D3.3 Report on filler material

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Authors E. Rojas, M. Rodriguez (CIEMAT), A. Bruch (CEA)
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**SUMMARY**

This document is the deliverable D3.3 of the project POLYPHEM, where, taking into account the filler material, the issues related to filler shape and its influence on the thermocline thermal and structural behaviour are discussed.

**Dissemination level**

PU (Public)

**Repository**

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Background: about the POLYPHEM project

The POLYPHEM project is a research and innovation action funded by the European Union’s H2020 program. It is implemented by a European consortium of 4 research centres and 5 industrial partners. The aim is to increase the flexibility and improve the performance of small solar tower power plants. The concept of POLYPHEM consists in implementing a combined cycle formed by a solarized micro gas-turbine and a Rankine organic cycle machine, with an integrated thermal storage device between the two cycles. The need for cooling is minimal.

Developed from a patented technology by CNRS and CEA, the pressurized air solar receiver is integrated in the micro-turbine cycle. The thermal efficiency targeted for the receiver is 80% with a cost of 400 €/kW. The innovative thermal storage uses thermal oil and a single thermocline tank with a technical concrete filler material.

The main expected impact of this project is to enhance the competitiveness of low-carbon energy production systems through the technology developed. The expected progress is a better fitting of electricity generation to variable local needs, an overall conversion efficiency of solar energy into electricity of 18% for an investment cost of less than 5 €/W and a low environmental impact. By 2030, the cost of electricity production targeted by the POLYPHEM technology is 165 €/MWh for an annual direct normal irradiation of 2600 kWh/m²/year (North Africa and Middle East) and 209 €/MWh under 2050 kWh/m²/year (Southern Europe). In addition to decentralized power generation, other applications are considered for the deployment of this technology used in poly-generation: industrial heat production, solar heating and cooling, desalination of seawater or brackish water.

A prototype plant of 60 kWel with a thermal storage of 1300 kWh is designed, built and installed on the site of the experimental solar tower of Themis in Targasonne (France). The objective of the project is to validate the technical choices under test conditions representative of actual operating conditions.

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 764048
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<tbody>
<tr>
<td>AALB</td>
<td>Aalborg CSP</td>
</tr>
<tr>
<td>ARRA</td>
<td>Arraela S.L.</td>
</tr>
<tr>
<td>CEA</td>
<td>Commissariat à l’Energie Atomique</td>
</tr>
<tr>
<td>CIEMAT</td>
<td>Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas</td>
</tr>
<tr>
<td>CNRS</td>
<td>Centre National de la Recherche Scientifique</td>
</tr>
<tr>
<td>CO</td>
<td>Confidential: only for members of the consortium (including the Commission Services)</td>
</tr>
<tr>
<td>Cp</td>
<td>Specific heat capacity</td>
</tr>
<tr>
<td>CSP</td>
<td>Concentrated Solar Power</td>
</tr>
<tr>
<td>D</td>
<td>Deliverable</td>
</tr>
<tr>
<td>ETC</td>
<td>Effective Thermal Conductivity</td>
</tr>
<tr>
<td>DEM</td>
<td>Discrete Elements Method</td>
</tr>
<tr>
<td>EURO</td>
<td>Euronovia</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Model</td>
</tr>
<tr>
<td>FISE</td>
<td>Fraunhofer Institute for Solar Energy Systems, ISE</td>
</tr>
<tr>
<td>HTF</td>
<td>Heat Transfer Fluid</td>
</tr>
<tr>
<td>KAE</td>
<td>Kaefer Isoliertechnik GmbH</td>
</tr>
<tr>
<td>ORC</td>
<td>‘Orcan Energy AG’ or ‘Organic Rankine Cycle’</td>
</tr>
<tr>
<td>PU</td>
<td>Public</td>
</tr>
<tr>
<td>STE</td>
<td>Solar Thermal Electricity (equivalent to Concentrated Solar Power)</td>
</tr>
<tr>
<td>TES</td>
<td>Thermal Energy Storage</td>
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### Nomenclature related to the choice of the filler

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
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<tr>
<td>$m$</td>
<td>oil mass flow through the filler/storage tank (kg/s)</td>
</tr>
<tr>
<td>$A$</td>
<td>heat transfer surface for each brick (m$^2$)</td>
</tr>
<tr>
<td>$Bi$</td>
<td>Biot number (non-dimensional)</td>
</tr>
<tr>
<td>$c_p$</td>
<td>heat capacity (J/kg·K)</td>
</tr>
<tr>
<td>$d$</td>
<td>diameter (m)</td>
</tr>
<tr>
<td>$D$</td>
<td>diameter of the filler bed (m)</td>
</tr>
<tr>
<td>$h$</td>
<td>convective heat transfer coefficient (W/(m$^2$·K));</td>
</tr>
<tr>
<td>$H$</td>
<td>height of the filler bed (m)</td>
</tr>
<tr>
<td>$k_s$</td>
<td>thermal conductivity of the body (W/(m·K))</td>
</tr>
<tr>
<td>$L$</td>
<td>characteristic length (m)</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number (non-dimensional)</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number (non-dimensional)</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number (non-dimensional)</td>
</tr>
<tr>
<td>$t$</td>
<td>time (s)</td>
</tr>
<tr>
<td>$V$</td>
<td>brick volume (m$^3$)</td>
</tr>
<tr>
<td>$v^*$</td>
<td>mean velocity of the oil through the solid matrix (m/s)</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>porosity (non-dimensional)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity (N·s/m$^2$)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>kinematic viscosity (m$^2$/s)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density (kg/m$^3$)</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>temperature change (K)</td>
</tr>
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### Subscripts

<table>
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<th>Meaning</th>
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<tr>
<td>com</td>
<td>related to commercial bricks</td>
</tr>
<tr>
<td>hollow</td>
<td>related to the hollows in the brick</td>
</tr>
<tr>
<td>oil</td>
<td>related to the oil</td>
</tr>
<tr>
<td>S</td>
<td>related to the solid</td>
</tr>
<tr>
<td>solid_brick</td>
<td>related to solid brick</td>
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</table>
1. INTRODUCTION

This deliverable presents specific issues related to the filler given by its material selection. The performed studies to define what filler shape is the most appropriate are here included. While stating the filler shape, simulation of thermal ratcheting was investigated.

This report uses the main outcomes and results of D3.1 Report on the designs and specifications of filler, tank and foundations.

2. SHAPING THE FILLER

Several materials have been considered to be used as filler. Options of using either concrete formulations (composed by an aggregate and a binder) or just the aggregate were under consideration (see D3.1). While the first option gives a structured bed, the second one implies working with a randomly packed bed. According to Papakokkinos et al. (1) the structured bed approach is burdened by the extra effort to implement the structure of the bed, whereas in the packed bed the tank is filled randomly with the filler materials. This extra effort may be translated as cost and longer energy payback periods. However, a carefully designed structured bed provides the capability to optimize the geometrical pattern in order to achieve the best compromise between thermal performance and pressure drop (low pumping energy), as well as to avoid the phenomenon of thermal ratcheting (2, see paragraph 3). Additionally, it seems that the influence of the binder in the heat capacity may be the predominant one (3). Therefore, the option of having a structured packed bed composed of bricks with a certain shape and size has been the preferred option in Polyphem project.

The bricks shape and geometrical pattern for the arrangement of the filler inside the tank should be easy to manufacture and reproduce in large-scale. A complex geometry with a high cost of manufacture would not comply with the overall objective of reducing the cost of the TES system. In that sense, solid bricks (see Figure 1), like the ones used for testing oil to concretes compatibility, were the first option to consider. Taking into account limitations when manufacturing, Arraela proposed 4 possible sizes, as illustrated in Figure 1.

![Possible brick sizes](image)

$
\begin{align*}
40\times20\times10 \text{ cm}^3 \\
40\times20\times4 \text{ cm}^3 \\
30\times15\times15 \text{ cm}^3 \\
25\times25\times10 \text{ cm}^3
\end{align*}$

Figure 1: Solid bricks

Several geometrical patterns for the allocation of the bricks have been proposed (Figure 2). The arrangement in Figure 2(a) imposes preferential vertical channels while the pattern in Figure 2(b) imposes directional changes in the oil flow (other than vertical), enhancing the heat transfer between the oil and the solid brick. Figure 2(c) shows a 3rd proposal where each layer of solid bricks is rotated in relation to its neighbour layers, so the tortuosity of the structured bed is even higher than with the pattern of Figure 2(b) and so the heat transfer. In any of these patterns, each brick needs four reference points to be marked in the surroundings bricks, which is seen as very time consuming when allocating the bricks as filler in a tank.

In order to see if, with this geometry, a homogeneous temperature can be expected in the brick bulk, the Biot number is calculated. The Biot number is a dimensionless quantity that relates the heat transfer resistances inside of a body and at the surface of a body. This ratio determines whether or not the temperatures inside a body will vary significantly in space, while the body heats or cools over time, from a thermal gradient applied to its surface. It is defined according to:

$Bi = \frac{h}{k_s/L}$

(Eq. 1)
where $h$ is a convective heat transfer coefficient (W/(m$^2$·K)); $k_s$ is the thermal conductivity of the body (W/(m·K)) and $L$ is a characteristic length (m) of the geometry considered.

Since $h = \frac{Nu}{k_s}$, it is necessary to calculate the Nusselt number, $Nu$, according to a specific correlation whose format is mainly given by the value of the oil Reynolds number, $Re = \frac{v \cdot L}{v_{oil}}$, $v = \left(\frac{m}{s}\right) = \frac{m}{\rho \cdot \sigma_{solid\_brick} \cdot \Delta_{tank}}$ and $Pr$ or oil Prandtl number, $Pr = \frac{cp \cdot \mu}{k_{oil}} = 13.9$. The porosity of the arrangements with solid bricks, $\varepsilon_{solid\_brick}$, is around 0.5.

In general, problems involving Biot numbers much larger than 1 indicate non-uniformity of temperature fields within the corresponding object, in this case, the brick. Thus, calculating Biot number playing with the different solid brick sizes (Figure 1) possibilities, there is none that can achieve such a low value for Biot number, meaning that using these solid bricks will not be an efficient enough heat transfer with the thermal oil. Additionally, since the porosity is higher than initially expected, the storage capacity would be lower. As a conclusion, and since it was possible to find out other options as it will be shown later, it was decided not to use the regular bricks geometries and configurations.

In previous works (4, 5, 6) the studied structured packed beds are erected from bricks that touch each other and the HTF channels appear because of the shape design of the individuals bricks (Figure 3).
Looking for commercial hollowed bricks made up of concrete, the geometries in Figure 4 were found. The idea, therefore, is to manufacture hollow bricks similar of any of those of Figure 4 but with the concrete mixture already studied and chosen in Polyphem project for the filler, i.e., HEATEK-RV. The expected result is, therefore, a solid matrix made of bricks full of vertical pipes obtained by aligning the hollows of every brick layer.

These commercial bricks may have the following technical data:

<table>
<thead>
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<th>Configuration</th>
<th>14 feedthroughs</th>
</tr>
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<tr>
<td>Solid index$^1$:</td>
<td>0.6-0.7.</td>
</tr>
<tr>
<td>Wall thicknesses ≥ 10 mm</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Nominal Dimensions</th>
<th>Length</th>
<th>Width</th>
<th>Height</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>215±3 mm</td>
<td>115±3 mm</td>
<td>100±2 mm</td>
</tr>
</tbody>
</table>

As previously, Biot number is calculated for this geometry: \( L \) in Eq. 1 is the hollow diameter \( (d_{hollow} = 3\times10^{-2} \text{m}) \) and the real mean velocity \( v^* \) (m/s) = \( \frac{v}{\rho e_{concrete} \mu_{concrete}} \) = 4.14 \times 10^{-4} \). Therefore \( Re = \frac{v^* d_{hollow}}{\nu_{e_{air}}} = 15.1 \) which implies laminar flow. For fully developed internal laminar flow, the Nusselt numbers tend towards a constant value of 3.66 (Incropera & DeWitt$^7$), giving a heat transfer coefficient of \( h = 13.8 \text{ W/m}^2\text{K} \).

\[ \text{Table 1: Sizes and dimensions of some commercial hollowed concrete bricks} \]

---

$^1$ Solid index is the relation of the solid volume to total one. It is related to porosity, \( \varepsilon \), by \( 1 - \varepsilon \).
In Table 2, the required information for the calculation of all these dimensionless numbers are shown.

<table>
<thead>
<tr>
<th>Oil properties @ 200 ºC</th>
<th>Filler properties</th>
<th>Filler bed parameters</th>
</tr>
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<tr>
<td>Material</td>
<td>Material</td>
<td>H (m)</td>
</tr>
<tr>
<td>Jarytherm DBT</td>
<td>HEATEK-RV</td>
<td>3</td>
</tr>
<tr>
<td>( \rho ) (kg/m³)</td>
<td>( \rho ) (kg/m³)</td>
<td>3105</td>
</tr>
<tr>
<td>910</td>
<td>3105</td>
<td></td>
</tr>
<tr>
<td>( c_p ) (J/kg K)</td>
<td>( c_p ) (J/kg K)</td>
<td>1000</td>
</tr>
<tr>
<td>2100</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>( k ) (W/m K)</td>
<td>( k ) (W/m K)</td>
<td>1.1</td>
</tr>
<tr>
<td>0.113</td>
<td>1.1</td>
<td></td>
</tr>
<tr>
<td>( v ) (m²/s)</td>
<td>( \varepsilon_{\text{com}} ) (-)</td>
<td>0.35</td>
</tr>
<tr>
<td>8.20 x 10⁻⁷</td>
<td>0.35</td>
<td></td>
</tr>
</tbody>
</table>

Since each brick wall is influenced, at least, by two holes, and the thickness of such walls is estimated around 1 cm (see Table 1), the characteristic length in Biot number \( Bi \) in Eq. 1 is assumed to be half of the brick wall thickness, i.e., 0.5 cm. Therefore, the obtained Biot number is 0.06. A value of 0.06 for Biot number assures, therefore, a uniform temperature within the hollow brick. The following calculation supports this statement too.

Let’s calculate how much time a brick requires to be heated/cool to a certain temperature, considering the figures obtained above and the Polyphem TES design conditions by the following energy balance:

\[
hA\Delta T = \frac{(c_p\rho V)\Delta T}{t} = \frac{(c_p\rho V)\Delta T}{hA} \Rightarrow t = \frac{(c_p\rho V)\Delta T}{hA}
\]

(Eq. 2)

where \( A \) is the heat transfer surface in the brick, \( A = 2\pi d_{\text{hollow}} \cdot 14 = 0.1319 \text{ m}^2; \) \( V \) is the solid volume in the brick, \( 1.6 \cdot 10^{-3} \text{ m}^3 \)

Therefore \( t = 273 \text{ s} \approx 4 \text{ min} \)

Taking into account that the oil mass flow is 0.7 kg/s, which implies a real oil velocity of \( 4.14 \cdot 10^{-4} \text{ m/s} \), the oil will flow along one brick in 241 s or 4 min, so the required time to heat it up is similar to the oil residence time in a brick.

Therefore, hollowed bricks with HEATEK-RV following the geometry figures of Table 1 will become appropriate filler for Polyphem storage system, from the thermohydraulic point of view, since the heat of the oil HTF can be effectively transferred to and stored in the filler.

When manufacturing the bricks it was observed that, due to the relatively high forge velocity of HEATEK-RV and the 1 cm wall thickness of the bricks, the mass segregates, breaking the bricks at the exit of the production machine. As result, some of the figures of Table 1 had to be changed to those of Table 3.

| Table 3: Sizes and dimensions of Polyphem HEATEK-RV hollow bricks |
|--------------------------|-------------------|-----------------------|
| **Configuration**        | 17 feedthroughs   |                       |
| **Nominal Dimensions**   | Length            | Width                 | Height                |
|                          | 250 mm            | 122 mm                | 100 mm                |
As can be easily seen in Figure 5, the thickness of the brick walls and hollow diameter are maintained. The porosity changes a little bit up to 40%, influencing the mean real oil velocity in the bed, \( v^* \), to \( 3.62 \times 10^{-4} \text{ m/s} \). The new figures for the Polyphem size of bricks are:

\[ Re = 13.2 \] (which implies laminar flow regime), so \( Nu = 3.66 \), which gives the same as before heat transfer coefficient, \( h \), and the same \( Bi = 0.06 \).

So no major differences with the figures obtained for commercial hollow bricks and so with the results: hollow bricks with HEATEK-RV and the geometry of Table 3 will assure a homogeneous temperature at each brick and an efficient enough heat transfer between the HTF oil and the filler (bricks).

This study and calculations have been presented in a poster at SolarPACES 2020, entitled *Thermal Storage Filler Material Distribution for the Polyphem Project* and authored by M. Rodriguez-García, E. Rojas and J.M. Caruncho.
3. THERMAL RATCHETING STUDY

3.1 CONTEXT AND PROBLEMATIC

Filling of the Polyphem’s storage tank was questioned and studied during significant time during the project, mainly regarding the material, the geometry, the shape of the filler material etc... For a long time from beginning of the project, pebble bed configuration, i.e. porous matrix made of small pebbles of concrete, was considered. This configuration, coupled with the inherent thermal cycles of the thermal storage, is accompanied by small inter-displacement between particles, and thermal mismatch between the container and the granular storage media. This is known to lead to thermal ratcheting. (Chen et al. 2006, Divoux et al. 2008, Dreißigacker et al. 2013) as illustrated in Figure 6.

Thermal ratcheting is threatening the mechanical integrity of the global system; so it has to be considered with care. To date, no engineer simple model can predict mechanical stresses appearing in the container. The only available solution is to use the Discrete Element Method, which is a simple but very computer intensive method. The DEM concept, shown in Figure 7, is in principle quite simple. It consists in considering each pebble as a separate element in interaction with its neighbors and/or walls and in applying, at each numerical cycle, Newton's second law of motion and a force-displacement law at the contacts. Up to now, this is the only approach allowing simulating the effective behavior of a granular bed submitted to thermal cycles and estimating the resulting effective mechanical constraints inside the bed and on the tank’s walls.

Figure 6: Illustration of the thermal ratcheting phenomenon in case of higher thermal expansion of the storage tank

CEA has already addressed the DEM approach for treating problems of cyclic deformation of granular media, for hydride storage where there is a chemo-mechanical problem (Galvis et al. 2017; Charlas et al. 2015; Salque et al. 2015) or for heat storage, where it is a thermo-mechanical problem (Sassine 2018). Even though hydride storage
involves a much larger volume swelling of particles, both problems are quite similar: a breathing\(^2\) media is entrapped in a finite size container (that can have its own breathing behavior). Note that the shape and direction of the expansion gradient (whether it is due to thermic in the case of heat storage or to phase change in the case of hydrides) may have an influence as well as the granular media by its own.

Those background studies on breathing granular material entrapped in a closed container have confirmed or revealed that:

- There is often a slow densification of the granular media in the container, leading to a progressive increase of the stress on the container walls;
- The maximum stress appears near the bottom of the container;
- A high slenderness ratio \(S_r\) (height of the granular bed over the diameter of the container) is detrimental, and can lead to rupture of the container. For example, for a \(S_r=2\), after a few cycles, the stress at the bottom can be 9 times the initial stress recorded after the container filing, for a nearly monosize particle distribution.

This method is thus promising for predicting mechanical problems of such type of storage, but:

1- These results need further experimental verifications. We have to investigate as well the influence of irregular shape particles with multi-modal size distribution;

2- A question is still present in terms of adequacy of the numerical integration as regard to the physics of the problem. For example, to accelerate the calculation time, the gravity is artificially increased, and/or the particle contact stiffness is decreased, and/or the temperature rate during cycling is increased, compare to reality. When focussing in the stress applied by the granular bed to the container, the change of these parameters is not harmless.

In this report point 2, which has never been properly addressed in the literature, is addressed. The study and results presented below will not give direct clues for the mechanical design of the Polyphem’s storage tank but are necessary to further assess the design of the container around a granular bed. The study has been performed using the DEM software Yade\(^{15}\) already used in the previous works of CEA on thermal ratcheting.

An executive summary of the study, mainly focused on illustration of the approach and results obtained, is presented in the following paragraphs. A more complete report is available in Annex.

### 3.2 Equations and Parameters Governing the Problem

The DEM approach and protocol using the YADE software are schematically presented in Figure 8.

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\(^2\) We propose to use the appellation "breathing media" for a media that sees its volume cyclically swelling and shrinking.
Basically, the main equations and phenomena to be considered are:

- The first principle of dynamics;
- The contact law between particles and with the walls;
- The particle swelling.

The parameters associated are listed in the Table 4:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>Young modulus</td>
<td>Pa=N.m$^{-2}$=kg.m$^{-1}$.s$^{-2}$</td>
</tr>
<tr>
<td>$r_{moy}$</td>
<td>Mean particle radius</td>
<td>m</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$H_{bed}$</td>
<td>Bed height</td>
<td>m</td>
</tr>
<tr>
<td>$g$</td>
<td>Acceleration of gravity</td>
<td>m/s$^2$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Swelling parameter</td>
<td></td>
</tr>
</tbody>
</table>

### 3.3 SUMMARY OF THE DIFFERENT TIME SCALES TO CONSIDER

An extensive study on the physical phenomenon involved has been performed to highlight the relevant value of the simulation time scale. Figure 9 is giving a summary of the different time scales to consider, as well as conditions to be respected. These latter conditions give us a frame in which parameters can be varied to obtain faster calculation times while keeping appropriate physical meaning of the simulated problem. A simplified version is proposed in Figure 10 as some parameters can be expressed as function of others parameters, so that we keep only the conservative conditions.

The difficult point is that there is no optimum situation, and the choice of parameters results in a compromise between several conditions.
3.4 Test cases and results

The previous study and definition of the equations, the relevant parameters and the associated time-scales and criteria have been applied on different test cases to assess their relevancy and their real meaning. Four different specific cases of increasing complexity have been considered as illustrated in Table 5.
### Table 5: Test cases

<table>
<thead>
<tr>
<th>Name</th>
<th>Geometry</th>
<th>Objectives</th>
</tr>
</thead>
</table>
| Test case 1  | ![Diagram](image1.png) | - Simple geometry  
- Small number of particles to ensure low calculation time and “easily understandable” results                                                                                                         |
| Test case 2  | ![Diagram](image2.png) | - Simple geometry  
- Introduction of the vibration component  

This study has permitted to conclude on adapted time stepping to avoid a self-vibrational mode when applying the particle swelling |
| Test case 3  | ![Diagram](image3.png) | - 2D geometry  
- Balance between the integration in a more complex and representative configuration and calculation times  

This particular geometry has permitted to enlighten that, depending on the choice of the contact stiffness, two regimes appear frankly:  
- one is an "elastic mode", where the force network between particles is quite stable, and varies in amplitude as swelling and shrinking of particle occurs;  
- the other is a "sliding mode" where particles tends to slide between each other, as well as with the container walls. In that case, forces are much higher, and show more unstable behavior. |
| Test case 4  | ![Diagram](image4.png) | - Representative problem with a sufficient number of particles  
- 1600 particles  

This simulation confirms that there is a transition between the elastic mode and the sliding mode if the contact stiffness is varied, but the transition is much less sharp. The bad news is that the real physics of the problem is the sliding mode, which corresponds to higher computation times. |
Some chosen results for Test case 4 are presented below. Several simulations have been performed, with varying the contact stiffness $E$. For each calculation, the initial construction of the pile is renewed. Approximately 1600 particles can randomly fit in the allowed space before pluviation. Looking at Figure 11, all the simulations exhibit a densification behavior of the granular bed as cycling progresses. A stabilized state is not reached, even for simulations with a high cycle number of 20. We had also to go further with the cycle number as solution for high $E$ are much more noisy and seems to need more cycles to exhibit a stabilized behavior. Note that a simulation with only 1600 particles will last two month with a $E=100\text{e}8$ Pa for 20 cycles.

Figure 11: Evolution of the pebble bed height variation and the porosity along cycling

Figure 12: Evolution of the stress ($F/S$) on the container walls (cylinder and base) as a function of the contact stiffness $E$
When increasing E, the signal is becoming more and more noisy, probably because there are more sudden changes in the force network between particles. Nevertheless, we have tried to plot the evolution of the maximum pressure (Fmax/S) applied by the particles to the container as a function of E in Figure 12. This exhibits that the pressure seems to show a saturation value, but the uncertainty is high and the force does not exactly shows a steady state. Results from Figure 12 confirm the potential impact of the thermal ratcheting on the mechanical design or a thermal storage tank filled with particles and the first order influence of the parameter E. It

3.5 Conclusion and perspectives

As a conclusion, the studies conducted up to now were necessary to really understand what is really calculated when using the Discrete Element Method to model the thermal ratcheting of a granular media. Imbrication of times scales makes the problem difficult in choosing adequate parameters to accelerate the calculation time. The conclusion is that the problem is quite locked, and the calculations time will be long. For example, for the choice of the contact stiffness, we can conclude that this parameter has to be chosen carefully in order to activate preferably the slide mode which is more physical. This choice was not done according this kind of new rules for the work available in the literature on thermal ratcheting using DEM approach.

The results show the importance of stiffness choice. The sliding mode is surely the calculation mode to aim, as it is closer to physical reality (which is something to ascertain by experimental confrontation). Previous studies on this subject were done ignoring the importance of stiffness choice. They should be checked under the light of our recent results. Next job is to perform simulations more in relation with the geometry of the tank design proposed recently.

Since this study on thermal ratcheting and DEM simulations started, the filling configuration has significantly changed. In particular, pebbles are no longer relevant and bricks are now considered. In this latest configuration, the porous media is structured and thermal ratcheting may be significantly reduced and, potentially, even suppressed.

Depending on the proposed geometry for the present solution using bricks, calculations related to the displacement of the bricks with thermal cycles may be interesting to address potential movement in the brick pile. This works can be done to finish the study concerning DEM modelling.
4. ANNEX 1: FULL REPORT ON DEM SIMULATIONS

4.1 PROBLEMATIC

Heat storage involves in essence thermal cycling of the particulate material adopted to store the heat. This is accompanied by small inter-displacement between particles, and thermal mismatch between the container and the granular storage media. This is known to lead to thermal ratcheting. Chen et al. 2006, Divoux et al. 2008, Dreißigacker et al. 2013. This phenomenon is threatening the mechanical integrity of the global system; so it has to be considered with care. To date, no engineer simple model can predict mechanical stresses appearing in the container. The only available solution is to use the Discrete Element Method (DEM), which is a simple but very computer intensive method.

4.2 BACKGROUND

At CEA, we have already addressed the DEM approach for treating problems of cyclic deformation of granular media, for hydride storage where there is a chemo-mechanical problematic (Galvis et al. 2017; Charlas et al. 2015, Salque et al. 2015) or for heat storage, where it is a thermo-mechanical problematic (Sassine 2018). Even though hydride storage involves a much larger volume swelling of particles, the problems are quite similar: a breathing media is entrapped in a finite size container (that can have its own breathing behavior). Note that the shape and direction of the expansion gradient (whether it is due to thermic in the case of heat storage or to phase change in the case of hydrides) may have an influence as well as the granular media by its own.

Those background studies on breathing granular material entrapped in a closed container have confirmed or revealed that:

- There is often a slow densification of the granular media in the container, leading to a progressive increase of the stress on the container walls;
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This method is thus promising for predicting mechanical problems of such type of storage, but:

3- These results need further experimental verifications. We have to investigate as well the influence of irregular shape particles with multi-modal size distribution;

4- A question is still present in terms of adequacy of the numerical integration as regard to the physics of the problem. In other words, in order to run faster calculations, a classical way is to increase the time step.
   a. For instance, a time step should be lower than the contact duration, which can be expressed as 
   \[ t_{contact} \sim \frac{m}{k} \]
   where \( m \) is the mass of a particle, and \( k \) is the contact stiffness. Very often, in order to increase the time step, a lower value of \( k \) is artificially adopted;
   b. Another time scale is present in the physics, it is the free fall time scale given by \( t_g = \sqrt{\frac{2r_{moy}}{g}} \). In real life this time scale is quite far from the contact time scale, and the calculation time is imposed by the smallest time scale. It is thus convenient to decrease the contact stiffness, or to artificially increase the gravity. But, increasing \( g \), or decreasing \( E \) (or \( k \)) has a direct consequence on the recorded stress of container wall for example;
   c. A third time scale is the cycling time scale, which we want to be close to the two other time scales mentioned above, so there is a will to decrease this value, but this may introduce some inertia problems.

3 We propose to use the appellation "breathing media" for a media that sees its volume cyclically swelling and shrinking.
In the following, we propose to address the point 2 that has never been properly addressed in the literature. The study and results presented below will not give direct clues for the mechanical design of the Polyphem’s storage tank but are necessary to further assessed design elements.

### 4.3 Equations and Parameters Governing the Problem

The DEM approach and protocol using the YADE software are schematically presented in Figure 13.

#### 4.3.1 Equations

**4.3.1.1 First principle of dynamics**

The problem consists for each particle in solving the first principle of dynamics:

\[
\begin{align*}
\mathbf{m}_i \ddot{\mathbf{x}}_i &= \sum \mathbf{F}_i + \mathbf{m}_i \mathbf{g} \\
\end{align*}
\]  

(Eq. 3)

It includes the gravity law:

\[
\mathbf{F} = \mathbf{m}_i \mathbf{g} 
\]  

(Eq. 4)

**4.3.1.2 Contact law**

During the breathing of the bed, particles are moving and overlap can happen, as illustrated in Figure 14.
Figure 14: Particle overlap

If FrictMat is used in the Yade software, from definition:

\[ F_n = k_n \delta l \]  
(Eq. 5)

\[ k_n = \frac{E_1 l_1 E_2 l_2}{E_1 l_1 + E_2 l_2} \]  
(Eq. 6)

With:

\[ \delta l = 2r_i \]  
(Eq. 7)

If \( E_1 = E_2 \) and \( r_1 = r_2 = r_m \oy \),

\[ k_n = Er_m \oy \]  
(Eq. 8)

4.3.1.3 Particle swelling

Principle of “breathing media” is that particles in it exhibit cyclic swelling and deflation, as illustrated in Figure 15.

Figure 15: Swelling of the particles

The swelling of a particle can be defined by the swelling parameter \( \beta \) as:

\[ V_2 = \beta V_1 \]  
(Eq. 9)

\[ r_2 = hr_1 \]  
(Eq. 10)

\[ \delta r = r_1 \alpha \Delta T \]  
(Eq. 11)

\[ h = 1 + \alpha \Delta T \]  
(Eq. 12)

with \( \Delta T \) the temperature variation of the particle and \( \alpha \) the coefficient of thermal expansion of the particle.

It comes:

\[ \beta = h^3 \]  
(Eq. 13)

Expressed in terms of particle radius variation:

\[ \delta r = r_1 (h - 1) = r_1 \alpha \Delta T = r_1 \left( \sqrt[3]{\beta} - 1 \right) \]  
(Eq. 14)

The rate of particle radius increase is:
\[ \delta r = r_1 \dot{h} \]  
(Eq. 15)

If we want to impose volume rate:

\[ \dot{\beta} = 3h \dot{h}^2 \]  
(Eq. 16)

\[ \delta \dot{r} = r_1 \left( \frac{\dot{\beta}}{3h^2} \right) \]  
(Eq. 17)

The period of cycling can be written:

\[ t_{cycle} = 2 \frac{\delta r}{\delta \dot{r}} = 2 \frac{r_{moy}(h-1)}{\delta \dot{r}} \]  
(Eq. 18)

The radius variation rate is:

\[ \delta \dot{r} = \frac{\delta r}{2t_{cycle}} = 2 \frac{r_{moy}(h-1)}{t_{cycle}} \]  
(Eq. 19)

Typical cycles can be illustrated by Figure 16.

Figure 16: Cycles of swelling and deflation, without pause

It can be convenient to add some pauses between cycling to wait for an equilibrated state. Time to reach an equilibrium should be low, otherwise it means that there are high inertia effects (Figure 17).

4.3.1.4 Problem parameters

The parameters are listed in the Table 6.
**Table 6: Parameters**

<table>
<thead>
<tr>
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<td>( H_{bed} )</td>
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<tr>
<td>( g )</td>
<td>m/s(^2)</td>
<td>Acceleration of gravity</td>
</tr>
<tr>
<td>( \beta )</td>
<td></td>
<td>Swelling parameter</td>
</tr>
</tbody>
</table>

Another unit system can be adopted, see for example the proposition to work in mm length in ANNEX

### 4.4 CONCERNING PHYSICAL PARAMETERS (CONTACT STIFFNESS AND SWELLING)

#### 4.4.1 Stiffness parameter \( \dot{E} \) to equilibrate interpenetrations

From the definition of the particle swelling, it comes:

\[
\delta r_{swell} = r_{moy} (h - 1) \quad (\text{Eq. 20})
\]

From the definition of the normal stiffness, it comes:

\[
\delta l = \frac{F}{E_{moy}} \quad (\text{Eq. 21})
\]

There should be an influence of whether the particle interpenetration (\( \delta l \)) is higher or lower than the particle radius change by swelling (\( \delta r_{swell} \)). This depends on how \( E \) parameter has been chosen compared to the threshold value \( \dot{E} \) defined by:

\[
\delta r_{swell} = \delta l \quad (\text{Eq. 22})
\]

It comes:

\[
\dot{E} = \frac{F}{r_{moy}(h-1)} \quad (\text{Eq. 23})
\]

An estimation of \( F \) can be the force expected between particles due to the particle column weight \( m_c \). In a cubic assembly, of height \( H_{bed} \), the weight is:

\[
m_c = \frac{H_{bed}}{2r_{moy}} \rho \frac{4}{3} \pi r_{moy}^3 = \rho \frac{4}{6} \pi r_{moy}^2 H_{bed} \quad (\text{Eq. 24})
\]

We can define the number of particle in the bed thickness (if cubic assembly is considered):

\[
n_p = \frac{H_{bed}}{r_{moy}} \quad (\text{Eq. 25})
\]

The corresponding force \( F \) is:

\[
F_g = m_c g \quad (\text{Eq. 26})
\]

The force is thus:

\[
F_g = \rho g \frac{4}{6} \pi r_{moy}^3 n_p \quad (\text{Eq. 27})
\]

So \( \delta l_g \) can be written:

\[
\delta l_g = \frac{4}{6} \pi r_{moy} H_{bed} \frac{\rho g}{E} \approx 2r_{moy}^2 n_p \frac{\rho g}{E} \quad (\text{Eq. 28})
\]
So the $E$ threshold writes:

$$E = \frac{2\rho g H_{\text{bed}}}{h-1}$$

(Eq. 29)

### 4.4.2 Interpenetration ratio

The interpenetration ratio is:

$$\frac{\delta r_{\text{swell}}}{\delta t_{\text{g}}} = \frac{1}{2H_{\text{bed}}} \frac{E(h-1)}{\rho g}$$

(Eq. 30)

### 4.5 Concerning time scales

In principle, time stepping is governed by the minimum time scale of different phenomenon. Hereafter, the different time scales are exposed.

#### 4.5.1 Contact time scale

The duration of a contact is given by the time period of a mass-spring oscillator:

$$t_{\text{contact}} \sim \sqrt{\frac{m}{k}}$$

(Eq. 31)

*Figure 18: Mass-spring oscillator*

Introducing the problem parameters:

$$t_{\text{contact}} = \frac{4}{3} \pi \frac{\rho r_{\text{moy}}^2}{E} = 2r_{\text{moy}} \sqrt{\frac{\rho}{E}} \approx 2r_{\text{moy}} \sqrt{\frac{\rho}{E}}$$

(Eq. 32)

In Yade software, they approximate this to:

$$t^{\text{Yade}}_{\text{contact}} = r_{\text{moy}} \sqrt{\frac{\rho}{E}}$$

(Eq. 33)

(in fact, $\sqrt{\frac{E}{\rho}}$ is the sonic speed in the constitutive material).

The ratio is:

$$\frac{t_{\text{contact}}}{t^{\text{Yade}}_{\text{contact}}} = 2$$

(Eq. 34)

The real oscillation period of two spheres linked by a spring with stiffness $k = r.E$ is:

$$T = 2\pi \sqrt{\frac{m}{k}} = 4\pi \sqrt{\frac{\rho}{\sqrt{3} r E}}$$

(Eq. 35)

which gives:
4.5.2 **Gravity time scale**

Another time scale is the time imposed by the free fall of a particle under gravity on the mean particle size distance, that is:

$$T = 2\pi t_{contact}$$  \hspace{1cm} (Eq. 36)

4.5.3 **Ratio of time scales**

$$\frac{t_g}{t_{contact}} = \sqrt{\frac{6E}{4\pi \rho g r_{moy}}} \approx \sqrt{\frac{E}{2\rho g r_{moy}}}$$  \hspace{1cm} (Eq. 38)

4.5.4 **Reducing time scale difference**

Very often, the problem is that $t_g \gg t_{contact}$ so the time step is imposed by the contact time step, and if $t_g$ is high compare to $t_{contact}$ the simulation will last very long. In order to reduce simulation time, there are two possibilities:

1. soften the contact stiffness, by taking a low value for $E$

   In that case, we may be careful to still respect the $\tilde{E}$ criterion, in order that the particle interpenetration is not too high compared to particle swelling.

2. increase gravity $g$

   In that case, what is the consequences on effort created between particles and walls, which is an important point of the calculation?

   The gravity $\tilde{g}$ that will equalize $t_{contact} = t_g$ is:

   $$\tilde{g} = \frac{E}{2\rho r_{moy}}$$  \hspace{1cm} (Eq. 39)

4.6 **CONCERNING FORCES**

An estimation of a maximum force due to gravity is (see part 4.4.1):

$$F_g = \rho g \frac{4}{6} \pi r_{moy}^2 H_{bed} = 2n_p \rho g r_{moy}^3 \frac{\pi}{3} = 2n_p \rho g r_{moy}^3$$  \hspace{1cm} (Eq. 40)

An estimation of a maximum force due to fully constrained particle is:

$$F_{swell} = Er_{moy} \delta l_{swell} = Er_{moy}^2 (h - 1)$$  \hspace{1cm} (Eq. 41)

The force ratio is:

$$\frac{F_{swell}}{F_g} = \frac{1}{2H_{bed}} \frac{E(h-1)}{\rho g}$$  \hspace{1cm} (Eq. 42)

The force ratio is equal to the interpenetration ratio. Indeed, it can be written:

$$\frac{F_{swell}}{F_g} = Er_{moy} \delta r_{swell}$$  \hspace{1cm} (Eq. 43)

$$F_{swell} = Er_{moy} \delta l_g$$  \hspace{1cm} (Eq. 44)

4.7 **INTRODUCING THE PARTICLE CYCLIC SWELLING AND SHRINKING**

We see two criteria to fulfill, one on interpenetration, the other on inertia effects.

4.7.1 **Interpenetration criterion**

The criterion is based on the idea that in a single calculation time, the increase in particle radius should be very small compared to the actual interpenetration.
This writes:

\[ \delta \delta r = \delta \dot{r} \cdot t_{\text{contact}} \ll \delta l \]  

(Eq. 45)

This gives a criterion on the swelling rate:

\[ \delta \dot{r} \ll \frac{\delta l}{t_{\text{contact}}} \]  

(Eq. 46)

When considering the swelling/shrinking period, the criterion becomes:

\[ t_{\text{cycling}} \gg \frac{2r_{\text{moy}}(h-1)t_{\text{contact}}}{\delta l} \]  

(Eq. 47)

From this we can define a minimum cycling time with the estimation of interpenetration due to gravity.

\[ t_{\text{cycling}}^{\text{min}} = \frac{2r_{\text{moy}}(h-1)t_{\text{contact}}}{\delta l} \]  

(Eq. 48)

\[ t_{\text{cycling}}^{\text{min}} = \frac{2(h-1)}{n_{\rho}g} \sqrt{\frac{E}{\rho}} \]  

(Eq. 49)

### 4.7.2 Inertia criterion

This criterion is assuming that the first criterion is fulfilled, that means that the particles are pushing on each other a nearly constant interpenetration (assumed very small in that case). If the swelling rate is too important, there will be high inertia effects.

As described in Figure 20, the velocity of the last particle of a pile can be written:

\[ v = 2n_{\rho}\delta \dot{r} \]  

(Eq. 50)
This velocity (inertia given to the particles) will have to be absorbed by the simulation, i.e. it has to have a negligible effect on the result. The time of flight of the last particle on top, which is assumed to be a time of inertia is:

\[ t_{\text{inertia}} = \frac{2v}{g} = \frac{4n_p \delta r}{g} \]  
(Eq. 51)

We have to keep this time close to the contact time:

\[ t_{\text{inertia}} < t_{\text{contact}} \]  
(Eq. 52)

It then gives a condition on the radius variation rate:

\[ \delta r < g \frac{t_{\text{contact}}}{4n_p} \]  
(Eq. 53)

The criterion on the cycling period can thus be written:

\[ t_{\text{cycle}} > \frac{8n_p r_{\text{moy}} (h-1)}{t_{\text{contact}} g} \]  
(Eq. 54)

From this we can define a minimum cycling time to limit inertia effect.

\[ t_{\text{cycling}}^{\text{inertia min}} = \frac{8n_p r_{\text{moy}} (h-1)}{t_{\text{contact}} g} \]  
(Eq. 55)

Leading to

\[ t_{\text{cycling}}^{\text{inertia min}} = \frac{4n_p (h-1)}{g} \sqrt{\frac{E}{\rho}} \]  
(Eq. 56)

This criterion leads to very high cycling time, we are wondering whether it is relevant.

Nota: The ratio between the two times \( t_{\text{cycling}}^{\text{inertia min}} \) and \( t_{\text{cycling}}^{\text{g min}} \) is:

\[ \frac{t_{\text{cycling}}^{\text{inertia min}}}{t_{\text{cycling}}^{\text{g min}}} = 2n_p^2 \]  
(Eq. 57)

This means that the time to take into account is \( t_{\text{cycling}}^{\text{inertia min}} \).

### 4.8 SUMMARY OF THE DIFFERENT TIME SCALES TO CONSIDER

Figure 21 is giving a summary of the different time scales to consider, as well as conditions to be respected. These latter conditions gives us a frame in which parameters can be varied to obtain faster calculation times while keeping some physical meaning of the simulated problem.

A simplified version is proposed in Figure 22 as some parameters can be expressed as function of others parameters, so that we keep only the conservative conditions.

The difficult point is that there is no optimum situation, and the choice of parameters results in a compromise between several conditions.
4.9 Test case 1 on Yade

These entire theoretical criteria have been checked on a simplified problem, to assess their real meanings.

4.9.1 Geometry studied

The simplified geometry is described in Figure 23.
4.9.2 Results for pluviation
The pluviation phase (or also called the jamming) is the phase when particles are initially piled up in the container. The method here consist in creating particle in space that are not in contact with other particles and then to let gravity build the pile. Particles are not far from each other in our case in order to have shorter falling times. An example of final state is shown in Figure 24. We did some simulation with some parameter variations, as presented in Table 7. The results are conform to what is expected (equations written in previous part).
### 4.9.3 Results for cyclic swelling and shrinking

Now, we test several parameters choices on the cycling phase.

The parameters adopted for the reference simulation presented in Figure 25.

**Reference case**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_1 )</td>
<td>12.5e-3 m</td>
</tr>
<tr>
<td>( H_1 )</td>
<td>4.0*10^2 r_1</td>
</tr>
<tr>
<td>( e_1 )</td>
<td>r_1/10.0</td>
</tr>
<tr>
<td>( L_1 )</td>
<td>4.0<em>r_1</em>1</td>
</tr>
<tr>
<td>( L_2 )</td>
<td>L_1</td>
</tr>
<tr>
<td>( n_1 )</td>
<td>2.5</td>
</tr>
<tr>
<td>( \varepsilon_{x1} )</td>
<td>r_1*0.01</td>
</tr>
<tr>
<td>( \varepsilon_{y1} )</td>
<td>r_1*0.01</td>
</tr>
<tr>
<td>( H_2 )</td>
<td>((2^*r_1)**2.0-((r_1+e_2/2.0)**2.0)**2.0)**0.5</td>
</tr>
<tr>
<td>( E_1 )</td>
<td>200.0e7 Pa</td>
</tr>
<tr>
<td>( n_1l )</td>
<td>0.2</td>
</tr>
<tr>
<td>( g_1 )</td>
<td>9.81 m/s²</td>
</tr>
<tr>
<td>( \rho_1 )</td>
<td>20000.0 kg/m³</td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>3.0e-6 kg/m/K</td>
</tr>
<tr>
<td>( \Delta T_1 )</td>
<td>250.0 K</td>
</tr>
<tr>
<td>( \mu_1 )</td>
<td>0.5</td>
</tr>
<tr>
<td>( n_{seu} )</td>
<td>1.0</td>
</tr>
<tr>
<td>( \alpha_{seu} )</td>
<td>10.0</td>
</tr>
<tr>
<td>( \Delta T_1 )</td>
<td>250.0</td>
</tr>
<tr>
<td>( H_1 )</td>
<td>1.0<em>alpha_1</em>\Delta T_1</td>
</tr>
<tr>
<td>( \beta_{seu} )</td>
<td>( H_1 )**3.0</td>
</tr>
<tr>
<td>( t_{contact} )</td>
<td>((4.0/3.0<em>3.14159</em>rho_1*r_1**2.0/E_1)**0.5</td>
</tr>
<tr>
<td>( t_{d} )</td>
<td>((2.0*r_1/g_1)**0.5</td>
</tr>
<tr>
<td>( F_{g} )</td>
<td>( rho_1<em>g_1</em>4.0/6.0<em>3.14159</em>r_1**3.0*(n_1*2.0)</td>
</tr>
<tr>
<td>( delta_{g} )</td>
<td>( 4.0/6.0<em>3.14159</em>r_1**2.0*(n_1*2.0)<em>rho_1</em>g_1/E_1</td>
</tr>
<tr>
<td>( delta_{max} )</td>
<td>( r_1*(H_1-1.0)</td>
</tr>
<tr>
<td>( t_{cycle} )</td>
<td>5000.0*t_{contact}</td>
</tr>
<tr>
<td>( t_{pause} )</td>
<td>t_{cycle}*0.05</td>
</tr>
</tbody>
</table>

**Figure 25: Parameters used for the reference case of Test case 1 in Yade**

The results of the reference case are shown in Figure 26. A graph is showing the ordering of the time scales and interpenetrations. The displacement of particles is quite regular, whereas the force evolution shows some unidentified vibrations (that are explained later in part 4.10).

Results obtain for several variations of the parameters are presented in Figure 27. It would be long to detail everything here, but we can retain the main conclusions of this study:

- The variation of the parameters are acting as expected by the theoretical equations written in the previous part;
- We see that if the proposed conditions to keep some physical meaning for the time scales are satisfied, the problem is well integrated (see green or red links between parameters), i.e. the curves are quite stables;
- Some unexpected vibrations appear, they are amplified when the parameters lead to unphysical behavior, but they still exist when parameters are in an acceptable physical range.
Figure 26: Results from the reference case
Reference case (t_cycle=5000, t_contact)

Case 1: slower cycling (10000)

Case 2: faster cycling (1000)

Case 3: very slow cycling (50000)

Case 4: very slow cycling but dt higher (50000, dt*10)

Case 5: faster cycling and Ex10 (t_cycle√10) (compared to Case 2)
4.10 Test case 2 on Yade

In order to understand the vibration, we have worked on a single particle system.

4.10.1 Geometry studied

The studied geometry is presented in Figure 28.
4.10.2 Simulations

The response to a sudden particle size increase (Figure 29) and to a continuous particle size increase (Figure 30) have been simulated. We can see that the oscillating mode of the system is activated, even with a continuous applied particle swelling (i.e. a continuous displacement applied), whereas we could expect that this solicitation mode can provide a solution where the particle speed is constant and equal the swelling speed. This stable solution can only theoretically obtained if the initial speed of the particle equals the speed imposed by the particle swelling, which can statistically never be the case in simulation of several particle packing.

So these vibrations cannot be avoided, but their amplitude can be limited. In next paragraph we propose a way to limit them.

Figure 29: Response to a sudden small particle size increase

Figure 28: One single particle movement geometry studied
4.10.3 Proposed condition to limit vibrations.

4.10.3.1 Solving the problem (without damping)

The problem without damping can be solved analytically. The equation to solve is:

\[ m \frac{d^2y}{dt^2} = -k(y - y_0) \]  \hspace{1cm} (Eq. 58)

Which gives:

\[ \frac{d^2y}{dt^2} + \omega^2 y = \omega^2 2 \delta \dot{r} \cdot t \]  \hspace{1cm} (Eq. 59)

With \( \delta \dot{r} = \dot{r} \) is constant, \( y_0 = 2 \dot{r} \cdot t \) with \( t = 0 \) at beginning of swelling.

Solution of this equation can be:

\[ y = A \cos(\omega t + B) + 2 \dot{r} \cdot t \]  \hspace{1cm} (Eq. 60)

At \( t=0 \), if we consider an initial speed of \( 2 \dot{r} \), we have:

\[ y = y_0 = 0 \]  \hspace{1cm} (Eq. 61)

\[ \dot{y} = 0 \]  \hspace{1cm} (Eq. 62)

This gives:

\[ B = \frac{\pi}{2} \]  \hspace{1cm} (Eq. 63)

\[ A = \frac{2 \dot{r}}{\omega} \]  \hspace{1cm} (Eq. 64)
The solution is thus:

\[ y = 2r \left( \frac{1}{\omega} \cos \left( \omega t + \frac{\pi}{2} \right) + t \right) \]  

(Eq. 65)

with:

\[ \omega = \frac{2\pi}{T} = \frac{1}{t_{\text{contact}}} \]  

(Eq. 66)

And:

\[ T = 2\pi \sqrt{\frac{m}{k}} \]  

(Eq. 67)

The amplitude can be written:

\[ 2A = 4\dot{r}t_{\text{contact}} \]  

(Eq. 68)

This is what has been measured in Yade.

The force oscillation is:

\[ F_{\text{oscill}} = m\ddot{y} = -mA\omega^2 \cos \left( \omega t + \frac{\pi}{2} \right) \]  

(Eq. 69)

The amplitude is:

\[ F_{\text{amp}}^{\text{oscill}} = 2mA\omega^2 = 4m\dot{r}t_{\text{contact}}\omega^2 \]  

(Eq. 70)

Replacing variable by their expression as function of primitive variables:

\[ F_{\text{amp}}^{\text{oscill}} = 8\rho r^2 \dot{r} \sqrt{\frac{E}{\rho}} \]  

(Eq. 71)

(which is homogeneous to a force : kg.m.s$^{-2}$)

Replacing \( \dot{r} \) by its value as a function of \( t_{\text{cycle}} \):

\[ F_{\text{amp}}^{\text{oscill}} = 8\rho r^3 2^{(h-1)} \frac{(h-1)}{t_{\text{cycle}}} \sqrt{\frac{E}{\rho}} \]  

(Eq. 72)

4.10.3.2 Proposed condition

In order that the oscillation does not disturb the simulation, we have to ensure:

\[ F_{\text{amp}}^{\text{oscill}} < F_g \]  

(Eq. 73)

We recall that:

\[ F_g = 2n_p \rho g r^3 \frac{\pi}{3} \]  

(Eq. 74)

This conducts to the minimum limit value for \( t_{\text{cycle}} \):

\[ t_{\text{oscill}}^{\min} = \frac{9(h-1)}{n_p g} \sqrt{\frac{E}{\rho}} \]  

(Eq. 75)

Let remark that:

\[ t_{\text{oscill}}^{\min} = 4 \frac{t_{\text{cycle}}^{\min}}{n_p g} \]  

(Eq. 76)

So the condition on the oscillation time \( t_{\text{oscill}}^{\min} \) is more conservative than the condition on the gravity interpenetration \( t_{\text{cycle}}^{\min} \), but in general case with a significant number of particles, the inertia time \( t_{\text{cycle}}^{\min} \) stays more conservative.
4.11 Test case 3 on Yade

In order to be more representative and to test the integration in a more complex problem, but still with a few particles to have short calculation times, another test case has been implemented.

4.11.1 Geometry studied

The geometry is shown on Figure 31.

![Figure 31: A 14 particle 2D geometry to further test the integration parameters. On right, geometrical parameters](image)

4.11.2 Results

The Figure 32 show some results when varying the contact stiffness between particles. It can be seen that the force evolution is quite different. When the stiffness is high, the maximum force is reached quickly, whereas for a low value of the stiffness, the ramp slope to attain the maximum force is decreasing, and for very low stiffness, the plateau disappears. This has been summarized on the following figures (Figure 33, Figure 34, Figure 35). It clearly shows that there is a transition between two deformation modes. When E is low, the particle pile is acting like a soft media that can absorb the swelling mismatch between the container and the particles. But when E is increasing, the force increases, and at some point, the global volume of particles is able to slide on the container walls, so that the volume mismatch between particles and the container is transformed into a global volume change of the particle pile. It has to be remarked that this happens approximately when the recorded interpenetration is becoming lower than the radial increase of a particle.

Changing the parameters (g, µ (friction), e1) is changing the critical value of the stiffness. But if we have a look to the calculation time, it does not change at all. If the sliding mode is desired, there is a minimum calculation time involved (see Figure 36)

We think that the physical situation is the sliding mode, with some small interpenetration between particles. This situation is correlated with a high calculation time, and this seems quite unavoidable.
Figure 32: Results for the simulation of test case 3 with a variation of the contact stiffness between particles. The graph in the middle shows the force evolution versus time. The graphs on right side shows a zoom on the force evolution just after the maximum force is attained (just after the swelling period). A graph is also indicating the intensity of the normal contact forces between the particles and the container.
Figure 33: Evolution of the maximum force ($F_{swell}$) and the minimum force ($F_{shrink}$) as a function of the contact stiffness $E$. The values of the maximum interpenetration is also compared to the value of the particle radius increase when swelling. Calculation time is plotted against the contact stiffness $E$.

$g=9.81$, $\mu=0.25$

Figure 34: Same kind of evolution than in Figure 33 but with other physical parameters.

$g=9.81$, $\mu=0.125$
Figure 35: Same kind of evolution than in Figure 33 but with other physical parameters

Figure 36: Evolution of the maximum force (divided by the varied parameters) plotted against the calculation time for different parameters

g=98.1 ; \mu=0.25
4.11.3 Toward a good choice for the particle contact stiffness and other parameters to reduce calculation time

Now there is the question of choosing the right parameters, especially the right contact stiffness to be in the sliding regime, but not too high in order to avoid useless calculation time.

4.11.3.1 Choice of the security factor in terms of time stepping

Some calculations (not shown here) have indicated that for the parameters given in Figure 37, the security parameters

- \( n_{\text{secu}} = 1.0 \)
- \( n_{\text{cycle\_steps}} = 2.0 \)

permit to have a good integration of the problem (the method was to decrease these parameters until the solution is becoming unstable)

\[
\begin{align*}
\text{n\_levels} &= 4 \\
n_{\text{secu}} &= 1.0 \\
n_{\text{cycle\_steps}} &= 2.0 \\
\text{Figure 37: Chosen parameters}
\end{align*}
\]

4.11.3.2 Choice of an optimal contact stiffness

For all the calculation done, when looking at \( \frac{\delta l_{\text{max}}}{\delta l_g} \) apparently it comes that the sliding (bed swelling) mode appears when:

\[ \delta l_{\text{max}} \approx 5 \delta l_g \]  

(Eq. 77)
In order to be sure that the sliding mode is ensured, this criterion has to be respected:

$$\delta l_{\text{swell}} > 2 \times \delta l_{\text{max}} \approx 2 \times 5 \times \delta l_g$$  \hspace{1cm} (Eq. 78)

With:

$$\delta l_g = 2r^2_{\text{moy}} n_p \frac{pg}{E}$$  \hspace{1cm} (Eq. 79)

$$\delta r_{\text{swell}} = r_{\text{moy}}(h - 1)$$  \hspace{1cm} (Eq. 80)

by using general security factors $\zeta_{\text{inter}} = 2$ and $\zeta_{\text{max}+g}$ it comes the criterion:

$$\frac{E}{\rho \cdot g \cdot r_{\text{moy}}} > \frac{2 \zeta_{\text{inter}} \zeta_{\text{max}+g} n_p}{h - 1}$$  \hspace{1cm} with $\zeta_{\text{inter}} = 2$ and $\zeta_{\text{max}+g} = 5$

**4.11.4 Proposition of an improved integration scheme**

In Sassine 2018, the integration algorithm follows this scheme:

1. increase particle size corresponding to 1°C;
2. find equilibrium of forces;
3. go to step 1.

This scheme is introducing large perturbation steps, and this may cause divergent calculations, or at least less stable calculations, potentially coupled with a higher calculation time.

In this work, we propose to have a progressive deformation of the particles, at each time step, the particle size is increased by a small increment. So the integration scheme is:

1. cycling time according to $t_{\text{cycling}} = 4n_p(h-1) \frac{E}{g} \sqrt{\rho'}$;
2. particle size increase by $\dot{r} \cdot \Delta t$;
3. let the simulation run straight, forces are calculated classically with the Verlet algorithm at each time step.

A test case has been performed with the same parameters as those used by Sassine. Results are presented on Figure 39. The solutions found are the same, except that:

- N. Sassine integration gives a more noisy solution;
- N. Sassine calculation time is 68 the calculation time of our algorithm.

---

**Figure 38: Evolutions of variation of main parameters with contact stiffness**
4.12 Test case 4 on Yade: Breathing of a 1600 particle column of particles

In order to further check about all of our hypothesis, a representative problem with a sufficient number of particles has been tested.

4.12.1 Geometry studied and parameters

A cylinder with a particle bed with a high slenderness ratio ($S_r=H/D$) have been constructed. The particle diameter is $d=25\pm10$ mm (randomly distributed). The diameter of the container is $D=7x d = 175$ mm. The height of the pile is approximately $H \sim 1300$ mm. The slenderness ratio is thus: $S_r=1300/175 = 7.4$.

Les parameters used in the simulations are listed in Table 8.
### Table 8: Parameters used in Test case 4

<table>
<thead>
<tr>
<th>#-------- Geom parameters (S.I. units)</th>
<th>#-------- Numerical parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>r1 = 12.5e-3</td>
<td>dp1 = 0.5</td>
</tr>
<tr>
<td>rFuzz = 0.4</td>
<td>n_secu = 1.0</td>
</tr>
<tr>
<td>R1 = 7.0*r1</td>
<td>n_cycle_steps = 3.0</td>
</tr>
<tr>
<td>H1 = 30.0*R1</td>
<td></td>
</tr>
<tr>
<td>epsi1 = r1*0.001</td>
<td></td>
</tr>
<tr>
<td>n1 = 10</td>
<td></td>
</tr>
<tr>
<td>N2 = 0.2*R1</td>
<td></td>
</tr>
<tr>
<td>nb_part = 2500</td>
<td></td>
</tr>
<tr>
<td>n.s_slice = 6</td>
<td></td>
</tr>
<tr>
<td>n.s_surf = 5</td>
<td></td>
</tr>
<tr>
<td>#-------- Physical parameters (S.I. units)</td>
<td>#-------- Times calculations</td>
</tr>
<tr>
<td>E1 = table.E1</td>
<td>t_contact = 2<em>r1</em>(rho1/E1)**0.5</td>
</tr>
<tr>
<td>nul = 0.2</td>
<td></td>
</tr>
<tr>
<td>g1 = 9.81 #m/s2</td>
<td>t_g = (2.0*r1/g1)**0.5</td>
</tr>
<tr>
<td>rho1 = 2000.0</td>
<td>F_g = rho1<em>g1</em>4.0/6.0<em>3.14159</em>r1**3.0*n1</td>
</tr>
<tr>
<td>alpha = 9.0e-6</td>
<td>deltal_g = 2.0<em>r1**2.0</em>np1<em>rho1</em>g1/E1</td>
</tr>
<tr>
<td>DT = 250.0 # K</td>
<td></td>
</tr>
<tr>
<td>frict1 = 0.25</td>
<td>t_g_cycling_min = 2*(h1-1.0)/n1*(E1/rho1)**0.5</td>
</tr>
<tr>
<td>alpha1 = 9.0e-6</td>
<td>t_inertia_cycling_min = 4.0*(h1-1.0)<em>n1</em>(E1/rho1)**0.5</td>
</tr>
<tr>
<td>DT1 = 250.0</td>
<td>t_oscill_cycling_min = 4.0*t_g_cycling_min</td>
</tr>
<tr>
<td>h1 = 1.0+alpha1*DT1</td>
<td>t_cycle = n_cycle_steps*t_inertia_cycling_min</td>
</tr>
<tr>
<td>beta1 = h1**3.0</td>
<td>t_pause = t_cycle*0.025</td>
</tr>
</tbody>
</table>

4.12.2 Results

Several simulation have been performed, with varying the contact stiffness $E$. For each calculation, the initial construction of the pile is renewed. Approximately 1600 particles can randomly fit in the allowed space before pluviation. A summary of the done is given in Table 9. We had also to go further with the cycle number as solution for high $E$ are much more noisy and seems to need more cycles to exhibit a stabilized behavior.

Looking at Figure 41, all the simulations exhibit a densification behavior of the granular bed as cycling progresses. A stabilized state is not reached, even for simulations with a high cycle number of 20.

The Figure 42 is showing the evolution of the (sum of the) forces on the cylinder and the base of the container. They follow the same kind of evolution (their values are different as the surface on which they are calculated are not the same, $S_{base}$< $S_{cylinder}$). For the low value of $E$, the evolution is quite regular (not noisy) and follow a sort of triangle evolution, which corresponds to a pronounced elastic mode described in section 4.11.2. As $E$ is increasing, the force signal is becoming more and more noisy, and the evolution shows a force return to zero when unloading happening in a shorter time (the triangle signal is less and less a triangle). A fast return to zero force goes along a non purely elastic deformation mode. The question is then: is it a purely sliding mode ? To try to answer this question it would be nice to see if a transition exists when varying the stiffness $E$. For this we plotted the maximum forces (see Figure 43 and Figure 44) to see whether we reach a constant value of the forces registered on the container walls after a certain value of $E$, like the one observed in 4.11.2.

This observation is not easy to do as when increasing $E$:

- The signal is becoming more and more noisy, probably because the pile of particle is becoming more and more unstable;
- There is a need to perform a high cycle number in order to reach a steady state, and this fact, together with the fact that taking high stiffness values $E$ is leading to quite long calculation times. For example, a simulation involving a $E$=100e8 Pa stiffness for 20 cycles is taking 40 days (1.3 month). See Figure 45.

Nevertheless, we have tried to plot the evolution of the maximum pressure ($F_{max}/S$) applied by the particles to the container as a function of $E$ in Figure 46. This exhibits that the pressure seems to show a saturation value, but the uncertainty is high and the force does not exactly shows a steady state.
Some other complementary simulation are running at the moment to strengthen this evolution (with a higher stiffness $E=200e8$, and with more cycles). Their individual duration is approximately 2.5 months.

<table>
<thead>
<tr>
<th>TC01</th>
<th>$E=1e8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC02</td>
<td>$E=5e8$</td>
</tr>
<tr>
<td>TC03</td>
<td>$E=10e8$</td>
</tr>
<tr>
<td>TC04</td>
<td>$E=1e8$</td>
</tr>
<tr>
<td>TC05</td>
<td>$E=5e8$</td>
</tr>
<tr>
<td>TC06</td>
<td>$E=10e8$</td>
</tr>
<tr>
<td>TC07</td>
<td>$E=50e8$</td>
</tr>
<tr>
<td>TC08</td>
<td>$E=1e8$</td>
</tr>
<tr>
<td>TC09</td>
<td>$E=5e8$</td>
</tr>
<tr>
<td>TC10</td>
<td>$E=10e8$, n_cycle_todo = 10.0</td>
</tr>
<tr>
<td>TC11</td>
<td>$E=50e8$</td>
</tr>
<tr>
<td>TC12</td>
<td>$E=1e8$, np1 = 100</td>
</tr>
<tr>
<td>TC13</td>
<td>$E=5e8$, np1 = 100</td>
</tr>
<tr>
<td>TC14</td>
<td>$E=50e8$, n_cycle_todo = 10.0</td>
</tr>
<tr>
<td>TC15</td>
<td>$E=100e8$, n_cycle_todo=10.0</td>
</tr>
<tr>
<td>TC16</td>
<td>$E=10e8$, n_cycle_todo = 5.0, np1=100</td>
</tr>
<tr>
<td>TC17</td>
<td>$E=50e8$, n_cycle_todo = 20.0</td>
</tr>
<tr>
<td>TC18</td>
<td>$E=10e8$, n_cycle_todo = 20.0</td>
</tr>
<tr>
<td>TC19</td>
<td>$E=100e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC20</td>
<td>$E=50e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC21</td>
<td>$E=1e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC22</td>
<td>$E=5e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC23</td>
<td>$E=10e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC24</td>
<td>$E=50e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC25</td>
<td>$E=100e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC26</td>
<td>$E=50e8$, n_cycle_todo=20.0</td>
</tr>
<tr>
<td>TC27</td>
<td>$E=100e8$, n_cycle_todo=20.0</td>
</tr>
</tbody>
</table>

Table 9: Performed calculations ($E$ is in Pa, np1 has been varied sometimes to evaluate its effect); “TC” means Test Case
Figure 41: Evolution of the pebble bed height variation and the porosity along cycling
Figure 42: Evolution of the sum of the forces recorded on the cylinder of the container and on the base on the container
Figure 43: Sum of maximum forces on the cylinder of the container (E is in Pa) along cycling

Figure 44: Sum of maximum forces on the base of the container (E is in Pa) along cycling
CONCLUSION AND PERSPECTIVES

As a conclusion, the studies conducted up to now were necessary to really understand what is really calculated when using the Discrete Element Method to model the thermal ratcheting of a granular media. Imbrication of times scales makes the problem difficult in choosing adequate parameters to accelerate the calculation time. The conclusion is that the problem is quite locked, and the calculations time will be long. For example, for the choice of the contact stiffness, we can conclude that this parameter has to be chosen carefully in order to activate preferably the slide mode which
is more physical. This choice was not done according this kind of new rules for the work available in the literature on thermal ratcheting using DEM approach.

The results show the importance of stiffness choice. The sliding mode is surely the calculation mode to aim, as it is closer to physical reality (which is something to ascertain by experimental confrontation). Previous studies on this subject were done ignoring the importance of stiffness choice. They should be checked under the light of our recent results. Next job is to perform simulations more in relation with the geometry of the tank design proposed recently.

Calculations dedicated to the Polyphem’s storage tank have not been performed yet. As explained above, a first step of validation and understanding of DEM tool and how to properly use it was necessary.

Further DEM simulations of thermal ratcheting will be adapted, depending on the choice of the filler for the polyphem’s prototype. The bad news is that the simulation may take a quite long calculation time (months), because of the new rule imposed of the stiffness choice, and the fact that time scales cannot be brought closer
5. ANNEX 2 - CHOICE OF A UNIT SYSTEM WITH DIMENSIONS IN MM

5.1 NEW SET OF PHYSICAL SIZES

There are three equations involving all the parameters:

\[ m_i \frac{d^2 \vec{x}_i}{dt^2} = \sum \vec{F}_i + m_i \vec{g} \]
\[ \vec{F} = k_n \delta l = E \epsilon_{moy} \delta l \]
\[ m = \rho \cdot V \]

Choosing to count \( x \) in mm, new variable \( \bar{x} \) leads to define the other measures as:

\( \bar{x} = 10^3 x \) expressed in [mm] (\( \bar{x} \) is \( x \) multiplied by 1000)

\( \bar{F} = 10^3 F \) expressed in [mN]

\( \bar{g} = 10^3 g \) expressed in [mm.s^{-2}]

\( \bar{E} = 10^{-3} E \) expressed in [kPa]

\( \bar{\rho} = 10^{-9} \rho \) expressed in [kg.mm^{-3}]

Checking: replacing the new variable in the original equation gives:

\[ m_i \frac{d^2 \bar{x}_i 10^{-3}}{dt^2} = \sum \bar{F}_i 10^{-3} + m_i \bar{g} 10^{-3} \]
\[ \bar{F} 10^{-3} = \bar{E} 10^3 \epsilon_{moy} 10^{-3} \delta l 10^{-3} \]
\[ m = \bar{\rho} 10^9 \cdot \bar{V} 10^{-9} \]

This leads to the new set of equations identical to the original one:

\[ m_i \frac{d^2 \bar{x}_i}{dt^2} = \sum \bar{F}_i + m_i \bar{g} \]
\[ \bar{F} = \bar{E} \epsilon_{moy} \delta \bar{l} \]
\[ m = \bar{\rho} \cdot \bar{V} \]

5.2 NUMERICAL APPLICATION

In order to check if dimension changes are all right with the excel calculation sheet:
<table>
<thead>
<tr>
<th>Unités non SI : dimensions in mm</th>
<th>Physical sizes</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>2.00E+08 kPa</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>rmoy</td>
<td>2.00E+03 mm</td>
<td>1.00E+03</td>
</tr>
<tr>
<td>Hbed</td>
<td>3.00E+03 mm</td>
<td>1.00E+03</td>
</tr>
<tr>
<td>g</td>
<td>9.81E+03 mm/s²</td>
<td>1.00E+03</td>
</tr>
<tr>
<td>rho</td>
<td>2.00E-06 kg/mm³</td>
<td>1.00E-09</td>
</tr>
<tr>
<td>alpha</td>
<td>9.00E-06 K⁻¹</td>
<td>1</td>
</tr>
<tr>
<td>DT</td>
<td>2.50E+02 K</td>
<td>1</td>
</tr>
<tr>
<td>h</td>
<td>1.00225E+00</td>
<td></td>
</tr>
<tr>
<td>beta</td>
<td>1.00677E+00</td>
<td></td>
</tr>
<tr>
<td>t_contact</td>
<td>4.09E-06 s</td>
<td></td>
</tr>
<tr>
<td>t_g</td>
<td>6.39E-02 s</td>
<td></td>
</tr>
<tr>
<td>Ratio between the two times</td>
<td>15600</td>
<td></td>
</tr>
<tr>
<td>Masse of a particle</td>
<td>6.70E-02 kg</td>
<td></td>
</tr>
<tr>
<td>Mass of a column of particles</td>
<td>5.03E+00 kg</td>
<td></td>
</tr>
<tr>
<td>Force applied on the base by a column of particles</td>
<td>4.93E+04 mN</td>
<td></td>
</tr>
<tr>
<td>Contact force if totally blocked</td>
<td>1.80E+08 mN</td>
<td></td>
</tr>
<tr>
<td>Ratio between forces</td>
<td>3650.35</td>
<td></td>
</tr>
<tr>
<td>Particle interpenetration delta_l</td>
<td>1.23E-05 mm</td>
<td></td>
</tr>
<tr>
<td>Particle swelling delta_r_swell</td>
<td>4.50E-02 mm</td>
<td></td>
</tr>
<tr>
<td>Ratio between the two delta</td>
<td>3650.35</td>
<td></td>
</tr>
<tr>
<td>modified gravity (to equalize times)</td>
<td>2.39E+12 mmm/s²</td>
<td></td>
</tr>
<tr>
<td>modified elasticity (to equalize interpenetrations)</td>
<td>1.82E+04 kPa</td>
<td></td>
</tr>
</tbody>
</table>
6. ANNEX 3 - RECALL FROM YADE USER MANUAL

The algorithm commonly used in Yade computes normal interaction stiffness as stiffness of two springs in serial configuration with lengths equal to the sphere radii (fig. spheres contact stiffness).

Series of 2 springs representing normal stiffness of contact between 2 spheres.

Let us define distance $l = l_1 + l_2$, where $l_i$ are distances between contact point and sphere centers, which are initially (roughly speaking) equal to sphere radii. Change of distance between the sphere centers $\Delta l$ is distributed onto deformations of both spheres $\Delta l_1 = \Delta l_2 = \Delta l$, proportionally to their compliances. Displacement change $\Delta l_i$ generates force $F_i = K_i \Delta l$, where $K_i$ assures proportionality and has physical meaning and dimension of stiffness, $K_i$ is related to the sphere material modulus $E_i$ and some length $l_i$ proportional to $r_i$.

$$
\Delta l = \Delta l_1 = \Delta l_2
$$

$$
K_1 = \frac{E_1}{l_1}
$$

$$
K_2 = \frac{E_2}{l_2}
$$

$$
K_i = \frac{F_i}{\Delta l_i} = F
$$

$$
K_1 \Delta l_1 + K_2 \Delta l_2 = F
$$

$$
K_1 = \frac{F}{\Delta l_1} = K_i
$$

$$
K_2 = \frac{F}{\Delta l_2} = K_i
$$

$$
K_1 + K_2 = K_i
$$

$$
K_1 l_1 = K_2 l_2
$$

$$
K_1 K_2 = K_i^2
$$

The most used class computing interaction properties $\text{u2}_\text{FockMat} \_\text{FockMat}_\text{FockPhys}$ uses $l_i = 2r_i$.

Some formulations define an equivalent cross-section $A_{eq}$ which in that case appears in the $l_i$ term as $K_i = \frac{E_i l_i}{A_{eq}} = K_i^{eq}$. Such is the case for the concrete model $\text{u2}_\text{ConMat} \_\text{ConMat}_\text{ConPhys}$, where $A_{eq} = \text{sad}(r_1, r_2)$.

For reasons given above, no pretense of equality of particle-level $E_i$ and macroscopic modulus $E$ should be made. Some formulations, such as [Hend2003], introduce parameters to match them numerically. This is not appropriate, in our opinion, since it binds those values to particular features of the sphere arrangement that was used for calibration.
7. REFERENCES

14 N. Sassine, Study of the thermo-mechanical behavior of granular media and interactions medium-tank, These de l’université UGA, France, 2018.
15 https://yade-dem.org/doc/