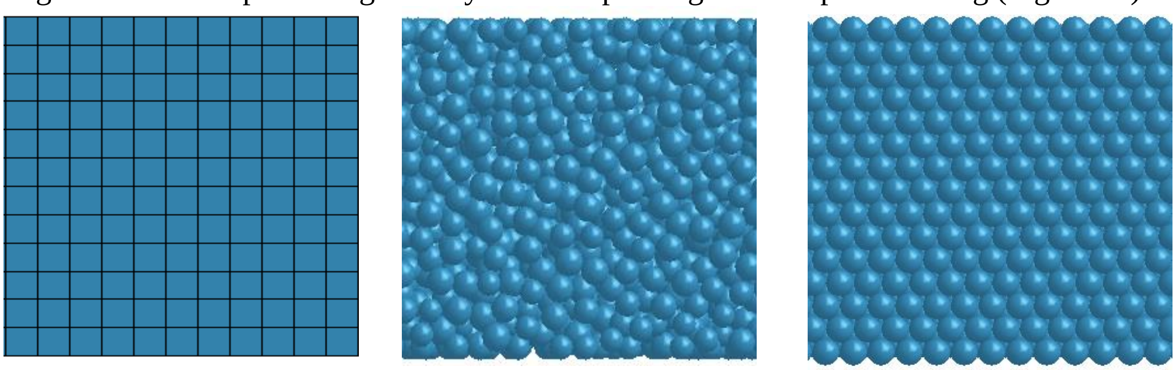


Figure 12: Finite elements and DES "mesh" illustration

For a good results correlation, the finite elements specimen mesh size is two times higher than the DES radius. For a good use of the DES-HBOND method, a failure criterion has to be defined. The DES-HBOND method implementation implies the needed criterion to be the energy release rate, which exclusively depends on the material properties. It is calculated as the area under the stress/strain curve.

The tensile tests results are presented in Figure 13. Three successive steps of the tensile test are illustrated: the initial state (a), the maximal necking state (b) and the failure state (c). For every

step the behavior of the three specimens is represented: the finite elements one (above), the compact stacked DES one (middle) and the randomly packed DES one (below).
The figure 13 shows that the finite elements specimen does not break. Indeed no failure criterion is defined for it. From a certain strain concentration at the specimen center (where necking appears), the finite elements sample is considered as broken and an eroding criteria should have been defined.
At state (b), the DES compact stacking specimen (middle one) shows a marked necking like the finite elements one. Their breaking elongations are also similar, with a failure angle about 45°, as predicated by the mechanical theory.
No necking occurs for the randomly packed DES specimen and its failure is too premature in terms of deformation. This behavior is due to the low spheres compactness. Indeed, there are too many “voids” between DES in the specimen which causes weak regions in the material (lack of matter).

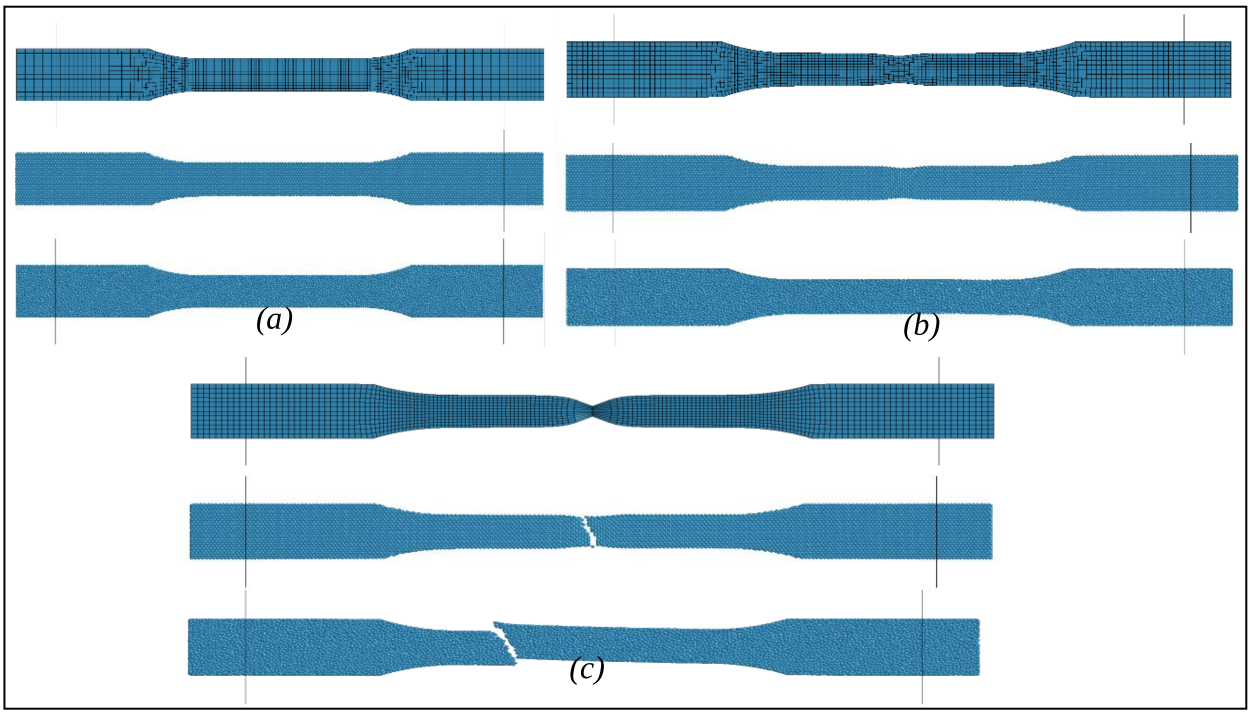


Figure 13: Screenshots of the three specimens behaviors at the initial state (a), at maximal necking (b) and at failure (c)

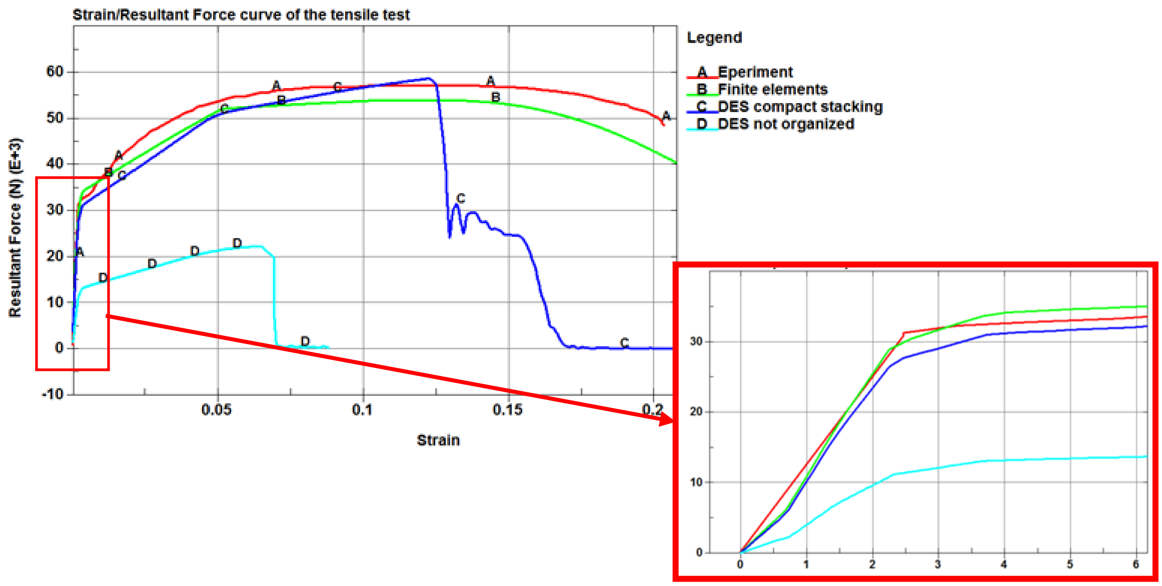


Figure 14: Force-strain curves of the experimental specimen (red), the finite elements one (green), the compact stacked DES one (dark blue) and the randomly packed DES one (light blue)

The middle cross section force-displacement curves of the experimental specimen (red), the finite elements one (green), the compact stacked DES one (dark blue) and the randomly packed DES one (light blue) are drawn on the Figure 14.

As expected (Figure 13), the randomly packed DES modulus and yield point are not well represented. Moreover, the Figure 14 shows that its resistance is much lower than the experimental result and that no necking occurs before failure. These results confirm that the randomly packed type of DES « mesh » is not usable for continuum modelling.

The Figure 14 demonstrates that finite elements and compact stacking DES modellings lead to good approximations of the experimental sample until necking:

The elastic domain is correctly modelled with finite elements and compact stacked DES.

The elasto-plastic transition is approximated by the « second linear part » occurring after the yield point of both curves (finite elements and compact stacked DES). The experimental soft passage of the matter from its elastic behavior to its plastic one (hard steel) is hard to model numerically. Indeed, this behavior causes a non-strict obedience to Hook's law's and necessitates the previous numerical definition of some conventional limits, like R_(e0.2%), which are not specified in those models.

The compact stacked DES plastic domain is modelled by a third linear part, and does not correspond to the expected behavior. This phenomenon seems to be specific to the DES modellings since both curves C and D have the same aspect.

The necking step is modelled in the compact stacked DES curve (Figure 13 (b)) and the necking occurs at the expected moment when comparing the curve with both experimental and finite elements ones. However the DES curve end shape does not correspond to the failure one represented on curves A and B.

Every step of the tensile test, applied to the compact stacked DES specimen, are detailed in Figure 15. These results are quite positive since every step of the compact stacked specimen force-strain curve can be identified with the experimental one.

Nevertheless, since the Discrete Element Method with Heterogeneous Bonds was recently implemented in LS-DYNA there still exists some improvements to make on the plastic domain modelling and on the failure one to make.

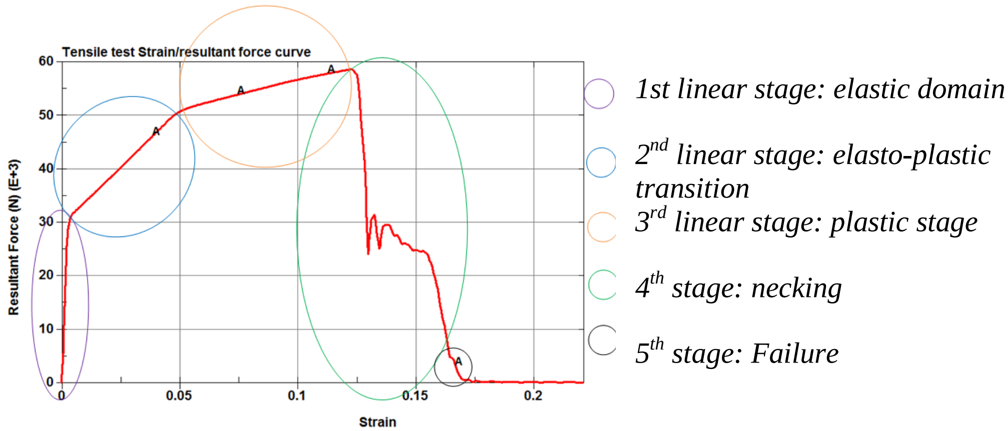


Figure 15: Description of the various stages of the compact stacked DES elasto-plastic behavior

4. Conclusion

Both the discrete and the continuous modelling approaches coming from the Discrete Element Method were studied in this paper: granular media modelling and continuum modelling. Numerical studies using the LS-DYNA® DEM permitted to determine the simplified model boundary conditions and loadings, as well as the spheres mechanical properties. Moreover, it has been established that a minimum finite element mesh size of around three times the spheres diameter is needed not to generate numerical noise on the cylinder. Also, a compaction procedure has been set up to obtain an acceptable granular media compactness before researching the cylinder mode shapes (gravity, small vibrations). It has been proved that a non-compressed media gives a too damped and noisy response. All these conclusions contribute to the project progress and our enhancement of knowledge on the DEM.
The second study helped in analyzing the DES-HBOND method ability to model damage in steel. It shows that the elastic mechanical behavior is well represented, but some improvements have to be brought to the plastic modelling, especially on the necking part. However, this new method is a real asset for the numerical failure modelling.

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