

Simulation of a randomly packed pebble bed
using the Discrete Element Method.

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Preface

This thesis represents my graduation work for the Bachelor in Applied Physics at Delft University of Technology. The thesis work was performed in the section Physics of Nuclear Reactors (PNR) of the faculty of Applied Sciences.

I would like to thank everybody at PNR for their support and suggestions.

Also a huge thank you goes out to C.R.A. Abrue, Assistant Professor, School of Chemical Engineering at State University of Campinas (UNICAMP), Brazil. The code used in this thesis was written and provided by him.

Erick Webbe

Abstract

A research has been performed on the radial porosity profile of a packed bed of multisized spheres. The beds have been simulated using a discrete element method. Next the results have been interpreted using MATLAB and a radial porosity profile has been calculated using line integrals. Goal of the research is to find a way to smoothen the radial porosity profile.

The results of the simulation have been compared to earlier experimental work to verify the accuracy of the calculations. Next a parameter sensitivity experiment has been conducted. Finally the model has been used to generate beds of multisized spheres.

A standard deviation of 0.7% in the average void fraction has been found. After comparison of the model with experimental research, the model is proven to be accurate using this deviation. The sensitivity experiment has yield similar results compared with the literature. The simulation of multisized pebbles did not finish as expected. The consequence is that no hard conclusions can be drawn from the data. There is however a strong indication that the use of multisized pebbles could smoothen the radial porosity profile.

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Chapter 1

Introduction

Climate change is a big issue in the international community. A lot of effort has been made to reduce the emissions of greenhouse gasses. The biggest international treaty is the well known Kyoto Protocol [1]. Recent research shows that the European Union is still on target to comply to the treaty [2]. Recently, president Obama and the USA also joined the global fight against global warming [3]. Despite all these efforts, it's widely accepted that for decades to come, we will still strongly depend on fossil fuels to meet our energy demands. Firstly because the technology of green energy isn't mature enough yet to supply the vast amounts of energy. Secondly because of the existing powerplants and means of transportation, and the investments that have been made in these fields. In the years to come, we need a midterm solution. Nuclear power is a very likely candidate, maybe even inevitable [4]. There are still a couple of problems facing nuclear energy. One of them is the safety aspect. The fear of an accident happening either because of human error or due to a terrorist attack is substantial. Conventional nuclear power plants stack defense systems one after the other to improve their defense-in-depth. This brings along quite some problems besides increasing the cost of the plant. The complexity of multiple systems makes it difficult to assess as to how safe the plant really is. Also the chance for human error could be larger with these complex systems. Modern plants, the so called Generation IV reactors [5], are designed to drastically decrease these problems.

1.1 Pebble-bed reactors

One of the six main Generation IV reactor types is the Very High Temperature Reactor (VHTR) which uses graphite moderation and an operation on temperature of around $1000^{\circ}C$. A possible design for this type is by using pebblebeds. In pebble-bed reactors the nuclear fuel is contained in pebbles of graphite instead of metallic rods. These rods are used in reactors like the BWR (Boiling-Water Reactor) and PWR (Pressurized Water Reactor). The graphite pebbles of typically $60[mm]$ in diameter contain 5000 to 20.000 coated triso particles. These triso particles contain a fuel kernel of UO_2 . A schematic of the pebbles can be seen in Figure 1.1.

The pebble-bed reactor has two major benefits. The first one is because of the gas coolant, since the pebbles act as a moderator, the reactor can be cooled with

an inert gas like helium. An inert gas is not reactive under normal circumstances and the gas does not get radioactive like water, which is used in conventional PWRs. Because of the higher operating temperature of the reactor the energy conversion efficiency improves. The low power density and the high temperature resistance of the core materials ensure that any decay heat will be dissipated and transported to the environment without the decay heat causing a meltdown. In Germany a pebble-bed reactor, the AVR (working group test reactor), was built in the sixties to serve as an experimental reactor and as a showcase to how safe this new form of technology was. However in the year 1988, after 21 years of service, the reactor was shutdown in the wake of the Chernobyl disaster and operating problems they had at the reactor. Currently there is one prototype of the pebble-bed reactor in China the so called HTR-10, standing for High Temperature Reactor ($10MW_t$). Multiple pebble-bed reactors are being designed for construction in South Africa to supply a large part of their energy needs and accepting pebble-bed reactors as a solution to their growing energy consumption.

FUEL ELEMENT DESIGN FOR PBMR

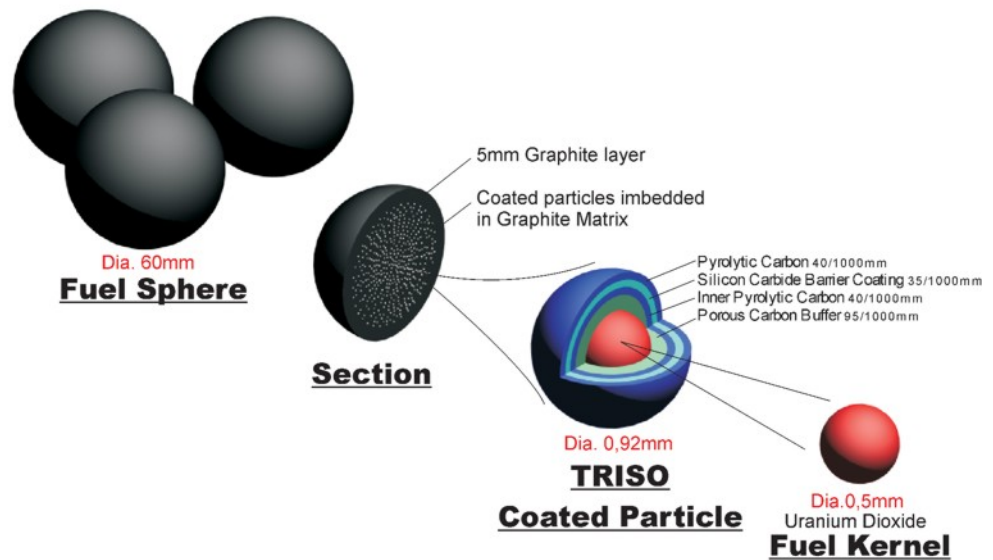


Figure 1.1: Schematic design of a pebble.

1.2 Previous work

Globally

An outline of previous work worldwide, relevant to the research will be provided in Chapter 2.

At Delft University of Technology

This thesis is the third on the topic of pebble beds, being researched at PNR at the Delft University of Technology (DUT). Previous work has been conducted by A. Ooms [6] and V. van Dijk [7].

The work by Ooms was aimed at simulating the packing and movement of pebbles in a bed. She compared different simulation techniques and has performed simulations based on static packing. Her conclusions contain a void fraction of 0.45 which is considered a bit high and a strong recommendation to perform a similar reasearch using a Discrete Element Method (DEM).

The work by Van Dijk was very experimental, using a setup called the PEbble Bed EXperiment (PebBEx). The goal was to make a scaled version of the HTR-10 reactor in China [8]. A setup has been developed to measure void fractions using gamma-ray tomography, an non invasive method. After this development has been completed, he measured the void fraction as a function of the radial position in the cylinder. His results have not yet been compared to results from simulated pebble-beds.

This thesis will continue the research, using the conclusions and recommendations of Ooms and Van Dijk. Also new experiments are done by J. Groen, using the setup of Van Dijk. His research focuses on improving the setup and testing the influence of multisized spheres on the radial void fraction. All of the research has been, and is being, supervised by dr.ir. J.L Kloosterman. The PebBEx facility has been realized with the assistance of drs. ing. A. Winkelman.

1.3 Problem description

Main point of interest in this thesis will be the void fraction in a pebble-bed as a function of the radial position. This fraction is found, and proven by Van Dijk, to be fluctuating near walls and boundaries. As will be described in Chapter 2, there is a big influence of this fraction on the operation of a nuclear reactor. There is a desire to have this fraction as constant as possible. To see if this can be achieved, a DEM will be used to simulate a pebble bed, as advised by Ooms. Secondly, these simulations will be tested for accuracy, using the results of Van Dijk. After this verification has been made, we can use the simulation to try different ways to smoothen the radial dependency function.

1.4 Outline of the thesis

In Chapter 2, the relevant theory on nuclear reactors and the packing of beds will be introduced. Chapter 3 will discuss the code used to simulate the pebble stacking, as well as the post processing of the data. Chapter 4 describes the calculations done with the code and the explanation why those calculations

have been selected. Chapter 5 shows all the results of the calculations and the comparisons with experiments. These results are interpreted in Chapter 6, which also contains the general conclusions of my research.

Chapter 2

Theory

In this chapter, the theory relevant for this thesis is introduced. The references provided in this chapter have more elaborate discussions on the subjects.

2.1 Power profiles

Static reactor flux and power distributions are of considerable importance in reactor design. A lot of research has been done for reactors in operation today, and many different setups have been developed [9]. Also an extensive study has been performed for the VHTR and the pebble-bed design by B. Boer [10]. His PhD thesis focuses a lot on power profiles as well. A good design usually yields a flat power profile. This is desirable for two different reasons. First it is advantageous from a thermal point of view. You would like to get an optimal temperature based on the core materials limitations without damaging the fuel pebbles. Also because a lot of parameters in the nuclear fission process, like micro- and macroscopic cross sections, depend on the temperature, you want to have good control over the temperature.

Secondly, a flat power profile also makes sure the fuel burn-up is equal for all pebbles. This is advantageous for the economy of the fuel pebbles and the efficiency of the reactor.

2.2 Sphere packing

Analytical analysis

The optimal packing of spheres in a volume is a well known problem in mathematics. In 1611, Johannes Kepler had conjectured a maximum possible density for both regular and irregular arrangements. This maximum was proven, with 99% certainty, in 1988 by Thomas Hales and equal to $\frac{\pi}{\sqrt{18}} \approx 0.74048$. The best known regular lattices are face-centered cubic (FCC) and hexagonal close-packed (HCP), a common lattice in crystals and solids [11]. This result only applies to an infinite three dimensional space, using only one size sphere. A similar result for spheres of multiple size, or in a fixed volume does not exist in analytical form. Approximations have been made [12], but only with limited applicability and for one size spheres.

Experimental research

Before computers were widely available and as powerful as today, sphere packing was studied using all kinds of experiments. G.E. Mueller has provided a nice overview in [13] (cited with updated references): “Roblee *et al.* [14] filled packed beds with paraffin and allowed it to solidify. Slabs were cut and annular rings were removed to determine the radial variations in the void fraction. Brosilow [15], and Benenati and Brosilow [16] poured lead shot into cylindrical containers and filled the system with liquid epoxy resin. Upon curing of the resin the solid cylinder was machined in stages. The weight and diameter of each cylindrical stage was measured and the radial variation of the void fraction was obtained. Scott [17] poured balls into a cylindrical container, filled it with molten paraffin, and then allowed it to cool. The three Cartesian coordinates of the balls in a roughly spherical cluster were obtained by using a modified standard optical comparator. The radial distribution was then obtained for intervals of one-fifth of the ball diameter. The technique of Ridgway and Tarbuck [18] used a packed bed contained in a cylindrical drum which was rotated about its axis so that any liquid present would form an annular layer at the surface of the cylinder. When a known volume of liquid was added the increase in the thickness of the annular layer was measured. This gave a measure of the voidage in the thin annular region. The method used by Thadani and Peebles [19] consisted of a vessel into which plastic spheres were poured. The packings were fixed in a plastic matrix and segmented. Each segment was radiographed and the point void fractions were determined by the radiograph emulsion point densities. Pillai [20] used a two-dimensional perspex bed with a measuring grid scribed on its outside face. The voidage distribution at the surface was quantified by counting the number of particles having their centers between successive grid lines. Goodling *et al.* [21] used precision polystyrene spheres and an epoxy mixed with finely ground iron to fill the void matrix. The solidified cylindrical packed beds were placed in a lathe and annular rings were machined from them. The change in mass and volume between cuts determined the void fraction at each radius. The above experimental data generally conclude that the radial void fraction has oscillations that are damped out at about four to five sphere diameters from the container wall.”

In his own research, Mueller used X-ray radiography to determine the center of a specially fabricated sphere with a metal core. With that data, he has setup a model to describe the radial void fraction. He compared his results with most of the former experiments, as also has been done in this thesis in Chapter 5.

Computational simulation research

There are a lot of different approaches possible for simulating a pebble-bed. A very nice summary can be found in the thesis of Ooms [6], Appendix B. This also contains a list of references of applications. In the literature, almost all implementations can be found. Over the last few years though, the DEM is most common. The change is due to better computer performance. Also the method provides good results in the research of densely packed bed, as are most common in nature.

Chapter 3

Computational Simulation

This chapter will describe the code used for the calculations. The code is written in FORTRAN, by Charles R. A. Abreu, who used it for his PhD thesis [22].

3.1 Discrete element method

The term discrete element method (DEM) is a family of numerical methods for computing the motion of a large number of particles like molecules or grains of sand. It consists essentially of integrating the equations of motion of the system numerically. In these equations you can add all the physics relevant to the system. The method can be viewed as a simulation of the system as it develops over a period of time. The fundamental assumption of the method is that the material consists of separate, discrete particles. These particles may have different shapes and properties. The method also often applies a neighboring lists method. In short this means that only the particles nearby a specific particle are assumed to influence that particle. This is done to greatly reduce the number of calculations.

More background and examples on DEM can be found in [23] and [24] for neighbouring lists.

3.2 Physical model

The parameters needed for displacement of the particles are speed and acceleration. The acceleration follows from Newtons law $F = m * a$. The resultant force is the superposition of all relevant forces. First we have gravitational and bouyancy forces:

$$F = \frac{4}{3}\pi r^3 g(\rho_p - \rho_f) \quad (3.1)$$

with r the radius of the pebble, g the gravitational acceleration and ρ the density of the pebble and the fluid in the volume.

Secondly there are a lot of frictional forces to be taken into account. The model uses the neighbouring lists to calculate all the pebble interactions under the assumption that pebbles outside of these cells will have no influence on the current pebble. For each pebble it is checked whether it is touching other pebbles around it. If they are touching, the drag is added to the resultant force. Also

changes in rotational speed due to drag is taken into account and considered in the next time step, as it influences the amount of drag. Also there is a check to see whether sliding occurs. A similar calculation is made for all pebbles which are touching the walls of the volume.

There is an option to have a fluid flow through the volume. The model takes drag force into account, so the fluid flow will influence the particles. The force is calculated using an empirical relationship:

$$F_D = C_D(Re)A_{\perp} \frac{1}{2} \rho v_r^2 \quad (3.2)$$

with C_D the dragcoefficient as a function of the Reynolds number, A_{\perp} the surface of the objects in the flow perpendicular to the flow's relative speed v_r and the fluid density ρ . More on this approximation and values for $C_D(Re)$ can be found in [25].

For the integration of the system, the Adams-Bashforth-Moulton predictor-corrector model is used. This method uses multiple prior positions to calculate the next position. The order of this method can be set for each simulation. Methods like Runge-Kutta or Euler [23] are alternatives but usually use only one prior step.

3.3 Input options

3.3.1 Initial parameters

All the parameters for system setup are stored in a **.inp* file. These files can easily be modified with a basic editor. This filename is also used as an argument when the calculation is ran. The initial parameters can be divided into three sections. For easier understanding these sections will be treated separately, though in the original file, the order of the lines of code will be different. In the next subsections, an example setup file is described. This example will generate a slender cilinder, containing fourty smaller and twenty larger pebbles.

Pebble properties

The file stores the number of different components, or pebbles in this case, to be used (NC). Also all the relevant physical properties of the pebbles can be set. This way you can simulate any type of pebble or wall, as long as properties like friction coefficients are known. All parameters are entered in the KMS-system, and well described by the comment above the line.

```
[Number of components - NC]
2
[Component properties (NC rows): Initial Number, Diameter(m),
Density(Kg/m^3), StiffNess(N/m), Shear StiffNess(N/m)]
0 0.001 2.45e3 1.e4 1.e4
0 0.002 2.45e3 1.e4 1.e4
[Normal coefficients of restitution of the component-component pairs
0.7 0.7 (NC by NC matrix)]
0.7 0.7
[Tangential coefficients of restitution of the component-component pairs
```

```

0.7 0.7 (NC by NC matrix)]
0.7 0.7
[Coefficients of friction of the component-component pairs (NC by NC matrix)]
0.3 0.3
0.3 0.3
[Normal coefficients of restitution of the component-wall pairs
0.7 0.7 (NC by NW matrix)]
0.7 0.7
[Tangential coefficients of restitution of the component-wall pairs
0.7 0.7 (NC by NW matrix)]
0.7 0.7
[Coefficients of friction of the component-wall pairs (NC by NW matrix)]
0.3 0.3
0.3 0.3

```

The coefficient of restitution is known as the ratio of velocities before and after a collision. A ratio of 1 is equal to an elastic collision, a ratio of 0 is equal to a completely inelastic collision.

Volume properties

The volume used in the simulation can be set, by defining walls to contain the pebbles. Both flat and conic walls are available. In the example below, a cylinder (line 1) with bottom (line 2) is created. Note that the position and the directional vectors of the walls take three arguments $[x, y, z]$, as the volume is three-dimensional. Again the relevant physical properties can be defined as desired. There also is an option to move individual walls. This could be used to simulate an earthquake. See also section 6.2.

```

[Box dimensions (m)]
0.01 0.01 0.05
[Number of Walls - NW]
2
[Wall properties (NW rows): Shape*, L1(m), L2(m), L3(m),
Stiffness(N/m), Shear-StiffNess(N/m), Position(m), U, W]
2 0.04 0.01 0.01 1.e4 1.e4 0. 0. 0.00 0. 0. 1. 0. 1. 0
2 0.00 0.00 0.01 1.e4 1.e4 0. 0. -0.02 0. 0. 1. 0. 1. 0
[Move walls?]
no
[Vectors A (m), f (1/s), and for wall velocities:
V = -2*Pi*A*sin(2*Pi*(f*t + )); (NW rows)]
* Shape = 1 - Flat wall:
L1: Length in the direction of U
L2: Length in the transversal direction [W - (W.dot.U)/(U.dot.U)*U]
L3: Anything
U and W: Linearly independent vectors denoting the wall plan
Shape = 2 - Conic wall:
L1: Height
L2: Anterior diameter
L3: Posterior diameter
U: Direction of the main axis of the wall

```

W: Any vector, provided that W and U are linearly independent

General properties

The *.inp file also contains general properties. These include the duration of the simulation, the options to start with an initial configuration or continue an incomplete one. The frequency to produce output statusfiles is also free to choose. Also you could have a fluid flow through the volume as discussed in section 3.2. Properties like fluid density are free to choose (in this case air). Finally there are options on the order of integration to be used (see 3.2) and the random number generator is seeded. For all of these properties, the comment in the preceding line is usually very clear.

```
[Read the initial configuration? (If yes, just type the file name)]
no
[Promote particle pouring? (If yes, just type the pouring file name)]
test.prg
[Periodical Boundary Conditions]
F F F
[Gravity Acceleration Vector (m/s2)]
0.0 0.0 -9.8
[Fluid density (Kg/m3)]
1.e0
[Seed for random number generation (a negative integer)]
-7384
[Base for file names (with no extension; maximum 100 characters)]
test
[Total time to be simulated (s)]
0.40
[Minimum number of time steps per collision]
10.
[Order of the predictor-corrector integration method (1-4)]
4
[Number of intervals in each initial euler time step]
100
[Time interval for saving the state of the simulation (s)]
0.05e0
[Time interval for saving snapshots of the simulation (s)]
0.01e0
[Time interval for reporting the progress of the simulation (s)]
0.01e0
[Resume simulation (if it was interrupted)?]
yes
[Consider fluid flow?]
no
```

3.3.2 Pouring parameters

All the parameters for pouring components into the volume is stored in a **.prg* file, with the *** equal to the name provided in section 3.3.1. It will store the number of pebbles that you want to be poured into your volume and the speed to do so. Also the shape and size with which to pour is entered here. An example is shown below:

```
[Number to be reached for each component (NC rows)]
40
20
[Shape of the pouring origin surface (Square/Circle)]
Circle
[Size of the pouring origin surface (m)]
0.01
[Maximum number of attempts for each time step]
10
[Time interval between pouring attempts (s)]
0.001
```

These files are easy to read and can easily be modified with a basic text editor. A parameter which can't be set is the order in which, or the ratio between two types of pebbles, to pour pebbles. This would be desirable if there are multiple sized pebbles.

A work around could be achieved by adding multiple lines, of the same type of pebble. The pouring algorithm chooses a pebble type randomly from the available types. If one type is present twice, the probability that this type is chosen effectively doubles. This would change the ratio in which the pebbles are poured from one on one, to one on n with n the times a line of one type of pebble added. The sum of numbers of pebbles of one type should of course stay the same.

3.4 Output processing

3.4.1 Visualization

After a simulation has been completed, the data is interpreted using MATLAB. Not only properties like average porosity and radial porosity can be calculated, there are also routines to make images (see Figure 3.1), and even movies, of the simulation.

The code has a very clear program flow and consists of easy understandable plotting routines, so it will not be treated in depth in this thesis.

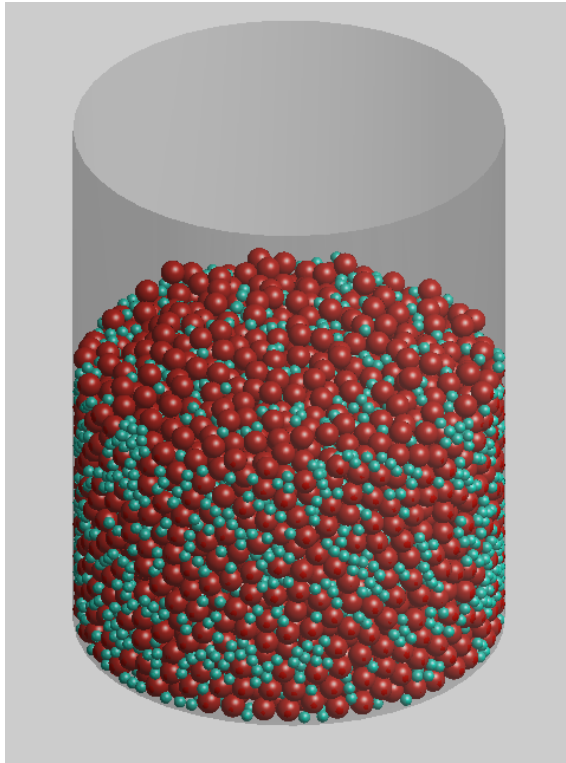


Figure 3.1: Example of an image created by MATLAB, based on simulation results.

3.4.2 Porosity calculation

The same data is used for the porosity calculations as for the visualization. An average porosity $\langle \varrho \rangle$ calculation is relatively simple:

$$\langle \varrho \rangle = \frac{\sum_i \frac{4}{3}\pi r_i^3}{2\pi R^2 z_{i,max}} \quad (3.3)$$

with i the number of pebbles, r_i the radius of the current pebble, R the radius of the cylinder and $z_{i,max}$ the height of the highest pebble. The bottom of the cylinder is at $z = 0$. One adaptation has to be made because in the simulation, you can't make a flat top layer, as with a real experiment. If now $z_{i,max}$ would be chosen as the top of the filled volume, there would be an overestimation of the void fraction. To prevent this, the z_{max} is chosen a few pebble diameters lower. The pebbles below this height are counted completely, the pebble with a center above this height are completely ignored. It is assumed that contributions of pebbles partially inside and outside the volume will average out.

The radial porosity calculation is a little more complex. It is done using line integrals, as described in [22]. This method calculates the amount of a tested radius being intersected by pebbles. This percentage is equal to the packing fraction for that radius. The value is evaluated for different radii, and averaged over different heights.

The method is implemented in a MATLAB algorithm. The algorithm will loop through a number of height and radial steps. During these steps, all the pebbles are evaluated individually. The first test is to see whether the pebble has a contribution to the plane at the tested height. If it has, then the height difference between tested height z_{test} and the pebble center is less than the radius of the pebble:

$$|z_{test} - z_i| \leq r_i \quad (3.4)$$

with z_i and r_i tested pebble height and -radius. If this condition is met, the actual contribution in the plane is the intersection of the pebble at the tested height. This radius is equal to:

$$r_{inplane} = r_{i,z=z_{test}} = \sqrt{r_i^2 - (z_i - z_{test})^2} \quad (3.5)$$

If there is a contribution to the plane, there is not always intersection with the tested radius. There are six possible situations, shown in Figure 3.3. The first two have no intersection, and are either completely within, or completely outside of, the tested radius. A pebble completely within the radius is tested using:

$$\begin{aligned} r_{test} &> r_{inplane} \\ r_{test} - r_{inplane} &\geq \sqrt{x_i^2 + y_i^2} \end{aligned} \quad (3.6)$$

with x and y the position of the pebble. A pebble completely outside of the radius is tested with:

$$r_{test} + r_{inplane} \leq \sqrt{x_i^2 + y_i^2} \quad (3.7)$$

The third case is when a pebble completely overlaps the tested radius. This will correspond to:

$$\begin{aligned} r_{test} &< r_{inplane} \\ r_{inplane} - r_{test} &\geq \sqrt{x_i^2 + y_i^2} \end{aligned} \quad (3.8)$$

Cases four through six correspond to partially intersecting pebbles. In all of these cases you calculate the angles at which the tested radius is intersected. The amount of a tested radius being intersected by a single pebble can be evaluated analytically. Figure 3.2 shows all the variables. In this Figure, the two centers are taken to be on the x-axis. This rotation does not influence the magnitude of the intersected angles, which will be used. The equations describing the two circles are:

$$\begin{aligned} x^2 + y^2 &= R^2 \\ (x - d)^2 + y^2 &= r^2 \end{aligned} \quad (3.9)$$

by combining the two we find, for x :

$$(x - d)^2 + (R^2 - x^2) = r^2 \quad (3.10)$$

$$\begin{aligned} x^2 - 2dx + d^2 + R^2 - x^2 &= r^2 \\ x &= \frac{d^2 - r^2 + R^2}{2d} \end{aligned} \quad (3.11)$$

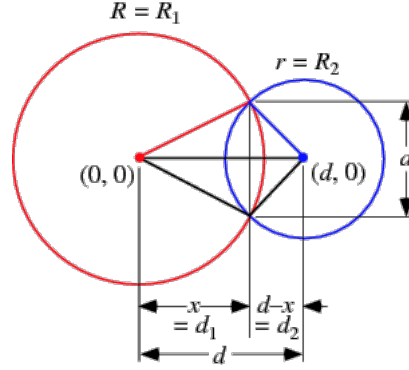


Figure 3.2: Intersecting circles and the parameters used in the calculation

and for y :

$$y = R^2 - x^2 \quad (3.12)$$

$$\begin{aligned} &= R^2 - \left(\frac{d^2 - r^2 + R^2}{2d} \right)^2 \\ &= \frac{4d^2 R^2 - (d^2 - r^2 + R^2)^2}{4d^2} \\ &= \frac{1}{2d} \sqrt{(-d + r - R)(-d - r + R)(-d + r + R)(d + r + R)} \end{aligned} \quad (3.13)$$

We can now find the angles at which the two circles intersect:

$$\begin{aligned} \theta_1 &= \arctan\left(\frac{y}{x}\right) \\ \theta_2 &= \arctan\left(\frac{-y}{x}\right) \\ \theta_{intersected} &= |\theta_2 - \theta_1| \end{aligned} \quad (3.14)$$

The final check is to see if the circle is intersected from θ_1 to θ_2 or the other way around. If $r_{inplane}$ is smaller than the tested radius (case 4) the contribution is equal to $2\pi \cdot \min(\theta_{intersected}, 2\pi - \theta_{intersected})$. If the $r_{inplane}$ is bigger than the tested radius, another check has to be done. A possible check is to see if the intersection point of the bisector of θ_1 and θ_2 and the contribution of the pebble in the plane lies outside (case 5) or within (case 6) the tested radius. The contribution of all the pebbles to a tested radius are added and scaled to find the radial filling fraction, $\rho(r)$:

$$\rho(r) = \frac{\sum_i \theta_{i, effective} \cdot r_{test}}{2\pi r_{test}} \quad (3.15)$$

The void fraction follows as $1 - \rho$.

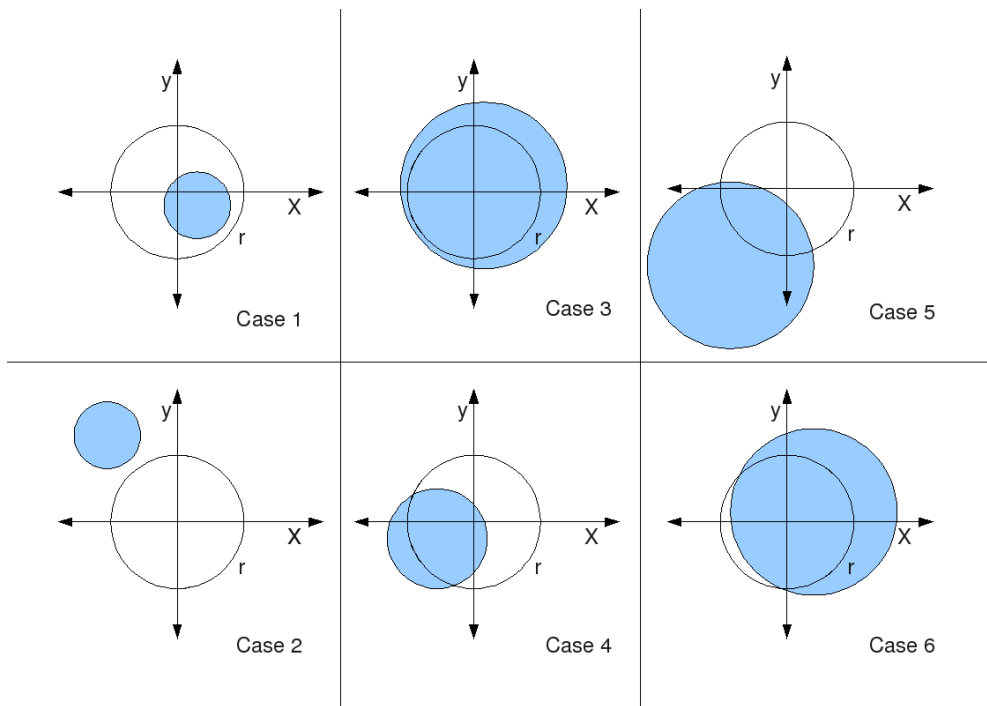


Figure 3.3: Visualization of the six different cases when a pebble has a contribution to the tested plane.

Chapter 4

Calculational Setup

Main point of interest of the experiment will be the dependence of the radial porosity profile on different numbers and types of pebbles. First of all the calculations will be compared to results obtained in previous experiments from Van Dijk [7] and research like Mueller [13]. This is done to validate the model. After this validation, the variance between calculations will be tested. This is done to get an idea of the variance of the results of the calculations, and to be able to tell if a change in porosity is significant or not. Also a parameter sensitivity test will be conducted, varying the friction coefficient between the pebbles. This is done to see how dependent the simulation is based on a single parameter. The friction coefficient is chosen based on results of Siiria [26]. Finally, calculations will be made with different ratios of pebble sizes. A possible application of the research is the optimization of the power profile of a pebble-bed reactor as described in section 2.1.

Chapter 5

Results

5.1 Estimation of the Variance

The result of the variance experiment is shown in Figure 5.1.

The results of the computation of the overall porosity is assumed to be normally distributed. A standard deviation is calculated, using the five results, as:

$$\sigma = \sqrt{\frac{1}{N} \sum_i (x_i - \mu)^2} \quad (5.1)$$

with μ the average of the measurements and N the number of data points. A standard deviation of 0.7% is found. This value will be used in later calculations as an indication whether results are significantly different.

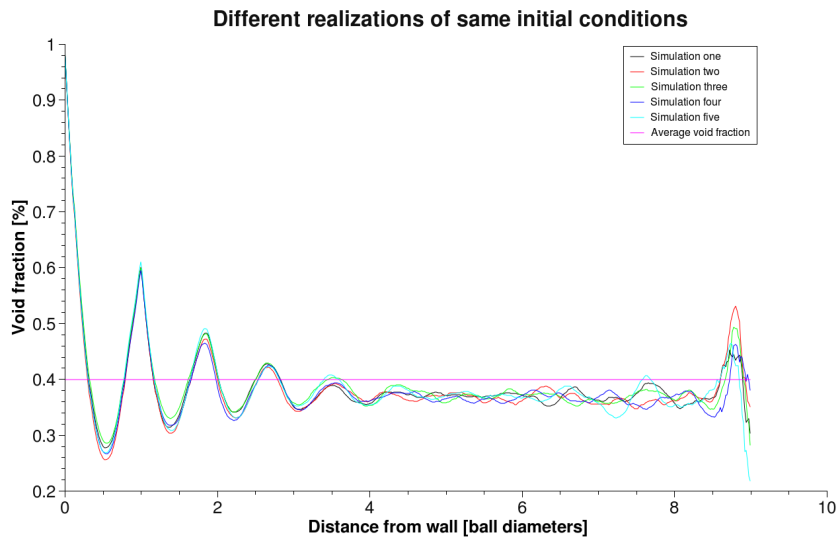


Figure 5.1: Graph of the radial porosity of five realizations. The integrator used 500 radial steps and 250 height steps. Also the average of all the average void fractions is shown as a horizontal line.

5.2 Parameter Sensitivity

The same calculation was done as [26]. In this calculation an estimation of the friction coefficient of perspex of 0.7 has been made, based on [27]. Next we ran simulations with small changes in this value. The changes were made $\pm 20\%$, $\pm 10\%$, $\pm 5\%$ and without any change. The results are shown in Figure 5.2. This graph shows no big dependence on the parameter in the tested range.

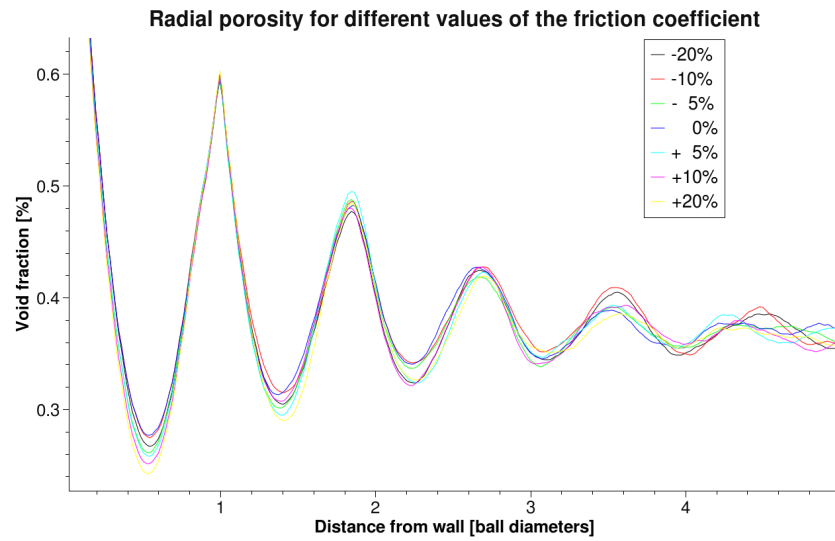


Figure 5.2: Graph of the radial porosity of seven realizations. The integrator used 500 radial steps and 250 height steps.

Figure 5.3 shows the same graph, only zoomed in on the first minimum. Here a dependence on the parameter can be seen.

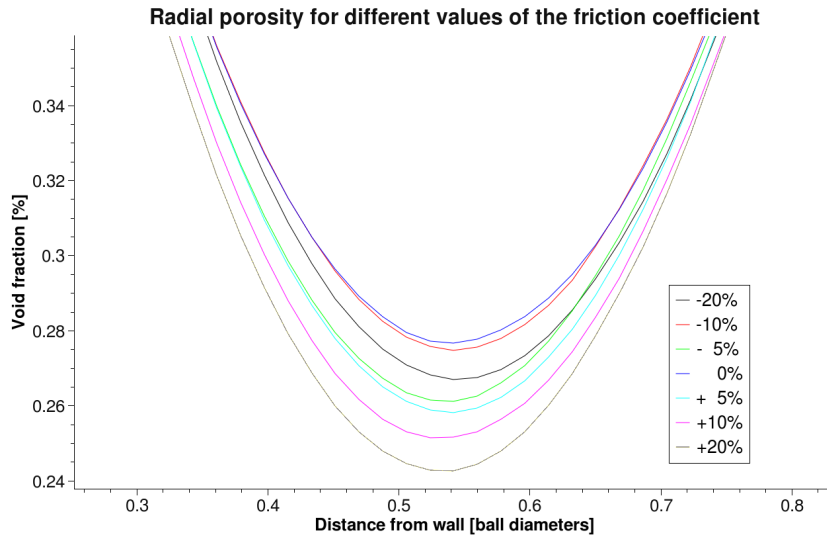


Figure 5.3: Same graph as Figure 5.2, but zoomed in on the first minimum. Roughly a same order is seen in the change in parameter and the order of the lines (from bottom to top: +20%, +10%, +5%, -5%, -20%, -10%, 0%).

Figure 5.4 shows the average void fraction versus the change in the friction coefficient. The order of average porosities is almost equal to the order found in Figure 5.3, from low to high: +20%, +10%, +5%, -5%, -20%, 0%, -10%. A linear fit has been made on the data. The negative slope of the fit corresponds to the results of Siiria [26].

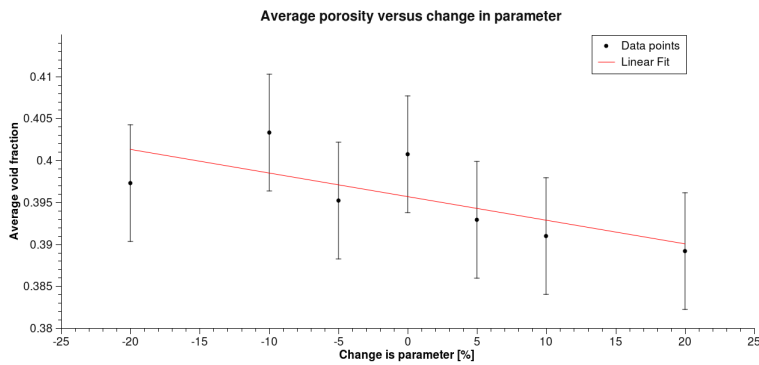


Figure 5.4: Graph of the average void fraction versus the change in parameter. Added are also the uncertainties in the void fraction based on section 5.1. A linear fit has been preformed in the form $y = Ax + B$.

5.3 Comparison with Experiments

An attempt has been made to simulate the experiment as done by Van Dijk. The initial setup for this experiment can be found in Appendix A. All the sizes and numbers as provided in his report have been used. Figure 5.5 shows his results compared with the results found in section 5.1. The fit has been positioned in the x-direction to best fit the graph, still equally scaled. This has been done to consider the problems described by Van Dijk, to find an accurate position of the wall.

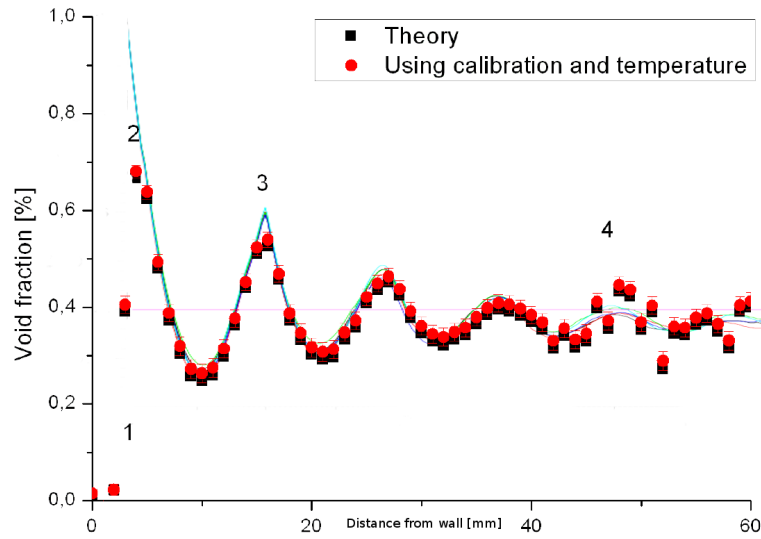


Figure 5.5: Comparison of the results of Van Dijk with the calculations. The same results have been used as in section 5.2.

A similar attempt has been made to compare the simulation results to other research. The comparison with the modelling results of Mueller [13] and the experimental results of Goodling [21] is shown in Figure 5.6.

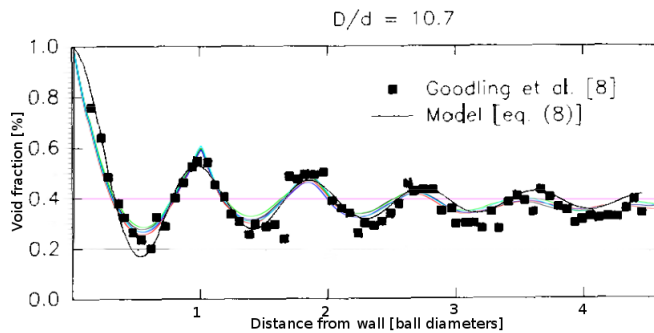


Figure 5.6: Comparison of the results of Mueller and Goodling with the calculations. The same results have been used as in section 5.2.

5.4 Different Sizes

The calculations for multisized pebbles did not complete as expected. After visual inspection of the data, it became clear that, in some cases, the fixed boundaries of the volume did not contain all the pebbles. In other cases, the pebbles completely disappeared. The simulation was completed correctly for the radial ratios 1 : 1, 1 : 1, 2 and 1 : 1, 3. The calculations of the radial ratios of 1 : 1, 4 through 1 : 2 with steps of 0, 1 have been used partially. Calculations of the ratios 1 : 2, 5, 1 : 3, 1 : 3, 5 and 1 : 4 completely failed. An example of a partially filled cylinder can be seen in Figure 5.7

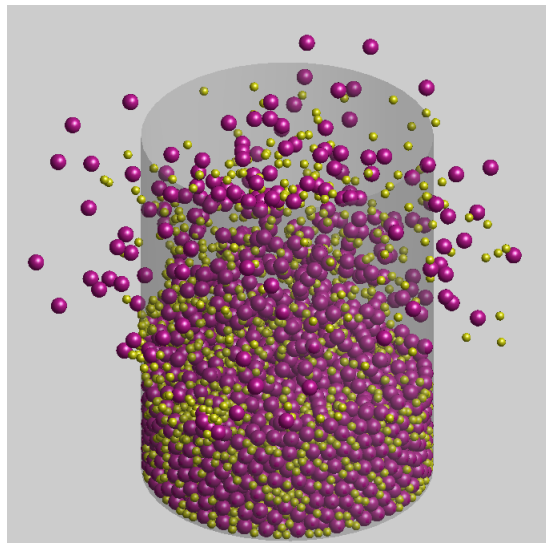


Figure 5.7: Visualisation of a unsuccessfull simulation. The Figure also shows that the layers at the bottom are still packed properly.

In most cases though, the bottom of the volume was filled upto approximately eight pebble diameters. The code in subsection 3.4.2 has been adapted to only integrate upto this height.

Figure 5.8 shows the porosity profile of three experiments which did finish as expected. A clear decrease in the amplitude of the wiggles can be seen.

Figure 5.9 shows the results of the simulations over a large range of multisized pebbles. There is a relatively large spread in average porosities, compared to Figure 5.1. This can be assigned to bad statistics because less pebbles are included in the calculations because the calculation only partially completed as expected. The Figure is zoomed in on the first wiggle to show an interesting phenomena. The amplitude of the wiggles keep decreasing and secondary peaks start to form. The position of these secondary wiggles have a strong correlation with the size of the secondary pebble. The order of the positions of the peaks also completely matches the order of the radial ratios between the pebbles.

Based on the results of Figure 5.9, an attempt has been made to calculate two separate sets of beds. Of these beds, the radial porosity would be calculated and super-positioned over each other. A result comparable with the mixed sim-

ulation would be an indication that by mixing different sized pebbles, you could make a flatter porosity profile. A calculation of the second type pebble also failed and gave results comparable with Figure 5.7. Due to failed calculations, a comparison with the experimental data of Groen (*not yet published*) could not be made.

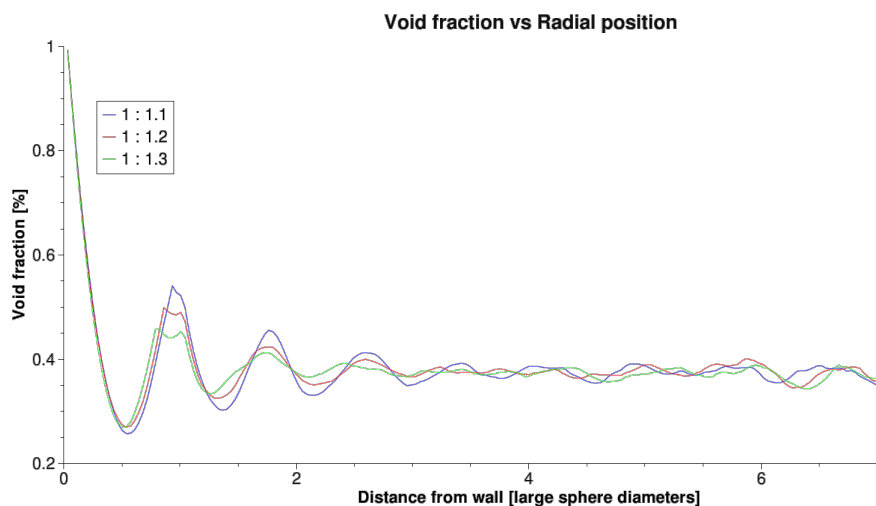


Figure 5.8: Radial porosity profile for three different ratios of multisized spheres. The ratios in the legenda are referring to the radius.

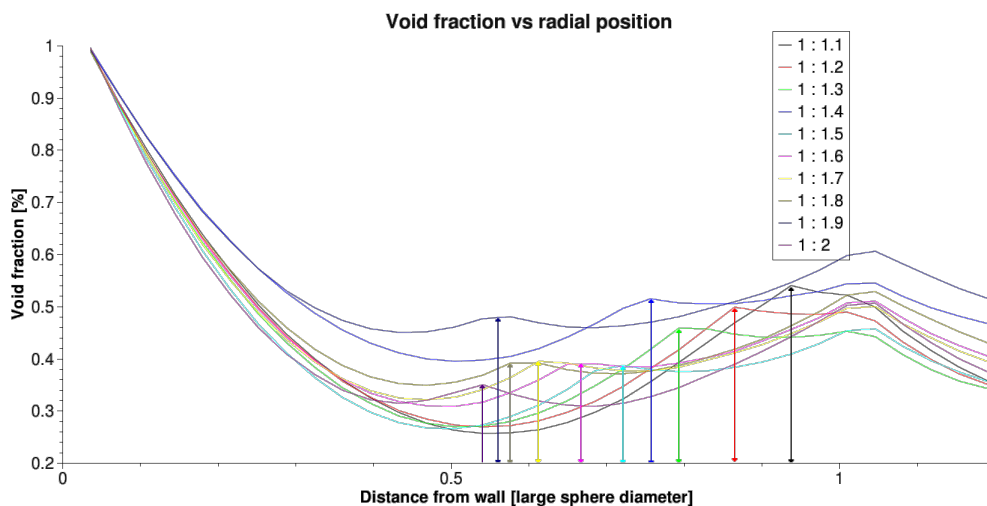


Figure 5.9: Radial porosity profile for ten different ratios of multisized spheres. The arrows indicate the position of the secondary peaks and have the same colors as the corresponding porosity profile. The ratios in the legenda are referring to the radius.

Chapter 6

Conclusions and recommendations

6.1 Conclusions

The conclusions drawn by Ooms are proven to be correct. The DEM is a good method to calculate random packed beds of pebbles. A lot of comparable research has been performed worldwide. An existing model has been obtained and adapted to simulate the PebBEx setup at DUT. The model is found to be very flexibel and easily adaptable to simulate more difficult geometries or use multiple types of pebbles at once. The fast amount of possibilities open doors to a lot more research on pebblebeds, using this model.

The model is also found to be in good compliance with experiments performed on packed beds. A standard deviation of the average void fraction of 0.7% has been found for these calculations, in Section 5.1. As seen in Chapter 5, the calculations yields results which are in good agreement with results found in different experimental studies. The comparison is not contradicting using the standard deviation of 0.7 %.

The study in multisized pebbles has shown some promising results but, due to bad statistics and bad reproducibility, no conclusions are drawn. There is however an indication that the use of multisized pebbles will flatten the radial porosity profile. Further research may find the error which caused the bad results.

6.2 Recommendations

In this section, I will provide some recommendations for follow-up research and improvements of the calculation. Main reason why this has not yet been done or implemented is the limited amount of time set for this research.

6.2.1 Follow-up research

Fixing the multisized calculations

The calculations analyzed in section 5.4 did not complete as expected. Also an explanation as to why this happened, has not yet been found. A higher number of Euler steps and a lower pouring speed did not solve this problem. If this problem is solved, the results presented in section 5.4 could be checked.

Different geometries

With the simulation, it is quite easy to make different geometries for the pebble container. A cone could be added to the bottom to better replicate an actual pebbled reactor. Also a second cylindrical wall could be added to simulate a co-centric wall.

Shaking the container

In many packings, the overall void fraction can be reduced by shaking the container. This shaking can be replicated in our simulation. This will often give a closer packed bed and a better representation of the actual situation. The effects of this packing on the radial voidfraction could be studied, and compared using the PebBEx setup.

Fluid flow

There is a possibility to have a fluid flow through the simulated volume. In an actual reactor this is also the case with the coolant flowing past the pebbles. This flow could be added to improve the reality of the simulation.

6.2.2 Calculation improvements

Conversion to linux

The FORTRAN code of the calculation could not be compiled for a Unix architecture. This would allow for the calculations to be performed on a Unix cluster. This would greatly improve the speed to simulate new setups. Problem lies in the use of the *FORM = binary*, in the FORTRAN code (Bin-FilesVF.f90, line 200). This is probably included in the Visual Fortran Compiler, which I could not get my hands on.

Knowing when to stop

The calculation allows for the user to set the total time to be simulated. Problem is that you will usually not know in advance how long a calculation will take to reach an equilibrium state. It is possible to make small steps, check if it is done, and if not continue the calculations, but this is a time consuming task. Automating these steps will also make calculation time decrease.

Appendix A: Example calculation input

This appendix will provide the reader with an example of the two input files described in Section 3.3, which also contains an elaborate discussion of the files. This example simulates the PebBEx setup as described by Van Dijk. An image of the result of the calculation is added.

The initial values *.inp

```
[Box dimensions (m)]
.5 .5 .5
[Number of components - NC]
1
[Component properties (NC rows): Initial Number, Diameter(m),
Density(Kg/m3), StiffNess(N/m), Shear StiffNess(N/m)]
0 0.0127 2.45e3 1.e4 1.e4
[Read the initial configuration? (If yes, just type the file name)]
no
[Promote particle pouring? (If yes, just type the pouring file name)]
test.prg
[Number of Walls - NW]
2
[Wall properties (NW rows): Shape*, L1(m), L2(m), L3(m),
Stiffness(N/m), Shear-StiffNess(N/m), Position(m), U, W]
2 0.3 0.229 0.229 1.e4 1.e4 0. 0. 0.15 0. 0. 1. 0. 1. 0
2 0.0 0.229 0.0 1.e4 1.e4 0. 0. 0.00 0. 0. 1. 0. 1. 0
[Normal coefficients of restitution of the component-component pairs
0.7 (NC by NC matrix)]
[Tangential coefficients of restitution of the component-component pairs
0.7 (NC by NC matrix)]
[Coefficients of friction of the component-component pairs (NC by NC matrix)]
0.3
[Normal coefficients of restitution of the component-wall pairs (NC by NW matrix)]
0.7 0.25
[Tangential coefficients of restitution of the component-wall pairs
0.7 0.7 (NC by NW matrix)]
[Coefficients of friction of the component-wall pairs (NC by NW matrix)]
```

```

0.3 0.3
[Periodical Boundary Conditions]
F F F
[Gravity Acceleration Vector (m/s^2)]
0.0 0.0 -9.8
[Fluid density (Kg/m^3)]
1.e0
[Seed for random number generation (a negative integer)]
-7384
[Base for file names (with no extension; maximum 100 characters)]
PebBEx
[Total time to be simulated (s)]
10.0
[Minimum number of time steps per collision]
10.
[Order of the predictor-corrector integration method (1-4)]
4
[Number of intervals in each initial euler time step]
100
[Time interval for saving the state of the simulation (s)]
0.05e0
[Time interval for saving snapshots of the simulation (s)]
0.01e0
[Time interval for reporting the progress of the simulation (s)]
0.01e0
[Resume simulation (if it was interrupted)?]
yes
[Move walls?]
no
[Vectors A (m), f (1/s), and for wall velocities:
      V = -2*Pi*A*sin(2*Pi*(f*t + )); (NW rows)]
[Consider fluid flow?]
no

```

* Shape = 1 - Flat wall:

```

L1: Length in the direction of U
L2: Length in the transversal direction [W - (W.dot.U)/(U.dot.U)*U]
L3: Anything
U and W: Linearly independent vectors denoting the wall plan

```

Shape = 2 - Conic wall:

```

L1: Height
L2: Anterior diameter
L3: Posterior diameter
U: Direction of the main axis of the wall
W: Any vector, provided that W and U are linearly independent}

```

The pouring values *.prg

```
[Number to be reached for each component (NC rows)]  
4800  
[Shape of the pouring origin surface (Square/Circle)]  
Circle  
[Size of the pouring origin surface (m)]  
0.2  
[Maximum number of attempts for each time step]  
1000  
[Time interval between pouring attempts (s)]  
0.0001
```

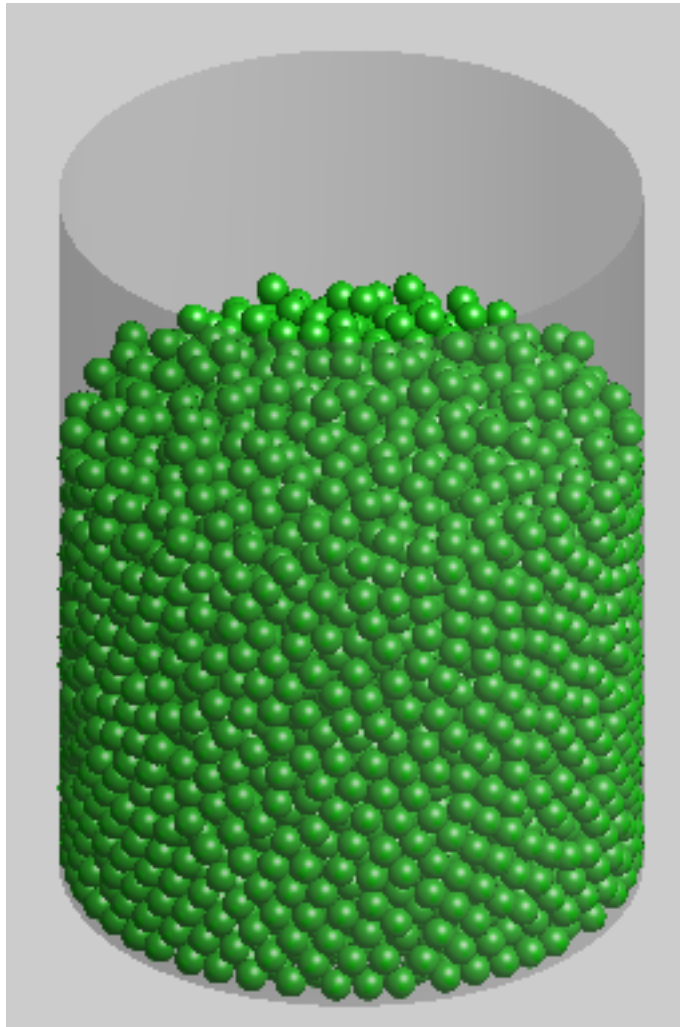


Figure 1: An image of the result of the calculation based on the input above.

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