Pore Scale Simulation of Packed Bed Reactor

Submitted In fulfillment of the requirements of

CHE F266 Study Project

By

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Abstract

The engineering design of packed bed based unit operations is very much influenced by the structure of thee packing matrix, which in turn is governed by the shape, dimensions and the loading of the constituent particles. For, say, reactor applications, optimum design of catalyst pellet in terms of shape configuration, internal pores and available surface area can promote catalytic activity and the prevalent transport properties of the system. In this project we develop an algorithm for packing of bed rectors using BLLENDER v2.7 as a tool for creating a simulation of the dynamics of the packing of the bed in terms of the interactions of the particles with themselves and the walls of the container. A realistic approach to the packing of beds is developed for spheres, spheres with an offset hole, sphere with two symmetric holes and spheres with four symmetric holes.

Rigid Body Simulation

Blender is the free and open source 3D creation suite. It supports the entirety of the 3D pipeline-modelling, rigging, animation, simulation, rendering, composting and motion tracking, even video editing and game creation. Blender v2.76 is a public project. The aim is to develop a packed bed of particles using Blender and get a more realistic approximation of how packing occurs in packed beds. Rigid body simulation module in Blender Physics is used to get a realistic packing. Once a geometry is created for basic spherical shapes, the same procedure can be extrapolated for different catalytic shapes such as cylinders, tri-lobes, etc. Porosity of the packed bed can be calculated by applying a mesh to the system and calculating the proportion of area mesh applied to the voids between the spheres and total mesh area.

The rigid body simulation can be used to simulate the motion of solid objects. It affects the position and orientation of objects and does not deform them. Unlike the other simulations in Blender, the rigid body simulation works closer with the animation system. This means that rigid bodies can be used like regular objects and be part of animation constraints and drivers.

Creating a rigid body:

Mesh objects can participate in the rigid body simulation. To create grid bodies, either click on *Rigid Body* button in the *Physics* tab of the Properties editor or use the *Add Active/ Add Passive* buttons in the *Physics* tab of the *Tool Shelf*.

There are two types of rigid bodies: Active and Passive. Active bodies are dynamically simulated, while passive bodies remain static. Both types can be driven by the animation system when using the animated option. During the simulation, the rigid body system will override the position and orientation of dynamic rigid body objects. Note however, that the location and rotation of the objects is not changed, so the rigid body simulation acts similar to a constraint. To apply the rigid body transformations you can use the Apply Transformation button in the *Physics tab* of the *Tool Shelf*.

Mesh based shapes:

These are calculated based on the geometry of the object so they are a better representation of the object. The center of gravity for these shapes is the object origin.

Convex Hull:

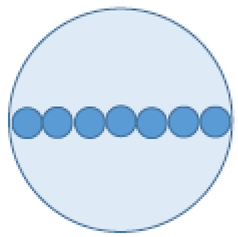
A mesh like surface encompassing (eg. Shrink wrap over) all vertices (best results with fewer vertices). Convex approximation of the object, has good performance stability.

Mesh:

Mesh consisting of triangles only, allowing for more detailed interactions than convex hulls. Allows to simulate concave objects, but is rather slow and unstable.

Simulation can be created for an array of a variety of shapes such as spheres, cylinders, donuts, tri-lobes, etc. For these shapes, N ratio should be considered and should not be very small or large either. N ratio is defined as no of particles placed side by side that can be accommodated on one diameter of the circular base.

Here, N=7



Ideal cases involve where N is between 6 and 8. A high N-number can cause a very loose packing of the bed leading to loss of efficiency while a very high N number corresponds to a very tight packing leading to large number of particles packed creating very large pressure drop across the length of the packed bed.

Algorithm for Bed Packing

Creating an array of numerous cubes crashing down:

- Cube—Settings—Add modifier—Array modifier—increase the count to 10—increase offset to 1.1 on x-axis.

Again,

- Add array modifier—count 10—relative off set=0 in x-axis and 1.1 on y-axis.

Again,

- Add array modifier—count 10—relative off set=0 in x,y-axis and 1.1 on z-axis.

Here, you have obtained 1000 cubes.

- Apply—Apply—Apply—array modifier to all the cubes.
- Now go to edit mode, and observe all as still a single object. Click P—'separate by loose part' to make them all separate objects. Go to object mode and you will have an array of 1000 separate cubes.

Adding Physics:

- Go to physics—rigid body—make weight to about 1000
- In rigid body collisions—select shape as 'mesh'.
- Physics toolbar on the left side of the tools panel and select copy from active to add same physics to all 1000 cubes.

Note: You'll get a green border after application of rigid body to all 1000 cubes.

- Click b and select all the cubes—click G to grab all objects and translate them all to a certain height (z=10)—click R to rotate the cube to a certain angle.

Adding a collision Plane:

- Add a plane from add objects –mesh-plane—Click S to scale the plane to about 10 times the size. This will be used as a platform on which the container will rest.
- Click Tab to go to edit mode and extrude region to add walls—Click X and delete the top face.
- Go to Object mode—Add rigid body—Passive rigid body—Shape Mesh.
- Run the simulation. You can observe some of the cubes passing through the platform which is not plausible and messes up the physics of the entire system.

Correction in the physics:

- Change where the origin of the cubes are.

Follow:

- Z—Wireframe
- B—Select many objects at a time (select entire cube)
- Ctrl+ Alt+ Shift+ C Origin to geometry

This will provide each cube with an origin point.

- Go back to the simulation in object mode and see the cubes shatter on the platform.

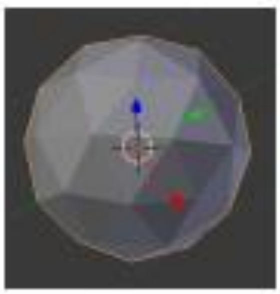
Adding the cylindrical container:

- Add objects—Mesh---Circle and change the coordinates of the circle to 0, 0, 0 on x,y and z axis.
- Click Tab to go to edit mode and extrude the region to get a cylinder
- Go to Physics—Add rigid body—Passive Body—Mesh

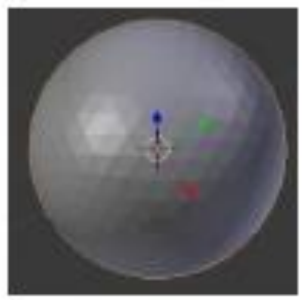
This is done to provide an interaction between the particles falling down and container along with the platform base.

Simulation with Spheres

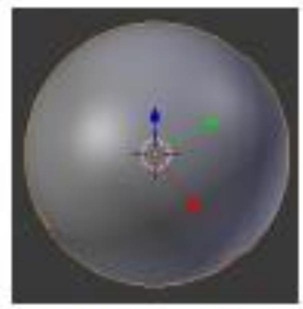
Spheres in blender are created using ico-spheres which are not exactly spheres by a mesh formed by triangles to give a polyhedron. Increasing the subdivisions gives a more spherical shape and fineness to the sphere and the maximum refinement (subdivisions=8) gives a perfect sphere.



subdivisions=2



subdivisions=4



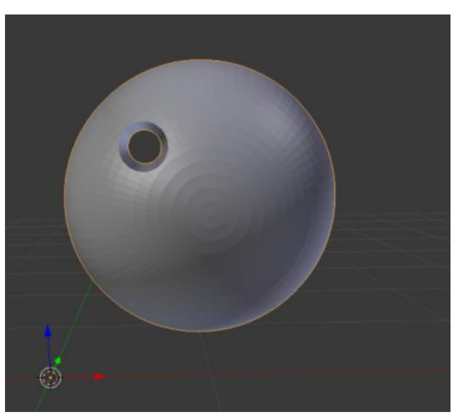
subdivisions=8

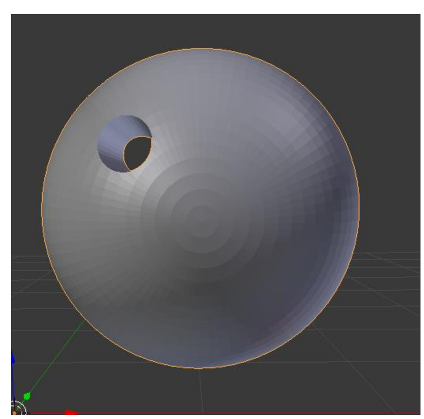
Due to the extreme fineness of the spheres sub-divisions 3 onwards, the rendering of the array creation of around 1000 spheres makes the software to crash.

However, packing was done for spheres of subdivision 3 to test the packing algorithm.

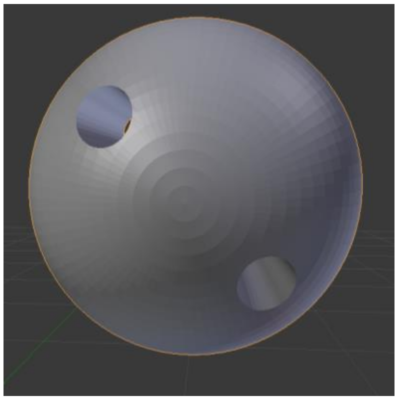
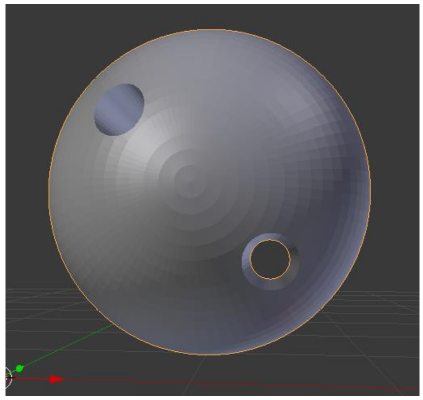
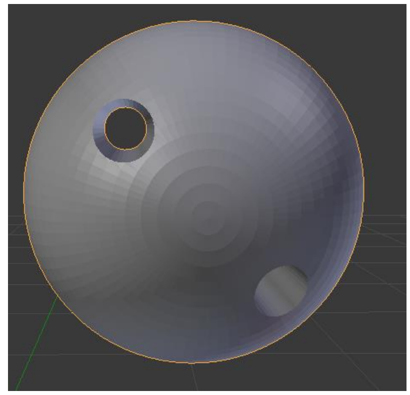
Further, geometries of spheres with holes were created in Solidworks 2016 as .STL files which can be imported to BLENDER for doing manipulations.

1 hole in a sphere with off-set form the center:

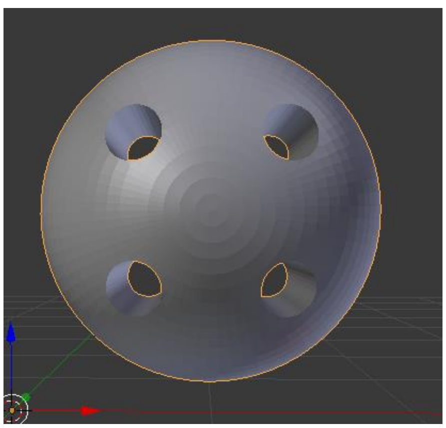
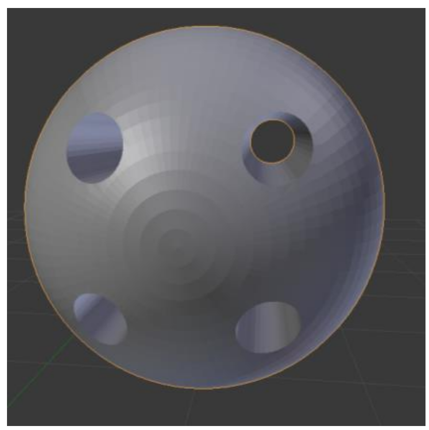




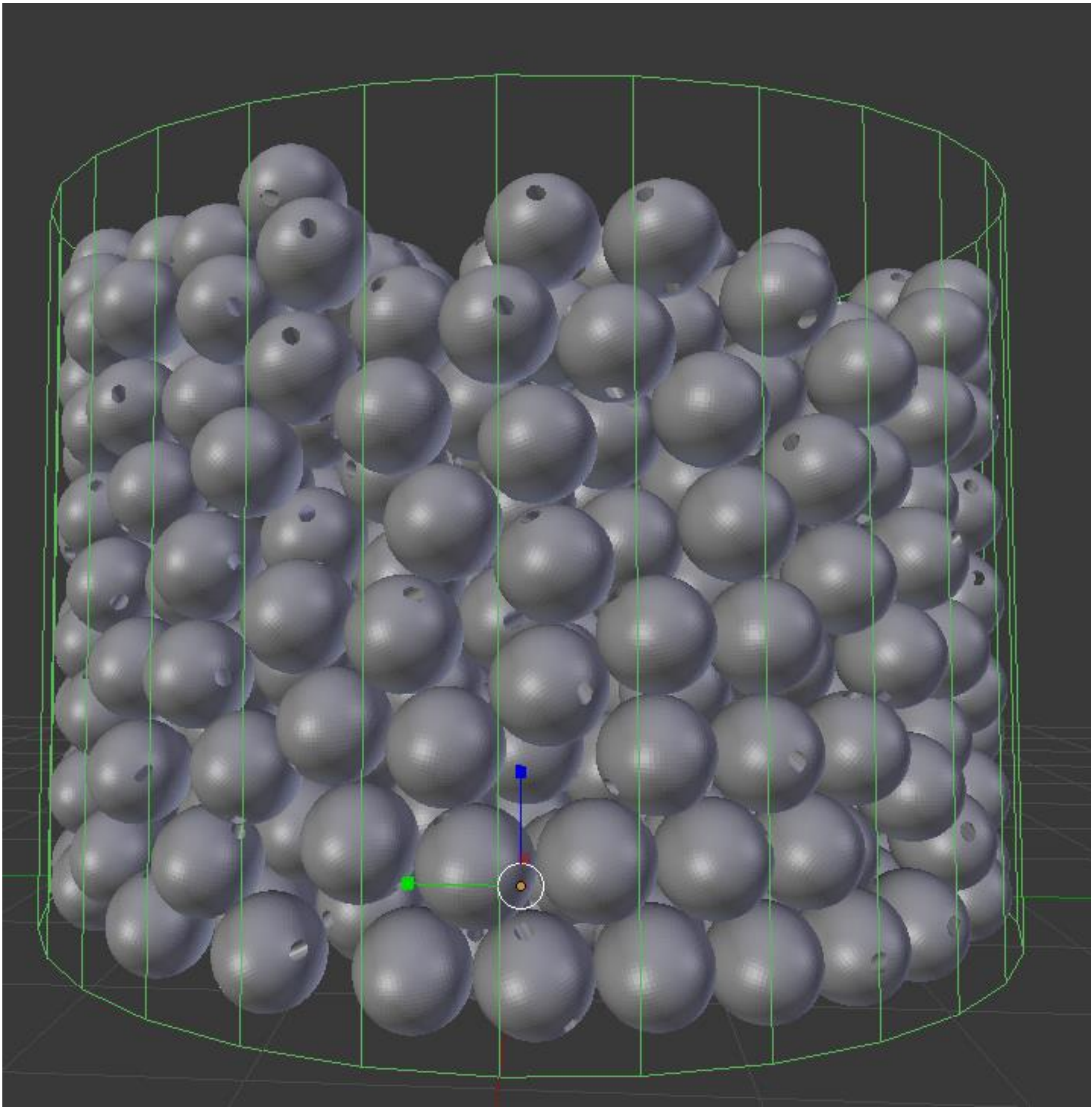
2 symmetric holes in a sphere:

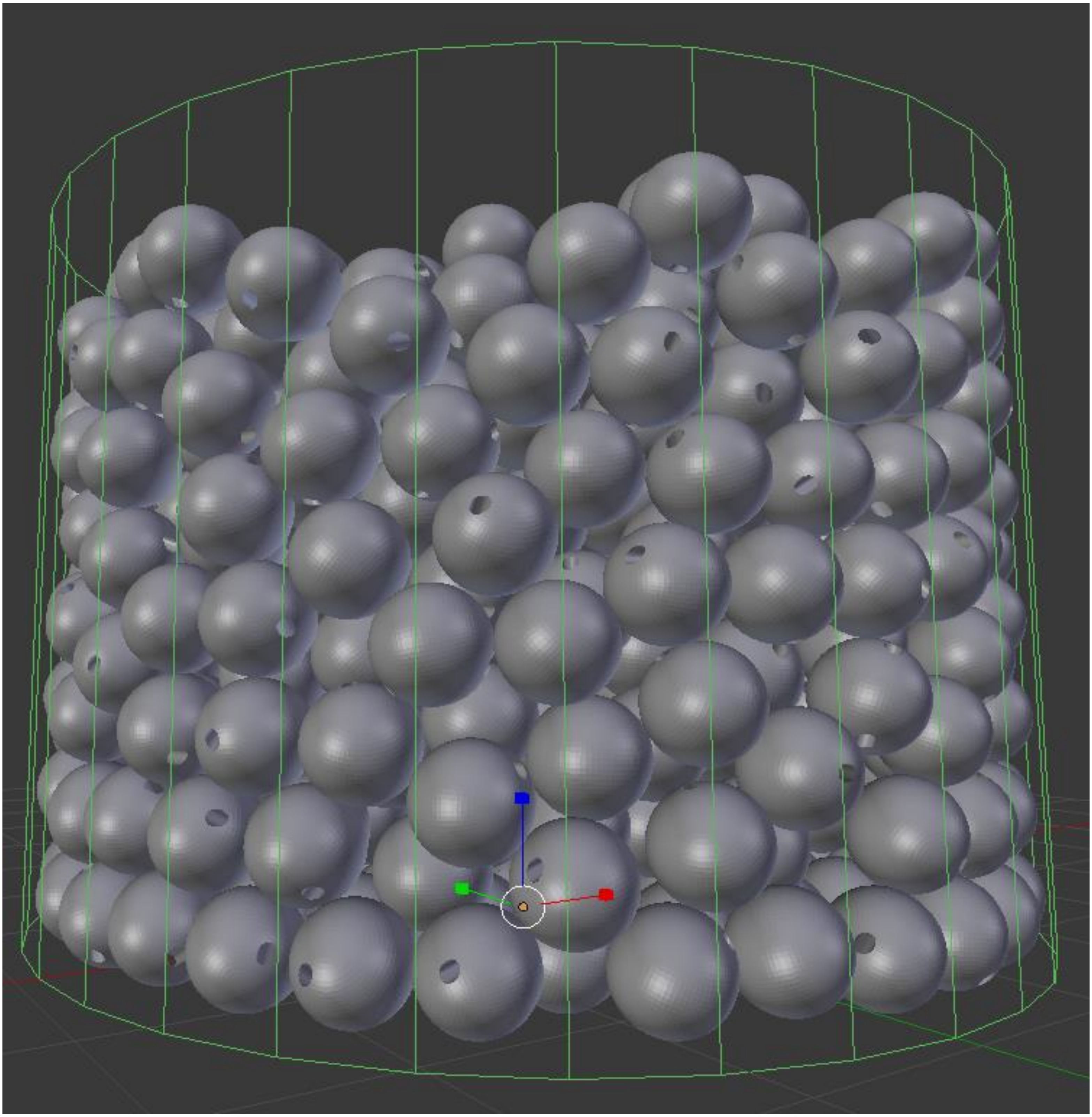




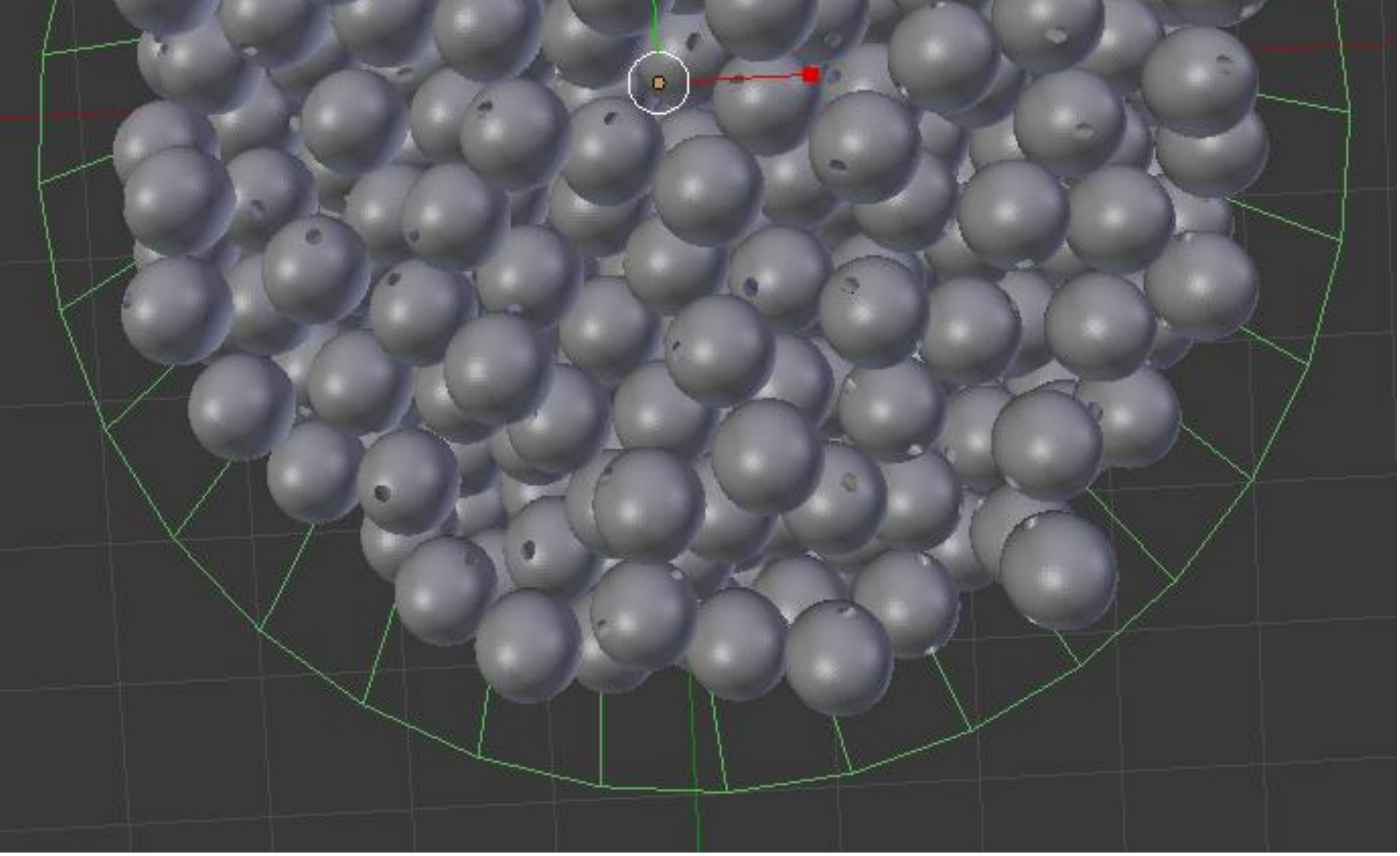
4 symmetric holes in a sphere:

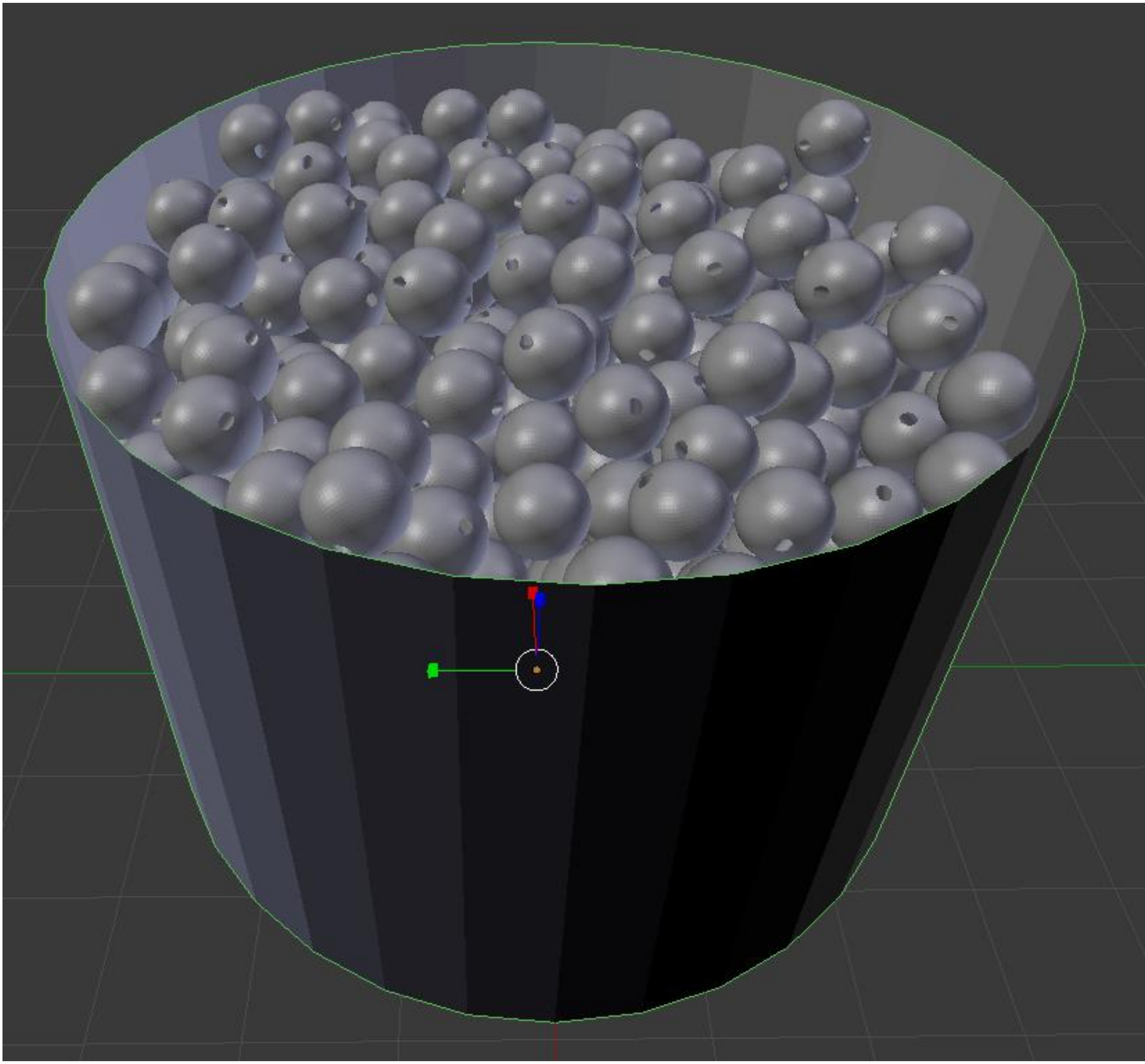



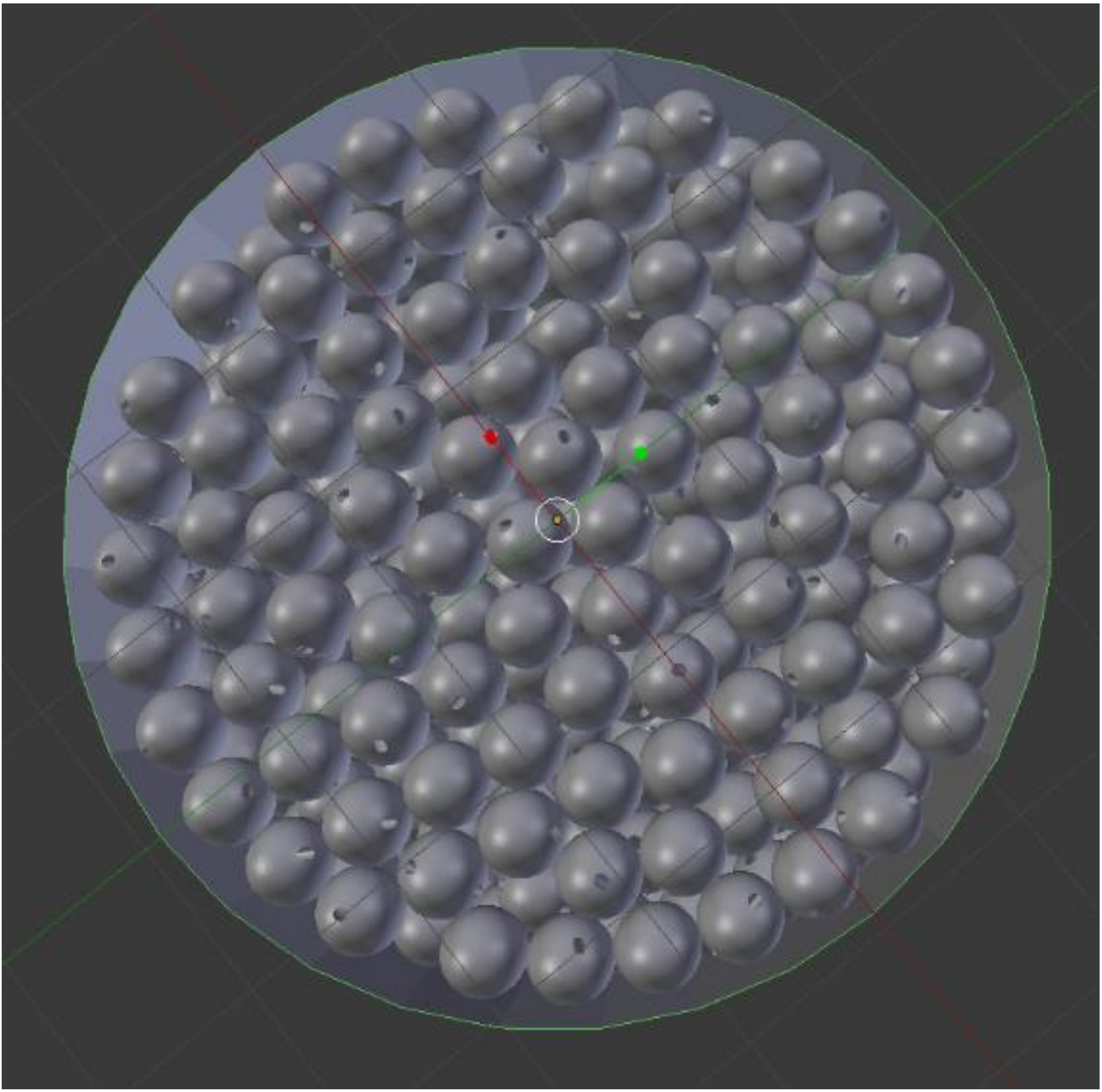
Simulation done for spheres with 1 hole:

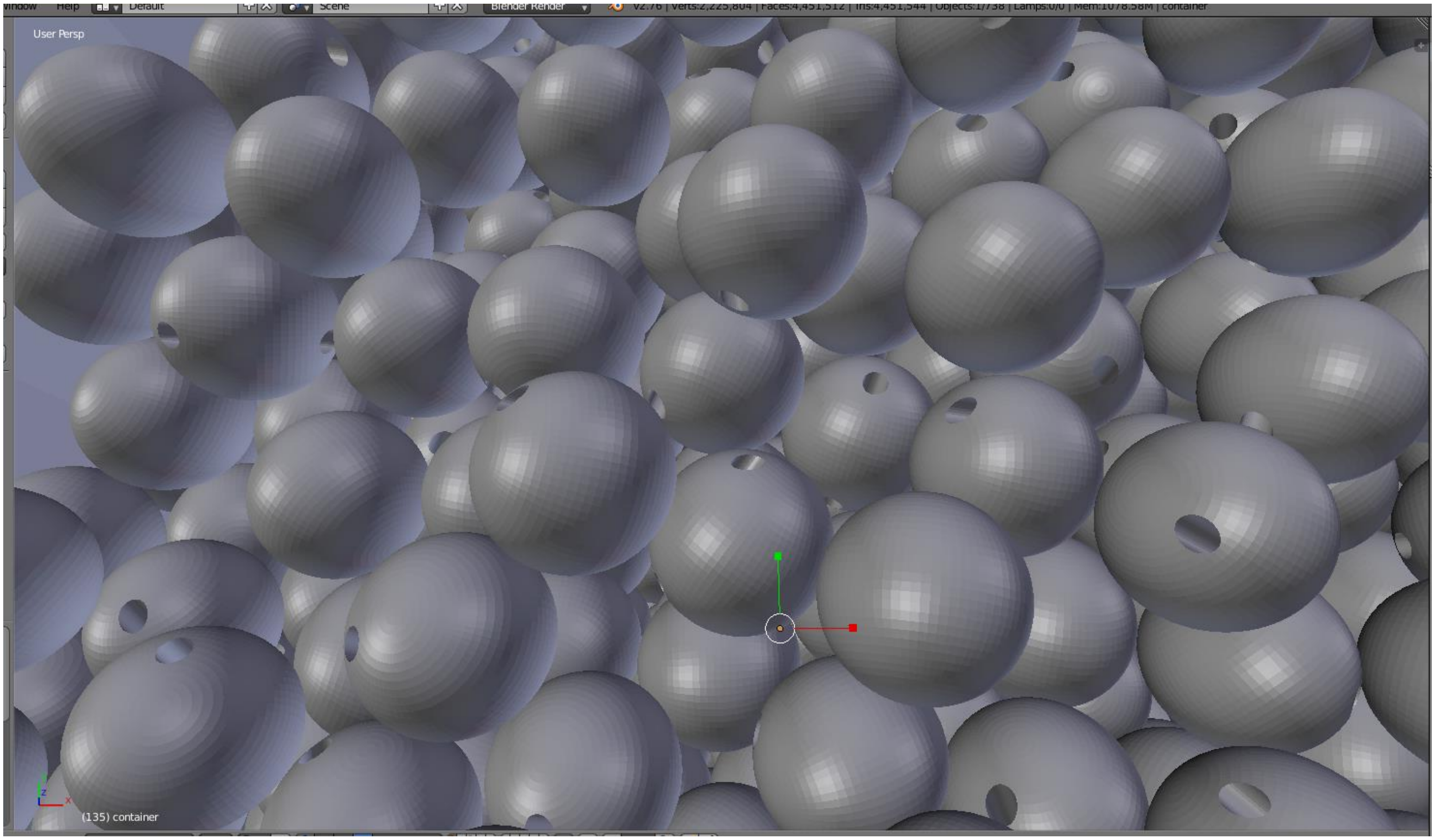






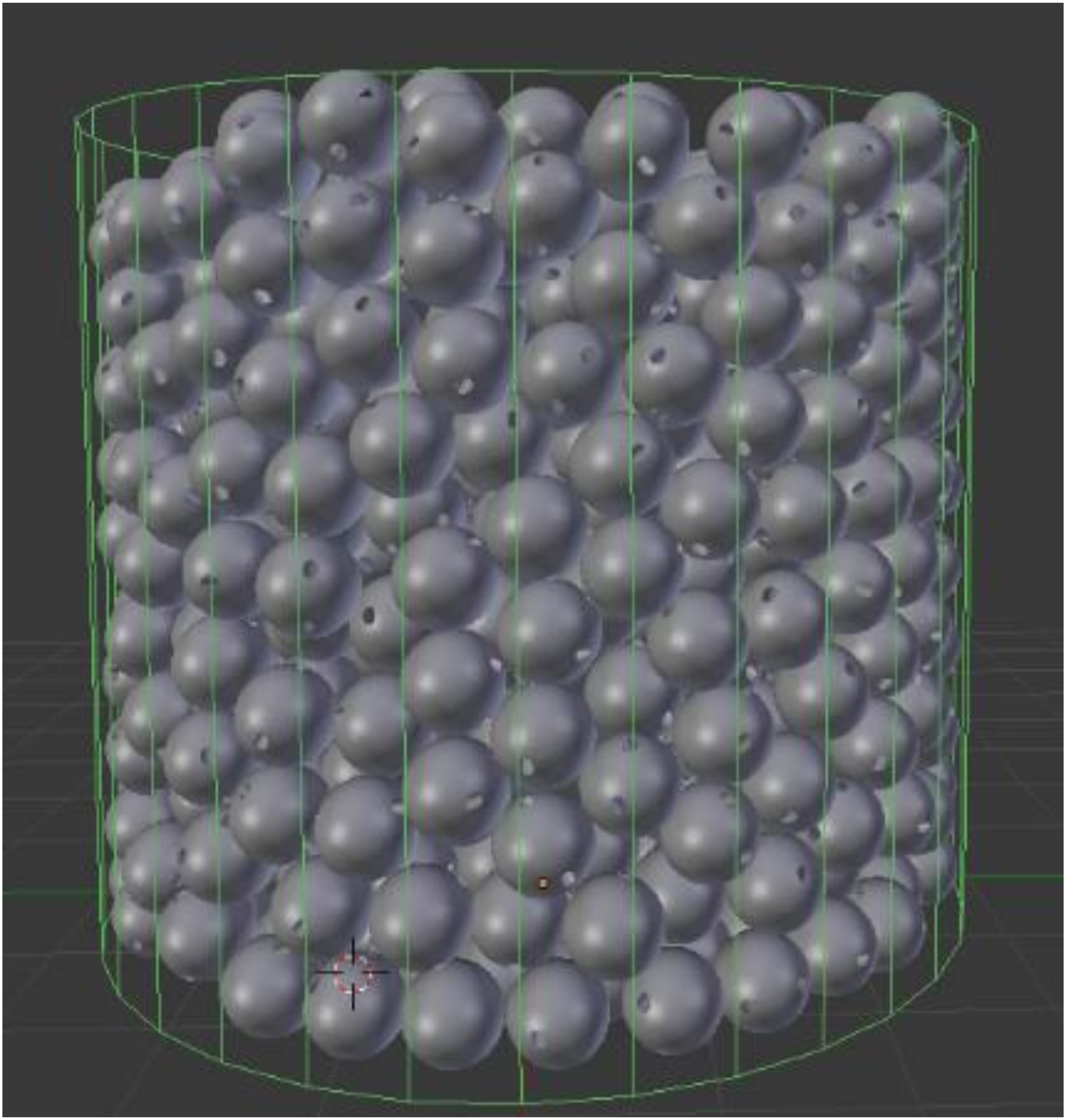


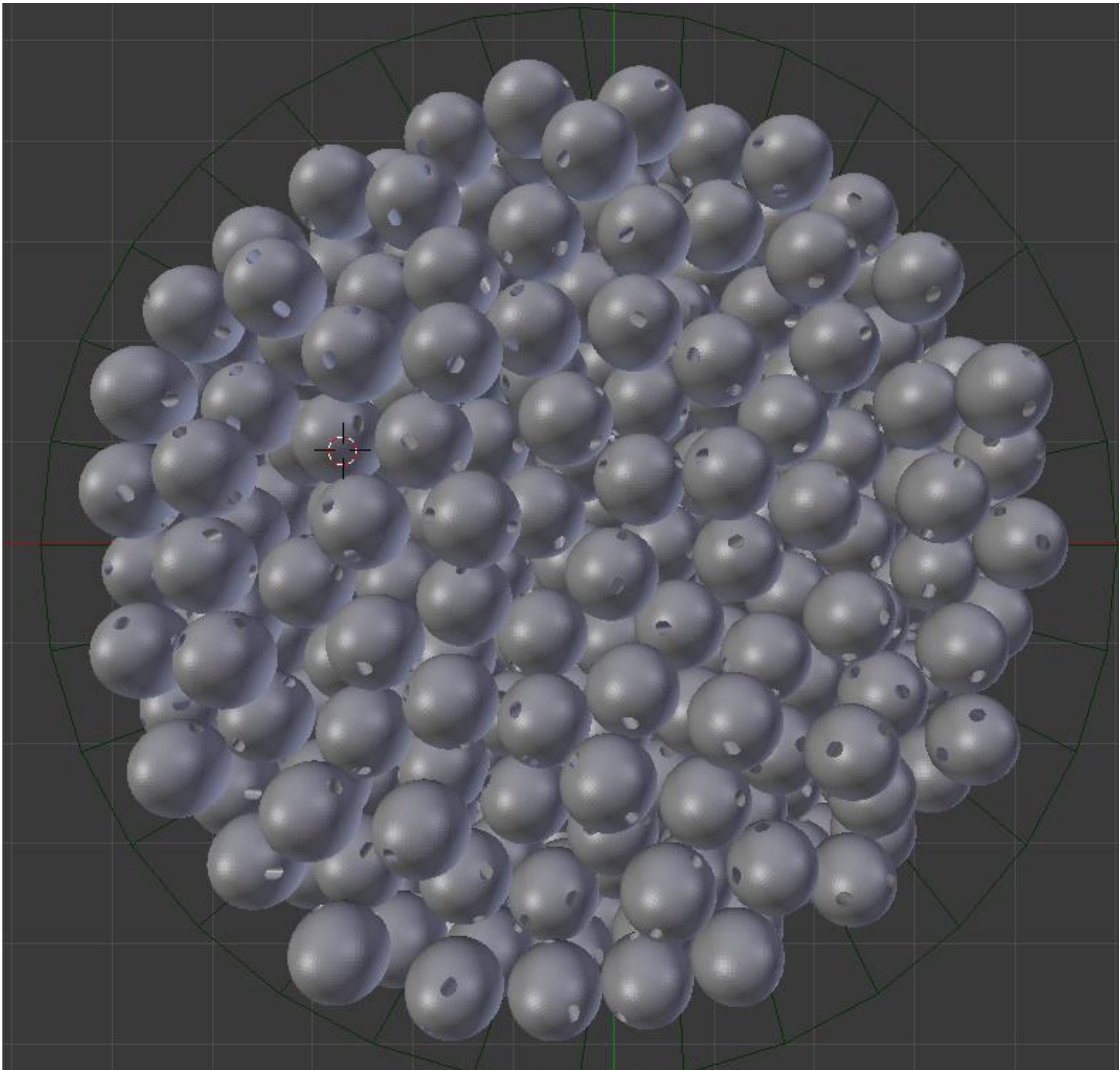


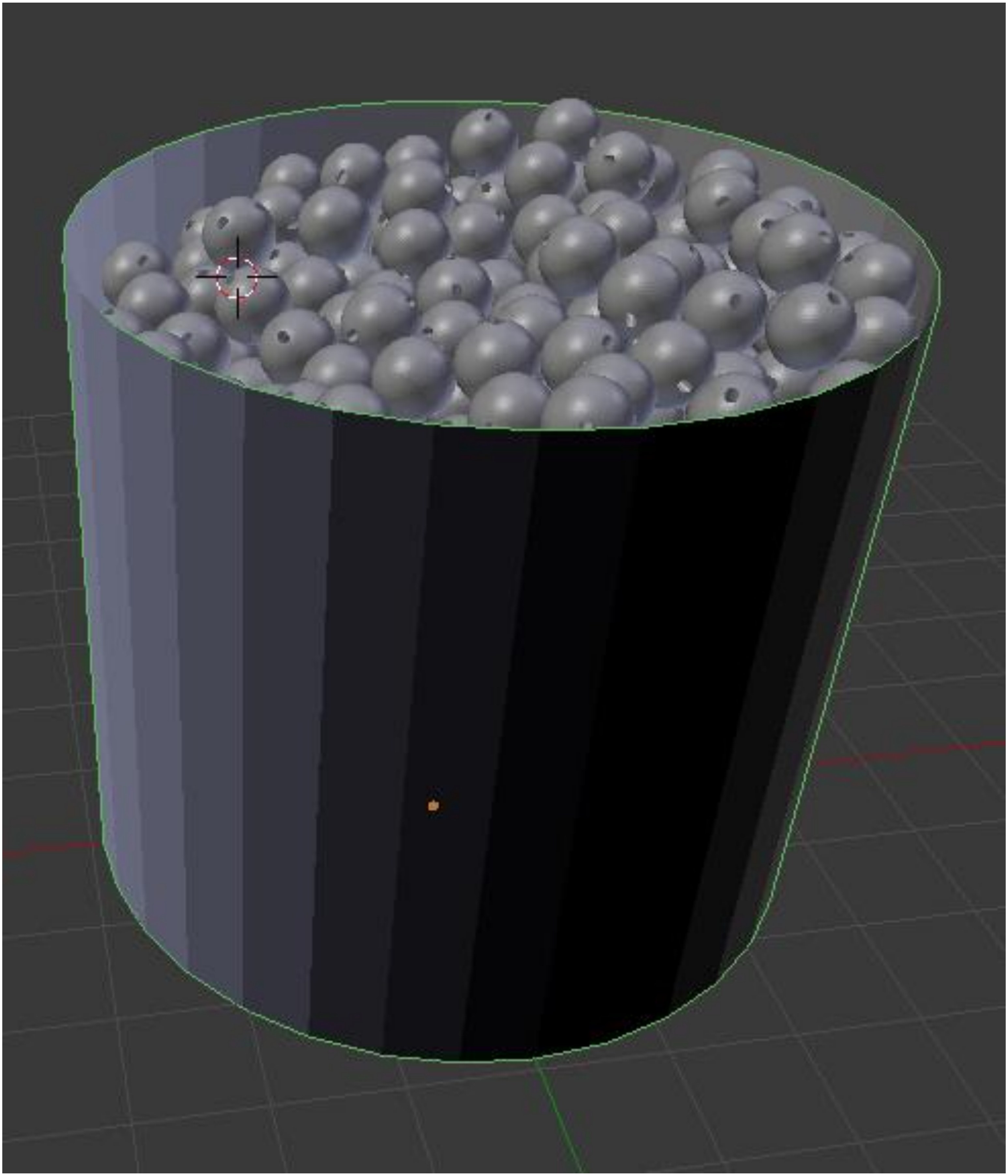


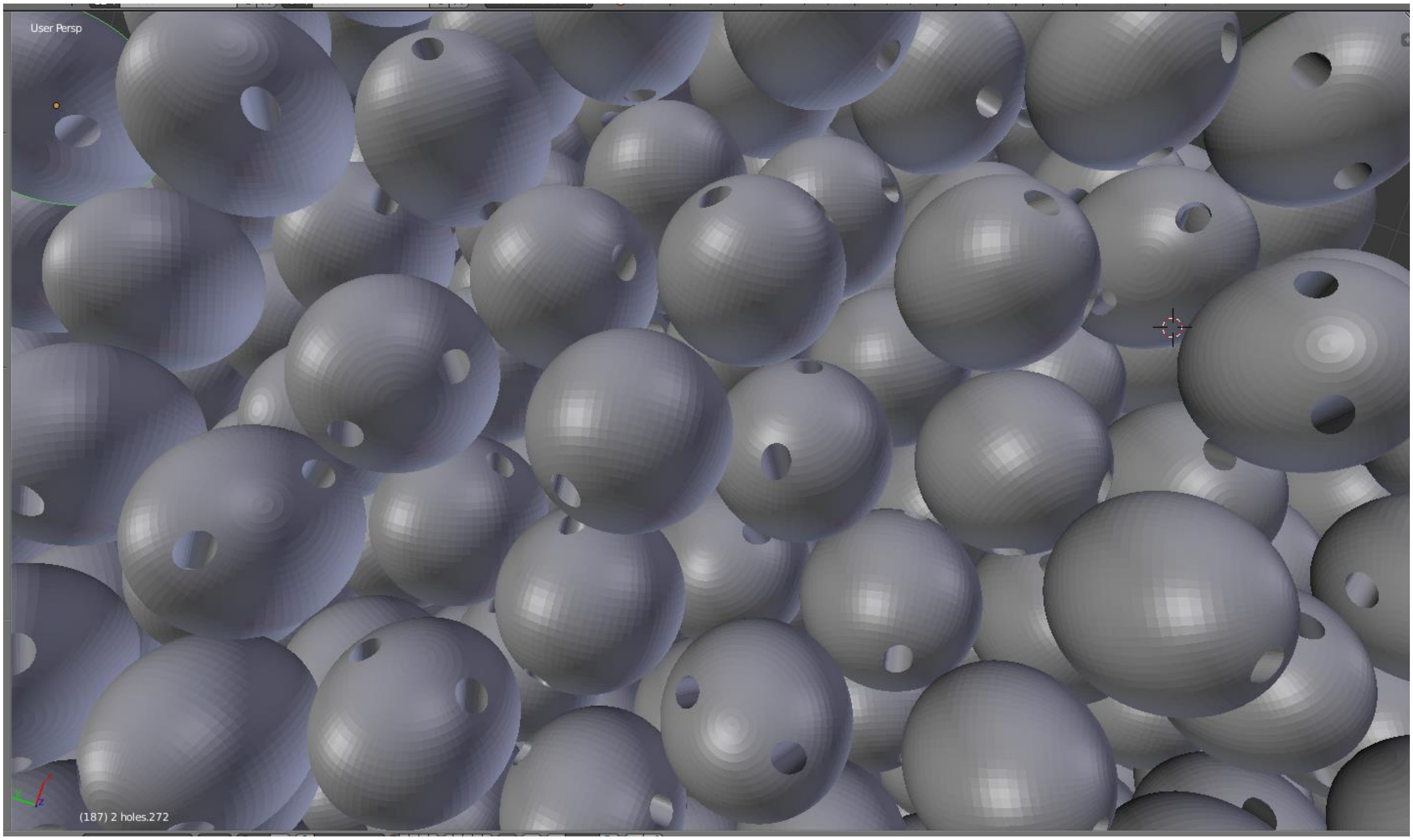
823 spheres are packed for aspect ratio of 5 for the container and N=10 spheres per diameter of container.

Simulation done for spheres with 2 symmetric holes:









861 spheres packed for an aspect ratio of 5 for the container and N=10 spheres per diameter of the container

Rendering geometry in BLENDER v2.76

A simple geometry of sphere with 1 hole (non-symmetric) and 2 symmetric holes are rendered in BLENDER.

The system takes around 4 hours to render the animation for packing a bed of spheres with 1 non-symmetric hole beginning with 1000 spheres and 6 hours to render the animation for packing a bed with 2 non-symmetric holed sphere beginning with 1000 spheres.

Representation in .STL file for 360° view

.STL conversion of files allows a 360 degree view of the packing of the spheres.

Also, if .STL files are not complex enough, can be transferred to the DESIGN MODELLER of ANSYS to perform fluid flow simulation.

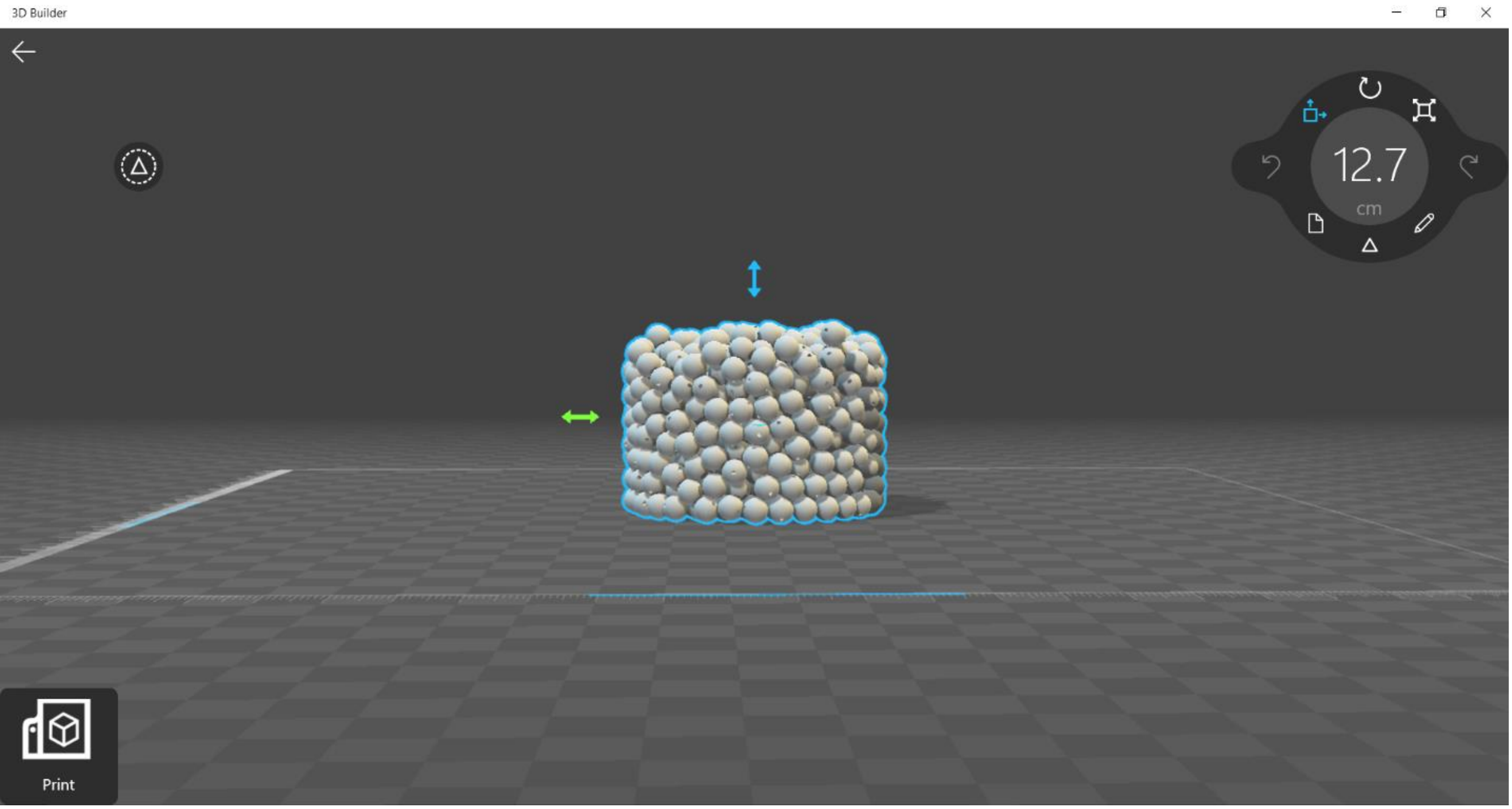
The image can be toggled with the mouse to obtain an overall view of the spheres.

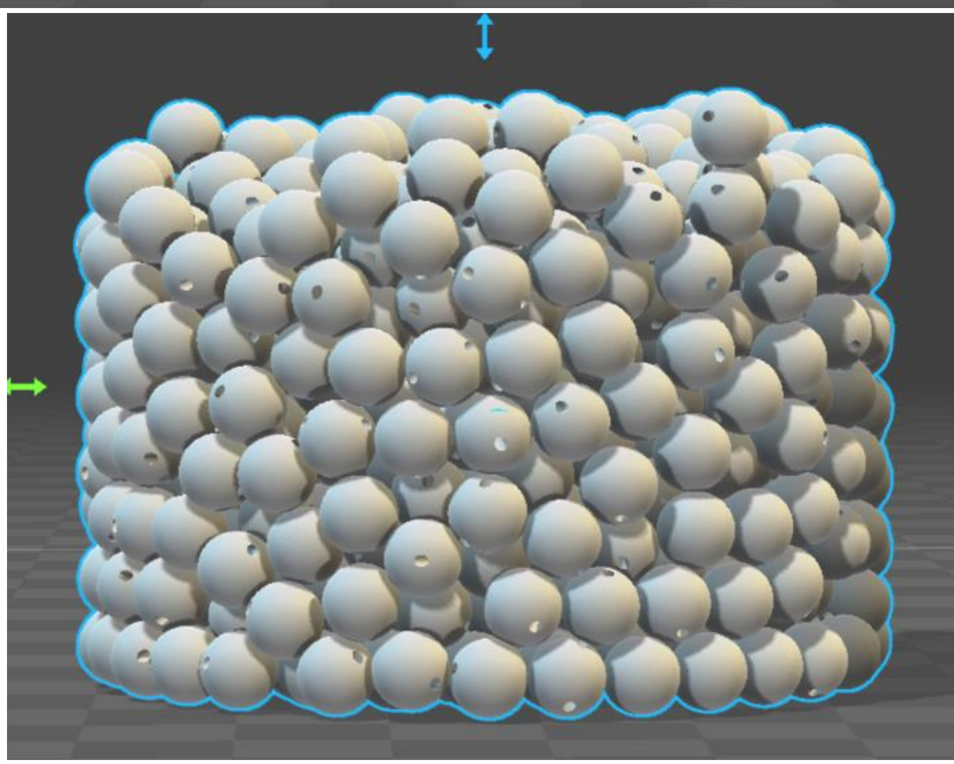
BLENDER supports the import and export of .STL files and hence a .STL file is created for spheres packed in the bed. However only the system comprising the spheres is exported as .STL file and the system of spheres along with the container cannot be exported together as .STL file.

Also .STL files can be directly used for 3D printing and for prototyping.

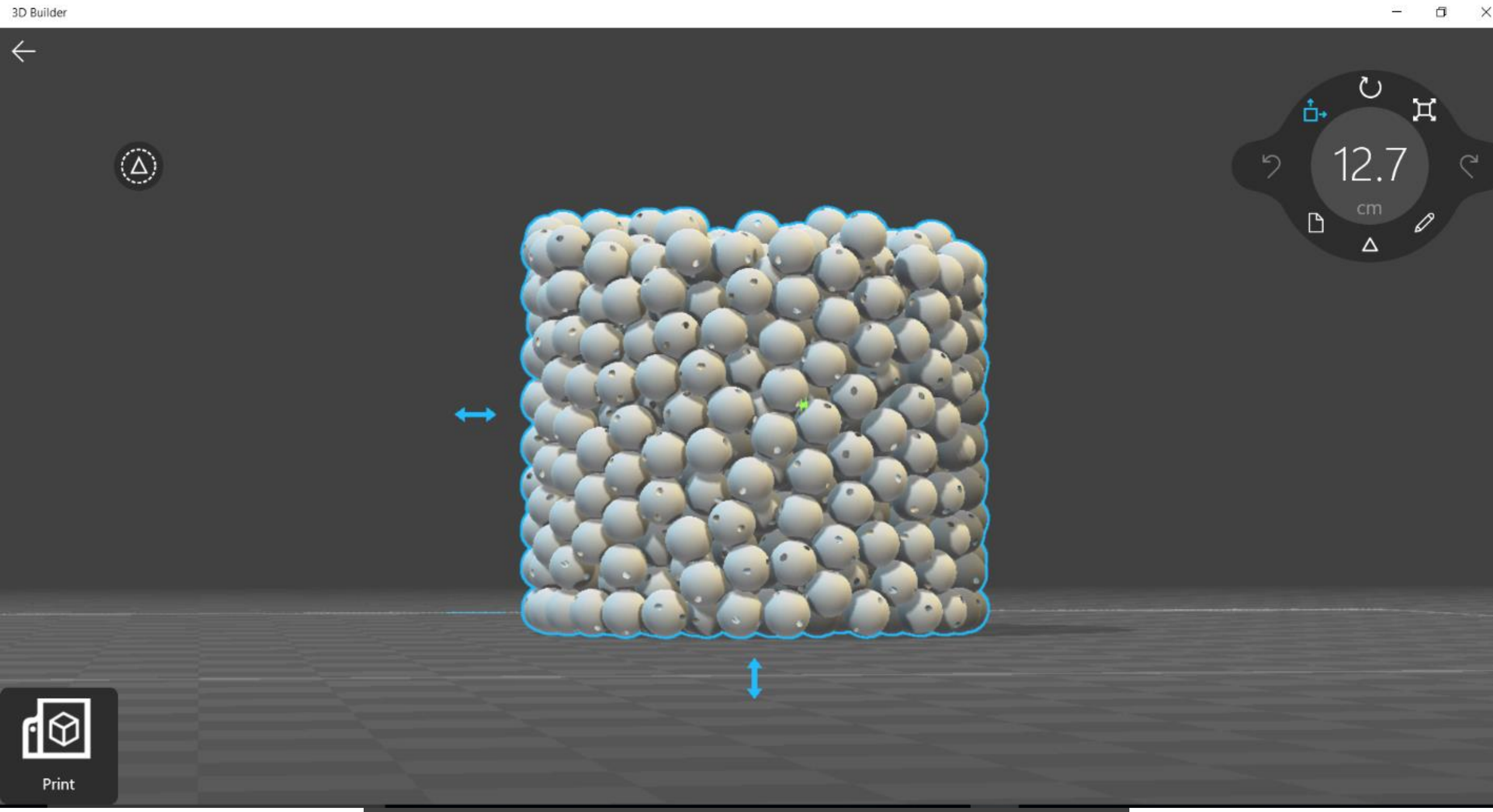
.STL file is imported in ANSYS student v19 for ANSYS Fluent simulation section and geometry is updated in ANSYS DESIGN MODELLER.

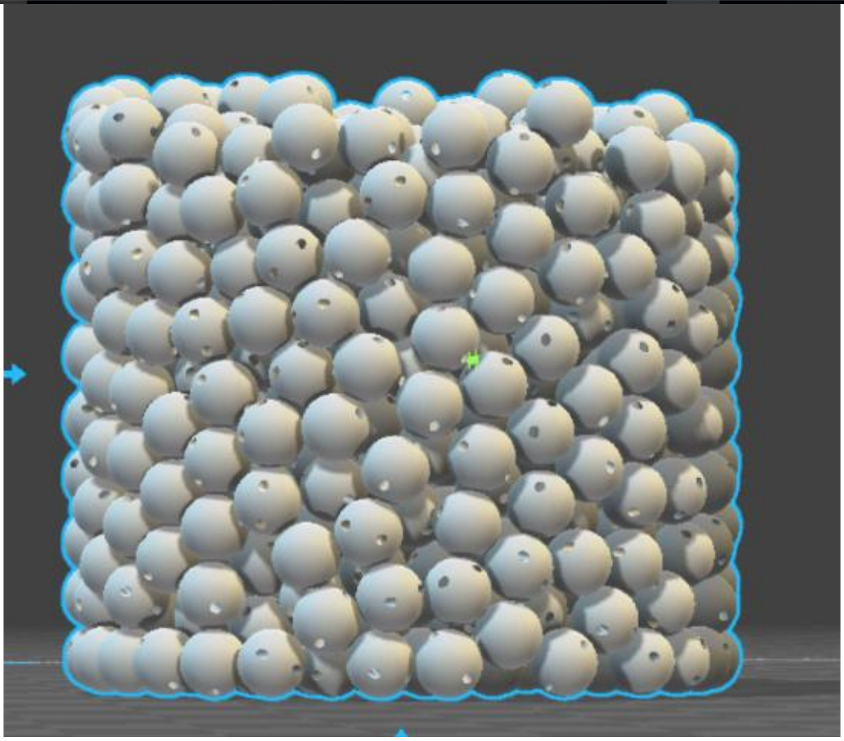
Sphere with 1 non-symmetric hole:



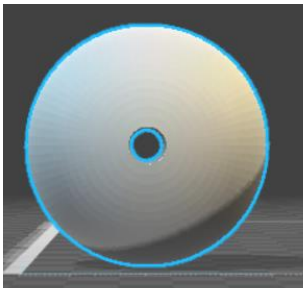


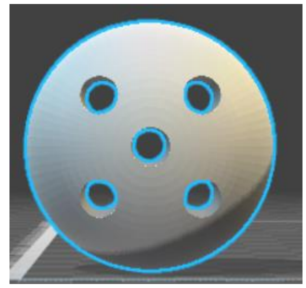
Spheres with 2 symmetric holes:

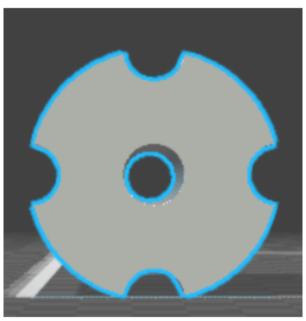


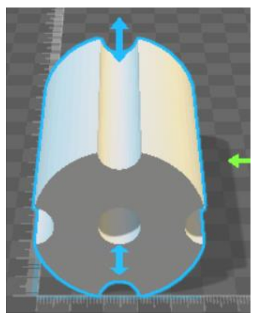


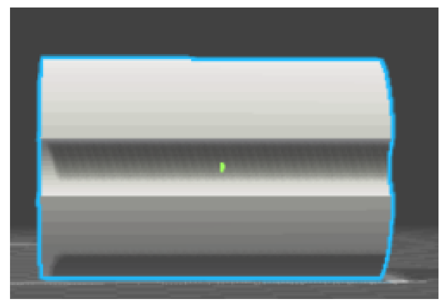
Modelling for sphere with 1 hole at the center, 5 holes in a sphere and cylinder cut out at the edges with hole through the length of the sphere:



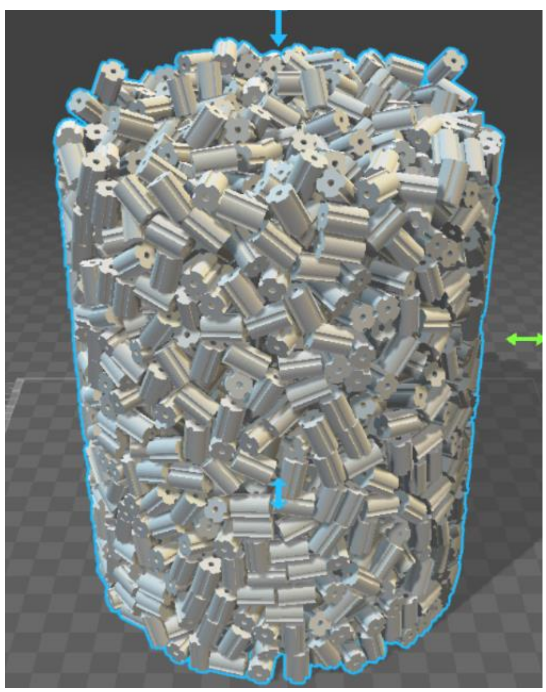


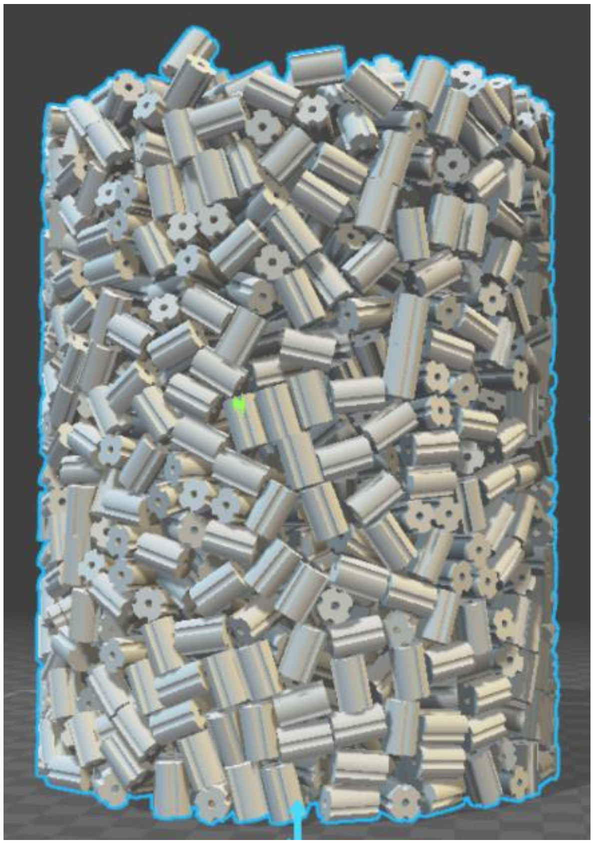


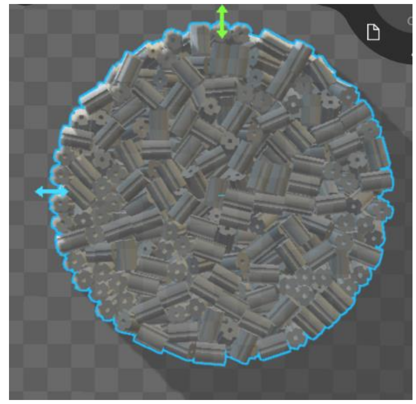


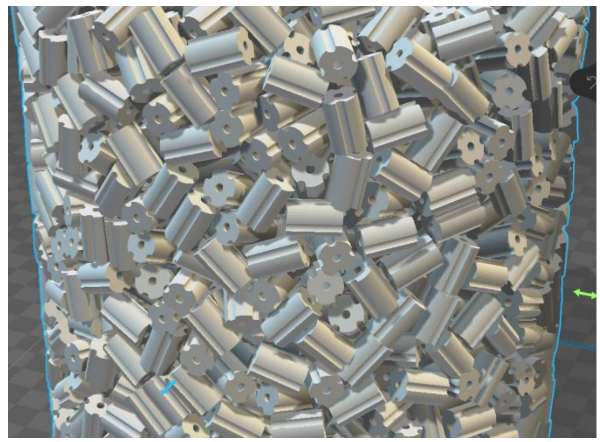


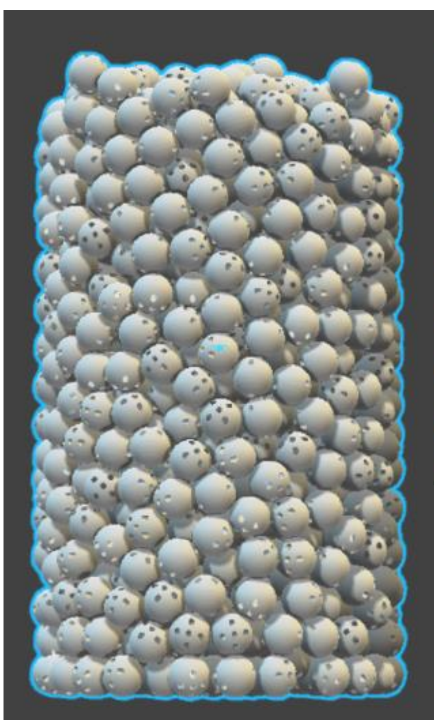
Simulation done for Cylinder with scrapping and hole through the length:

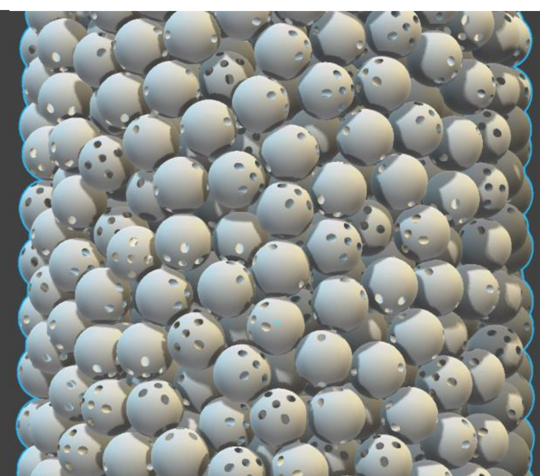


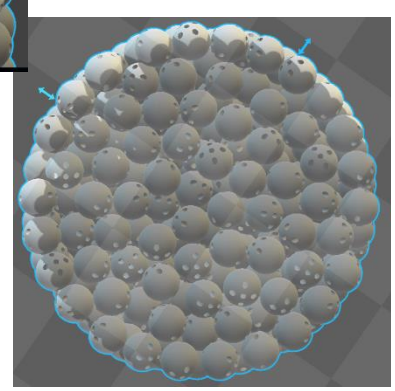












Conclusion

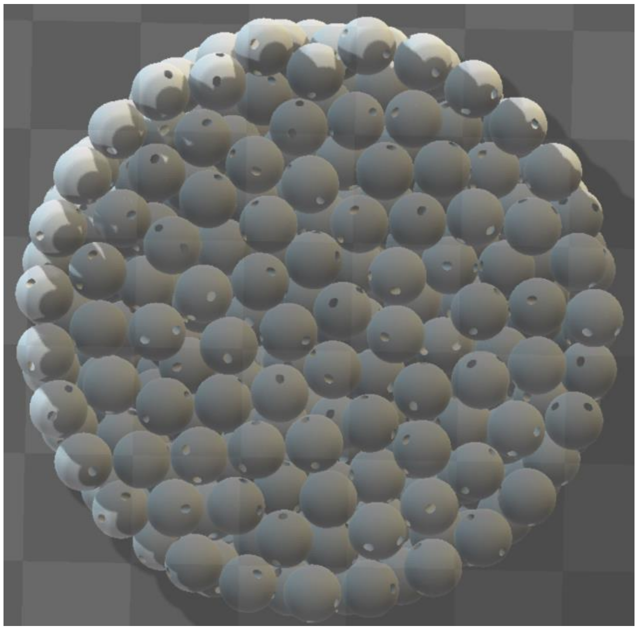
The geometry of packed bed creation for spheres with 4 symmetric holes is not created since the system crashes while rendering such a fine geometry. This is because in rigid body physics, collision type: mesh is used and creation of 2 additional holes will add more surface area for mesh for one sphere. Since the simulation is to begin with 1000 spheres, the amount of surface area created for additional mesh is too large and makes the system unstable.

The system of packed spheres was successfully exported in ANSYS and geometry was updates indicating that the spheres are ready for simulation in ANSYS. Since container cannot be exported in .STL file along with the spheres, in the DESIGN MODELLER or the SPCAECLAIM section of ANSYS, a cylindrical container can be easily drawn as a means of packing container for the spheres.

All the different geometries can be either created in BLENDER or any other CAD software such as ANSYS Design Modeller, Solidworks, OpenSCAD and can be imported as .STL files in BLENDER. The above mentioned algorithm has to be followed for an efficient method for the packing of the container. The demerits of using BLENDER is that we can only specify the aspect ratio for the cylindrical container (Height:Diameter) and accordingly specify the N number(number of spheres per diametric length of the container). However, once the packing is done, the geometry of packed spheres only can be exported as .STL file and can be opened in Windows 3D Builder and the dimensions [um cm mm in m ft] in 3D builder. Hence the dimensions will be set accordingly.

For example,

When the set of spheres is imported inn 3D builder, and dimensions set to cm, 5.6 cm diameter of the base of packing, 10 spheres can be packed per diameter length. Hence the size of each sphere will be approximately 5.6/10 cm ~ 5.6 mm and the container height can be calculated accordingly.



Base of the container.

Another benefit for using BLENDER is that we can generate a randomness in the packing. If the randomness factor were not included, an exact amount of 10 spheres would have been in line in the diameter. Whereas we can clearly see the non-uniform packing of the container. Also, a better way to perform the packing would be to create the geometry inn another CAD software and then importing the .STL file. The reason for this is that the ico-spheres used in BLENDER do not provide the exact sphericity and going to larger subdivisions, means a high rendering time. Hence, creating a geometry elsewhere and then using it in BLENDER is efficient.

A major advantage of the algorithm is that it can be used for packing of any kind of catalyst shape and configuration. Despite of the weight/shape/size of the catalyst, algorithm allows a randomness in the generation of the reactor bed.

Roadmap to Completion for fluid flow analysis:

The limitation of BLENDER is that we cannot know the porosity of the packed bed. For this, wither the geometry needs to be exported to ANSYS or OpenFOAM and mesh commands can be used to calculate the porosity of the bed.

Porosity = (volume of mesh on particle)/ (Total Volume of mesh)

References:

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2. Baker, *CFD simulation of flow through packed beds using the finite volume technique*, University of Exeter, 2011.