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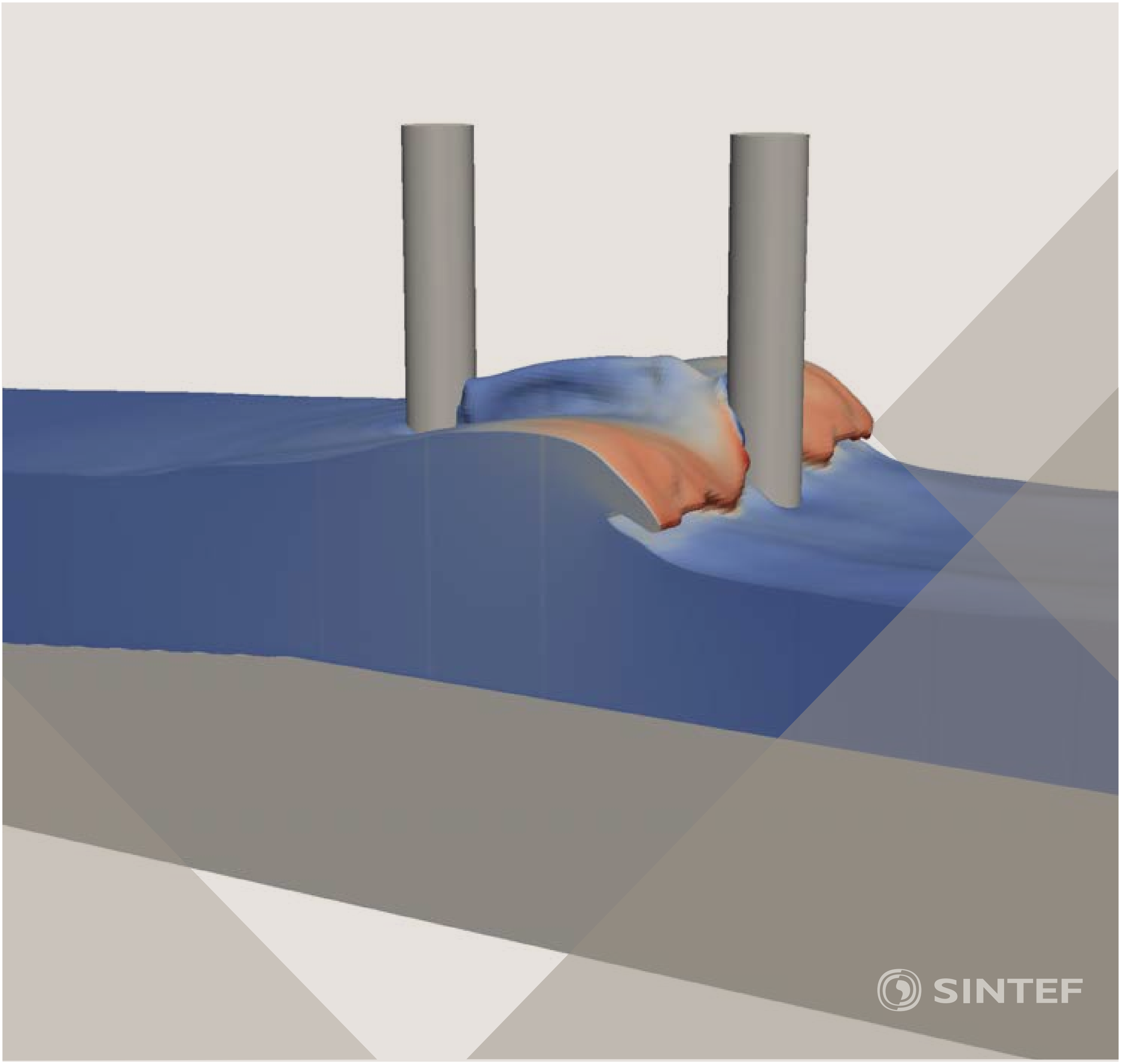
Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



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Editors:
Jan Erik Olsen and Stein Tore Johansen

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

NUMERICAL INVESTIGATION OF PARTICLE TYPES INFLUENCE ON PACKED BED ADSORBER BEHAVIOUR

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ABSTRACT

Packings are an inseparable part of Chemical Engineering processes like adsorption. Computational Fluid Dynamics (CFD) simulations on fully resolved packed beds can provide local flow information (e.g. wall effects and flow bypasses) which cannot be identified using ―black box" and/or one-dimensional modelling, which can have severe influence on the adsorption characteristics.
Creation of random packed beds is one of the main challenges in studying fully resolved packings; this can be covered using Discrete Element Methods (DEM). In this study the effect of using different types of particles on the fluid flow pattern in the packings was investigated. Three different types of particles (mono-disperse spheres, mono-disperse cylinders and poly-disperse cylinders) were packed into beds with identical dimensions (same height, same diameter) using custom DEM code and meshed using open source tools.
CFD simulations were performed using adsorpFoam, a newly developed solver for modelling adsorption, based on open source CFD code OpenFOAM®. In this stage of study particles were considered as non-reactive to investigate fluid flow only.
From simulated packings porosities as well as particle arrangements and positions have been analysed. Frequency and positions of high velocity spots were extracted. The residence time distributions were also analysed.
Furthermore, experiments with the identical types of particles were performed to verify the validity of the packing structure and global simulation results. The pressure drops derived from simulations were compared to the measured values from the beds in the lab and also available correlations and a good agreement was observed.

Keywords: Computational Fluid Dynamics, Packed bed, Particle, Discrete Element Method, Bypass, Pressure drop, OpenFOAM®.

NOMENCLATURE

Latin Symbols
D Bed diameter [m]
d Particle diameter [m]
m Mass [kg]
p Pressure [Pa]
q Energy [J]
S Source term [kg/m³/s, J/m³/s]
T Temperature [K]
u Velocity [m/s]
Y Mass fraction

Sub/superscripts
fluid Fluid phase
solid Solid phase
M Mass
E Energy
i Specie i

INTRODUCTION

In chemical engineering operations usually large contact surface areas are required for improving mass and heat transfer between phases. Packed beds are devices used for providing large surface area between fluids and solids. They are used in different processes like adsorption and chromatography. Packed beds are typically a column filled with solid particles. The shape of column, particles and D/d can have a critical effect on the performance and efficiency of the packed beds. A not optimally packed bed can have bypasses which causes small contact time and area between fluid and solid or it can have dead zones where there is no flow and that can cause very low mass and heat transfer (which are mainly driven by diffusion) and creation of hot spots inside the bed (Wakao and Kagei, 1982). There are different approaches to study design and packing of packed beds, e.g. zero or one dimensional process simulation approaches. Among available approaches computational fluid dynamics (CFD) can provide three dimensional spatial resolution besides time resolution which makes this tool very promising for studying local effects (e.g. bypasses and hot spots) in the packed beds (Calis et al., 2001).
Eppinger et al. (2010) introduced a new meshing method of beds filled with mono sized spherical particles by flattening the particle-particle and particle-wall contact points. They studied the pressure drop and the porosity of the beds with D/d between 3 and 10 using CFD. Behnam et al. (2013) suggested a new approach for modelling radial thermal convection based on averaged radial and axial velocity components from detailed CFD simulation of spherical packed beds. Dixon and Nijemeisland (2001) showed how CFD can

be used as a tool for studying packed beds in detail. They suggested development of reduced models which are detailed enough to be used for design purposes based on the detailed CFD simulations. They studied low D/d (2-4) bed behaviour for spherical particles. Taskin et al. (2010) used CFD for refining cylindrical particles for investigation of the flow, transport and reaction interactions in this beds and they observed non-uniform and non-symmetric surface and intra-particle variations and also steep temperature gradients at tube wall. Bey and Eigenberger (1996) performed experiments on different sphere, ring and cylinder sizes (3.3 < D/d < 11) and measured the radial velocity profiles below the beds and used the data for derivation of a model for predicting the porosity inside the beds. Beavers et al. (1973) performing experiments studied the effect of bed size on the porosity and flow characteristics of spherical random packed beds and they found out the porosity of the beds is not influenced by the bed size for D/d > 15. Experimental measurements performed by Ribeiro and Pinho (2010) on random packed beds of mono sized spheres were used for developing of a correlation for average bed porosity. Haughey and Beveridge (1969) analysed regular and random packed beds of spheres as a basis for examination of more general random packed beds. Dixon et al. (2011) studied the meshing of a single spherical particle and its effect on the quality of the simulations for heat transfer and fluid flow, they (Dixon et al., 2013) used this pre-study to investigated the effect of meshing and mesh quality at particle-particle and particle-wall contact points of spherical packings on the fluid dynamics and heat transfer inside the beds. They suggested using bridges between particles and also between particles and wall to reduce the error in calculated drag force and heat transfer.

Usually previous studies on packed beds limited to low D/d ratio or just one type of particles. The presented approach in this study is has been used with packings with D/d > 25 and including functionalized particles (e.g. adsorption) with internal heat and mass transfer and different particle types and particle size distribution. With this analysis it would be possible to investigate local overheating effects during e.g. adsorption process etc. However due to experimental limitations the columns with D/d ~6 was used for this validation study.

Spherical and cylindrical particle types are commonly used in packed beds (Mueller, 1992 – Giese et al., 1998). In this study three different types of particles (spheres, mono disperse cylinders and particle size distribution) were packed in the identical bed geometries using an in-house discrete element method (DEM) code. Similar packings were also built in the lab to verify the packing creation, meshing and CFD simulation of the beds. Different packing parameters from CFD/DEM (e.g. porosity, velocity distribution…) were investigated and compared for these three packings.

SIMULATION WORKFLOW

Packing creation

The first step in preparation for CFD simulations was creation of packings. For this purpose an in-house discrete element method (DEM) code was used. DEM is a numerical approach for modelling large number of particles interacting with each other and the surrounding geometry (Munjiza, 2004). Granular mediums of random shapes can be modelled with different methods. Multi-sphere approach is a powerful method for modelling random shapes. In this approach each particle is represented by a set of overlapping spheres which are treated as a unit and move together. However the diameter of spheres representing a particle is smaller, a more accurate representation of the particle shape is created. On the other hand by increasing the number of sub-spheres computational efforts also increases, therefore it is important to select a reasonable sub-sphere number to get the best possible simulation of the particles in reasonable time (Kruggel-Emden, 2008).

Table 1: Particle types and sizes.

Packing	Distribution type	Characteristic diameter [m]	Characteristic Length [m]
Sphere	Mono sized	0.006	-
Cylinder type 1	Mono sized	0.00506	0.00513
Cylinder type 2	Particle size distribution	0.0039 (0.0025 – 0.0044)	0.0054 (0.0029 – 0.0094)

Particle types and their sizes can be seen in table 1. Mono-disperse sphere particle and two types of cylindrical particles were packed into the beds. The cylinder type 2 particles have a varying aspect ratio (l/d) from 0.8 to 2.3. Particles were released into a cylindrical bed with inner diameter of 0.032 m from the height of 0.2 m from bottom of the bed. Particles were falling freely into the bed by gravity (9.8 m/s^2) in the direction of main bed axis.

Figure 1: Packing creation for mono-disperse cylinders: a – filling the beds with DEM code, b – correcting the bed heights to 0.013 m and exporting the STL, c – merging the main bed and particles STLs.

The filling was continued till a filling height more than 0.13 m was achieved (figure 1-a). Then the heights of beds were corrected to 0.13 m by keeping only the particles which were complete below this height. Particles were exported as STereoLithography (STL) file format (Jacobs, 1992) from the DEM code (figure 1-b). Bed geometry were also drawn in Catia® (3DS, 2017) and exported as STL. Particles and bed STLs were merged to create the final STL for meshing (figure 1-c).

Meshing

Prepared geometries in STL format were meshed using an open-source tool snappyHexMesh® which is an automatic mesher supplied with OpenFOAM® (OpenFOAM, 2017).

Figure 2: Mesh created for mono-disperse cylinders: a – mesh on the particles surfaces, b – mesh on the vertical centre cut plane, c – mesh on the horizontal centre cut plane.

In this mesher the main geometry is mapped into a base hexahedral mesh by refining the mesh close to STL surfaces and removing of the parts of the mesh which are not needed and snapping the mesh to STL surface (figure 2). The background mesh had a cell size [cubes] of 0.005 m and was refined on the STL surface up to four levels. In each level, the mesh is cut into half in each direction. The final meshes had around 1.5 million cells. In this study a new method for treating the contact points between particles and particles and walls was introduced. Creating the meshes using this method a bridge connection between the particles was created similar to Dixon et al. (2013) and Ookawara et al. (2007). Unlike their approach in this study the bridge is introduced by mesh and its size can be controlled by the minimum mesh size. The meshes had good quality and for improving the quality the very few skewed cells (< 10 cells in total) were removed from the meshes.

Solution

For simulating the flow through the packed bed a solver based on the open-source CFD code OpenFOAM® was developed. The new solver (adsorpFoam) is capable of modelling adsorption in the packed beds. In adsorption process target molecules are removed selectively from fluid by the solid (De Boer, 1956).

In the figure 3 the algorithm for adsorpFoam is shown. At the beginning of the time step the coupled Navier-Stokes and continuity equations are solved using the pressure implicit with splitting of operator algorithm (PISO) based on the pressure and velocity values from previous time step or initial conditions. Using the calculated pressure and velocity fields and based on the adsorption model applied, sink and source terms for heat and mass transfer are calculated. In the next step mass and heat transfer equations are solved and boundary conditions and also fluid and solid properties are updated.

Since the focus in this study is on the flow structure in the packed beds, the adsorption was deactivated to just simulate the flow through the beds.

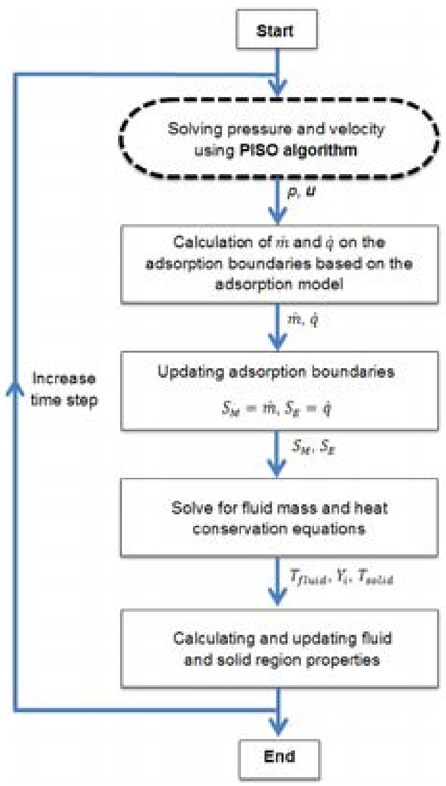

Figure 3: adsorpFoam algorithm.

Data extraction and evaluation

For analysing the simulation results data were extracted using open-source tool ParaView® (ParaView, 2017). An automation script was written for ParaView® to extract the radial and axial data from simulated beds. Two types of data were extracted and compared form beds:

- Geometrical information: number of particles, average porosities, particle centre positions, particles angles and axial porosities.
- Flow properties: bypasses, velocities, velocity distribution along radius and height, high velocity points, pressure drops and residence time distributions (RTD).

As it can be seen from figure 4 two sets of angles were extracted and analysed for cylindrical particles. The first angle (in this text it is referenced as ―Horizontal angle”) is the angle between the axial particle centre line and the horizontal plane (figure 4-a) and the second angle (in this text it is referenced as ―Radial angle”) is the angle between the particle centre line and the line which passes from centre of bed to the centre of mass of the particle (figure 4-b).

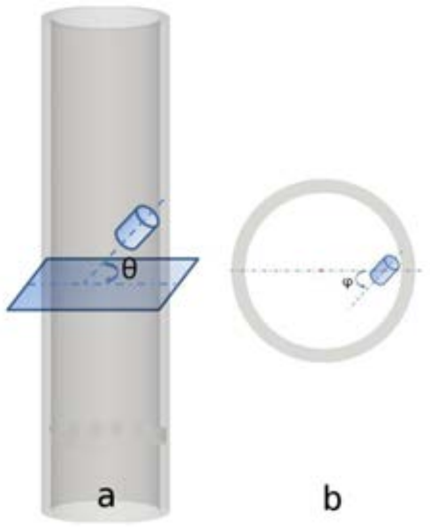

Figure 4: Particles angles: a – Horizontal angle: angle with horizontal plane, b – Radial angle: angle with line passing centres of particle and bed central axis.

EXPERIMENTAL

To verify the work flow for creation and simulation of the packings a similar bed with the same dimensions was built and packed with similar particle types.

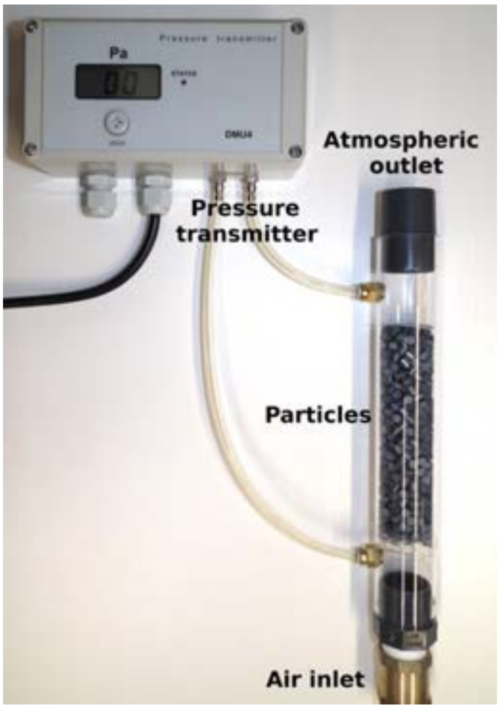

Figure 5: Experimental setup for mono-disperse cylinder packed bed.

As it can be seen in figure 5 air at ambient conditions (298 K and 10^5 Pa) enters the bed at the bottom and exits after passing the particles from atmospheric outlet. Average porosity and number of particles for all three types of particles were measured and compared to the results from DEM simulation. Also the pressure drop at different inlet velocities was measured and compared to the simulations.

SIMULATION SETTINGS

Identical to the experiments the fluid used for simulations was air at ambient conditions (298 K and 10^5 Pa). Walls and particles surfaces were treated with no-slip and isothermal boundary conditions. The outlet was set to pressure-outlet with absolute constant pressure of 10^5 Pa and zero-gradient velocity. For comparison between simulation and experiments the simulation inlet was set to velocity inlet and it was varied from 0.1 m/s to 1.6 m/s. The comparisons between simulations of three different types of packings were done at an inlet velocity of 0.829 m/s. No turbulence model was used since the Reynolds number in the packings are less than 2500 based on both Reynolds definitions: superficial velocity and bed diameter and also local velocities and particle diameters.

RESULTS AND DISCUSIONS

Simulations verification

Similar packings using DEM code and in lab were created. The beds were packed (for both experiments and DEM) by releasing the particles from the plane positioned at distance two times the final beds height (26 cm) from bottom of the beds to create consistent packed beds in both methods.
Different values from simulations were compared to the lab experiments. In table 2 in the second column (Number of particles) needed particles to fill the bed up to 0.13 m for both simulations and experiments were counted and compared. As it can be seen there is less than 2 % difference between number of particles packed into the beds using the DEM code and particles which were packed into the beds in the lab. In the third column the calculated and measured porosity from both methods are compared. In this case the deviation between simulations and lab experiments is bigger compared to the number of counts; it is mainly because the meshing in the areas where two particles collide, these regions were not fully resolved to keep the mesh computationally affordable. Also the particles used in reality were not perfect (especially cylinders) and that also caused larger deviation between the simulation and lab results.

Table 2: Comparison between DEM simulations and experimental measurements (the deviation between two methods is shown as percentage).

Packing	Number of particles (DEM/Reality)	Overall porosity (DEM/Reality)
Sphere	533/525 (Δ = 1.5 %)	0.429/0.432 (Δ = 0.7 %)
Cylinder type 1	599/605 (Δ = 1.0 %)	0.406/0.38 (Δ = 6.4 %)
Cylinder type 2	1007/1000 (Δ = 0.7 %)	0.418/0.393 (Δ = 6.0 %)

Figure 6 shows the measured and simulated pressure drop for spheres at different inlet (superficial) velocities. The results are also compared to very well-known Ergun equation (Ergun, 1949). As it can be seen good agreement between simulation, correlation and experiment can be observed.

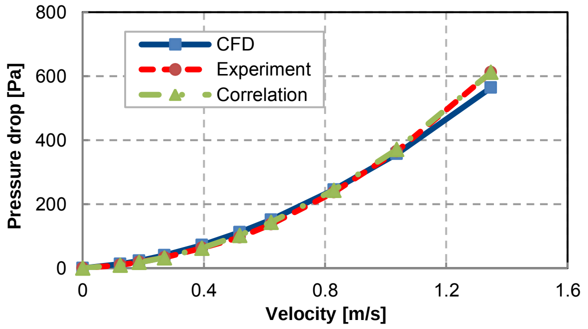

Figure 6: Pressure drop for spheres packed bed, simulation, correlation (Ergun) and experiments.

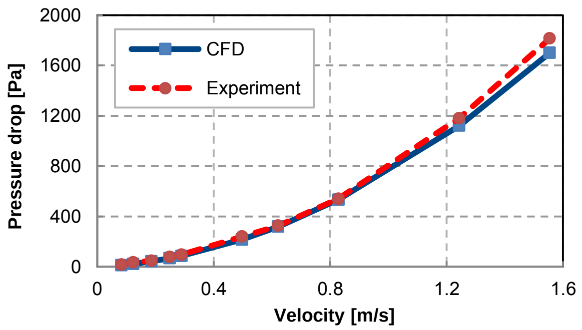

Figure 7: Pressure drop for cylinders type 1 packed bed, simulation and experiments.

The same comparison was also performed for the packed bed with cylindrical particles. The measured values from lab setup were compared to the simulations and good agreement was observed (figure 7 and figure 8). The slight deviation between measurements and experiments can be justified by the small difference in the created and simulated packed beds porosities.

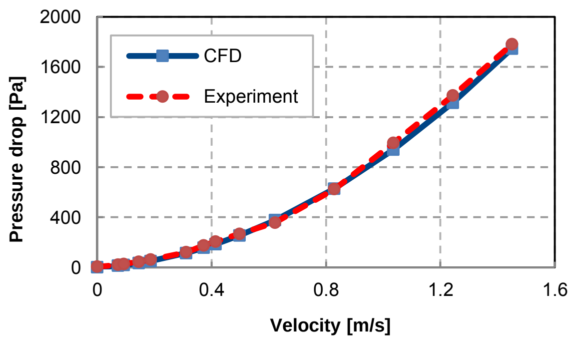

Figure 8: Pressure drop for cylinders type 2 packed bed, simulation and experiments.

Radial and axial porosities

Besides overall porosities calculated and reported for all three types of particles (table 2), local porosities in the bed radial direction and also bed axial direction were extracted and analysed.

As it can be seen from figure 9 by moving from centre of bed towards the walls the porosity fluctuates and reaches its maximum at bed walls (the data was extracted from 64 co-centric cylindrical cuts). The porosity for spherical particles was also compared to available correlations from literature (De Klerk, 2003) and a good agreement can be observed in the predicted frequency and amplitude of porosities fluctuations.

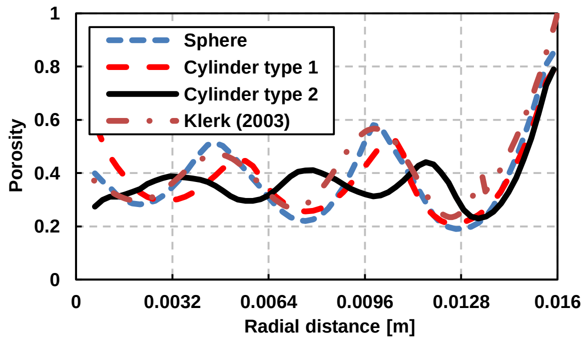

Figure 9: Average porosity on cylindrical co-centric cuts for all three types of particles vs. distance from centre of beds and also comparison to available correlation for spheres.

Higher porosity at walls creates possible fluid bypasses at walls. As it can be seen spheres have the biggest fluctuations in the porosity along the radius compared to the cylindrical packings. By changing the particle shape from spheres to cylinders these fluctuations reduces and in the case of cylinder type 2 particles (cylindrical particles with particle size distribution) packed into the bed the fluctuations in the porosity are smallest. The frequency of repetition of these fluctuations correlate with particles equivalent diameters which can be seen more clearly in figure 10, where the centres of mass of all of the particles are mapped to the top view. With spheres a clearer pattern in the centres of particles can be seen and this fades with going to particle size distribution cylinders.

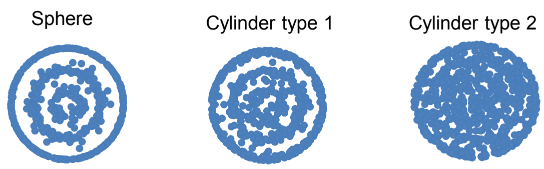

Figure 10: Centres of mass of particles mapped on the top view.

Figure 11 shows how the porosity changes over bed height for the different types of particles (data extracted over 520 planes along the bed height and the moving average of porosity with 20 points).

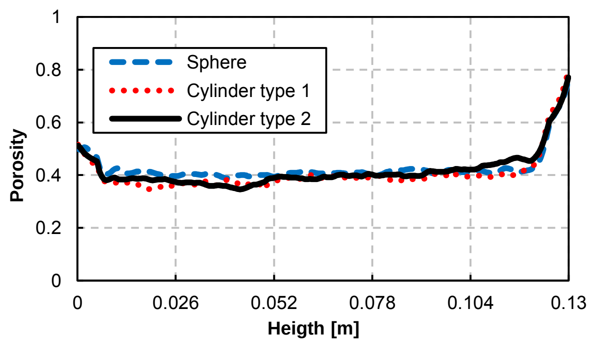

Figure 11: Moving average porosity along bed height for all three types of particles.

The porosity is almost constant and close to average porosity for spheres but it increases slightly along the bed height for cylinders because of the shaking effect of particles during the filling and repositioning of already filled particles. At the beginning and end of the bed the porosity increases, because of the end effects of particle contact with inlet section and also not smooth end of the bed.

Particles alignment

Another interesting parameter to be investigated for cylindrical particles is how particles align during their packing in the beds and effects of size distribution on their arrangement. If the particles tend to align along a specific direction (e.g. bed main axis) it is more probable channelling happens and that causes low fluid residence time and (short contact between fluid and solid) and decrease in adsorption performance.

Figure 12 shows how horizontal angle varies for cylinder type 1. As it can be seen for the full packing particles tend to be positioned more horizontally/vertically compared to incline in the bed.

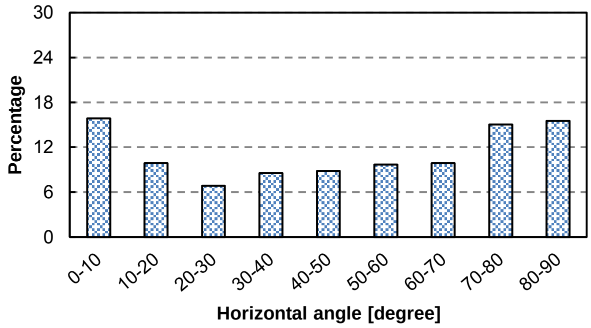

Figure 12: Horizontal angle distribution for mono-disperse cylinders.

In comparison particles distribution at all radial angles (figure 13) is similar and particles are frequently positioned more randomly compared to their horizontal angle.

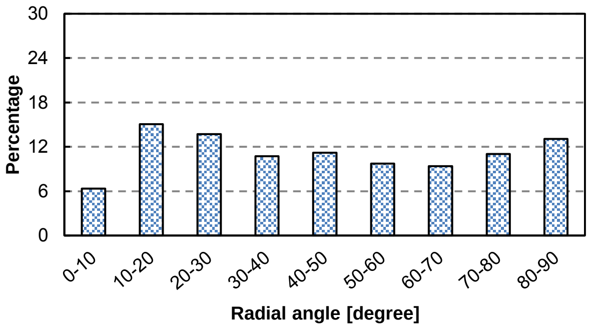

Figure 13: Radial angle distribution for mono-disperse cylinders.

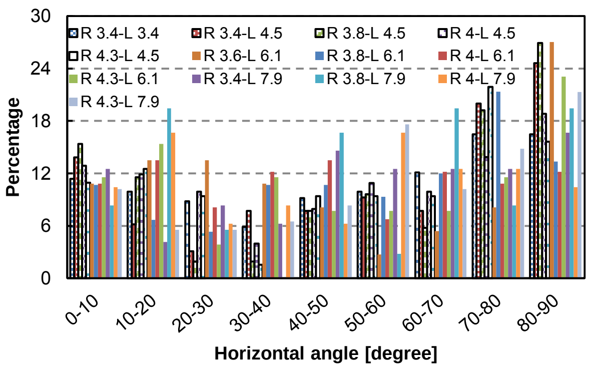

Figure 14: Horizontal angle distribution for particle size distribution cylinders.

In the bed with cylinder type 2 (particle size distribution) particles tend to be more vertical than horizontal or inclined. As particles become shorter in length they are more positioned vertically compared to longer particles (figure 14).

As it can be seen in figure 15 like mono-disperse cylinders, cylinder packing with particle size distribution has also more random spread of particles radial angles.

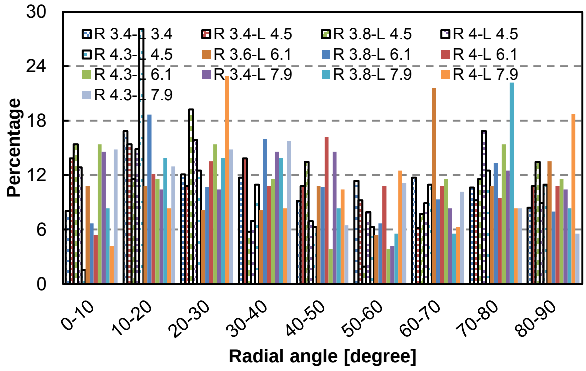

Figure 15: Radial angle distribution for particle size distribution cylinders**.**

Pressure drop

One of the parameters in operating cost of packed beds is the bed pressure drop. However this pressure drop is higher more energy is needed to pass the fluid through the bed. In figure 16 pressure drop for the beds is shown and compared. Pressures are average pressure extracted over 11 equally spaced planes along bed height. As it can be seen cylinders with particle size distribution have the highest pressure drop compared to the other two types of packings (as they have lowest void fraction). The pressure drop for sphere packing is more linear compared to the other beds, since the spheres are positioned more arranged and do not reposition and become denser by adding layers of particles. In the beds with cylinders adding more layers cause the lower layers to rearrange and become denser. This caused denser packing at the lower parts of the bed and contributed to the higher slope of the pressure drop curve in the lower zone. This effect can be seen more in the bed with particle size distribution.

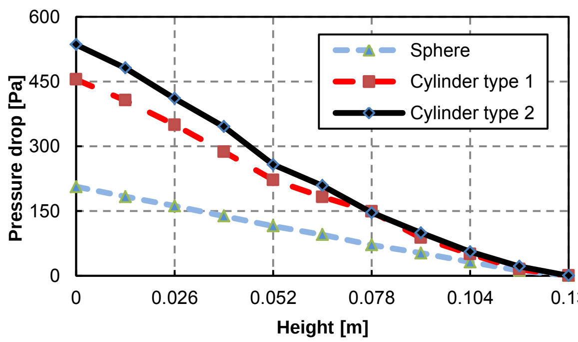

Figure 16: Pressure drop along bed height for different types of packing**.**

Velocity

Table 3 shows the average physical velocity magnitude (axial velocity difference less than 1 %) and also the peak velocities occurring in the beds (inlet and outlet sections are excluded). The average velocity is very similar the same in all of the beds since the average porosity was also similar. But maximum velocity in the beds is much higher in the bed with particle size distribution particles (more than two times more than spheres bed).

Table 3: Average and maximum physical velocity for the beds.

Packing	Average velocity magnitude [m/s]	Maximum velocity magnitude [m/s]
Sphere	1.93	7.5
Cylinder type 1	2.04	13.2
Cylinder type 2	1.98	15.6

Figure 17 shows how this high velocity points are distributed along the height and radius of the bed geometry. All the regions with velocity eight times bigger than inlet velocity are extracted and shown in this figure. In the upper part of the figure the beds are shown from front view and high velocity points are coloured with their distance from centre of the bed. In the lower part of the figure the same high velocity points are shown on the top view but coloured with their height from beginning of the packings.
As it can be seen and high velocity points happen more often in the cylindrical packed beds compared to sphere bed. In the sphere bed there are just a few high velocity points which shows the homogeneous distribution of the flow in the beds compare to the other beds. High velocity points are located mostly close to walls which can be justified by wall effects and higher porosities at the walls and they are randomly distributed along the bed height.

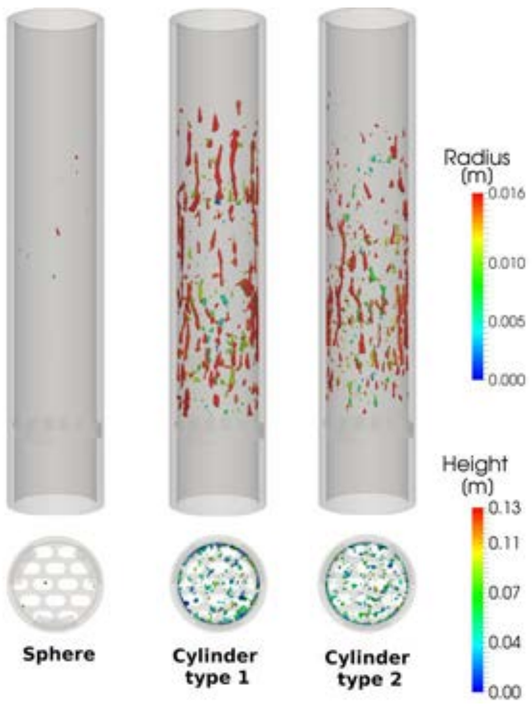

Figure 17: High velocity points (higher than eight times inlet velocity) in the beds: upper picture coloured with their distance from centre of the bed, lower pictures coloured with their distance form bottom of the packings.

The radial and axial velocity distributions in the beds follow similar pattern as the radial and axial porosity in the beds. Overall the velocities are higher close to walls compared to centre of the beds (figure 9).

Residence time distribution

Using residence time distribution (RTD) the amount of time a fluid element spends inside the beds can be evaluated and compared to the behaviour of a plug flow reactor. For simulating RTD a tracer was inserted uniformly at the beds inlet and its concentration at the outlet was recorded and compared for all three beds over the time.

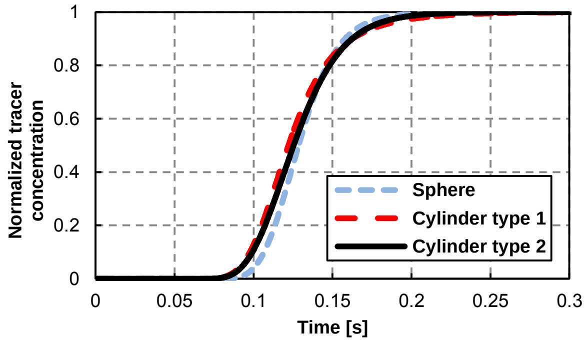

Figure 18: Residence time distribution for all three beds**.**

Figure 18 shows the RTD for three different types of bed. RTD curves look very similar since the porosities are comparable. Just in the sphere bed the breakthrough curve is steeper which shows it has a closer behaviour to plug flow and less channelling inside the bed. Tracer iso volumes (normalized concentration higher than 0.5) at t = 135 ms can be seen in figure 19.

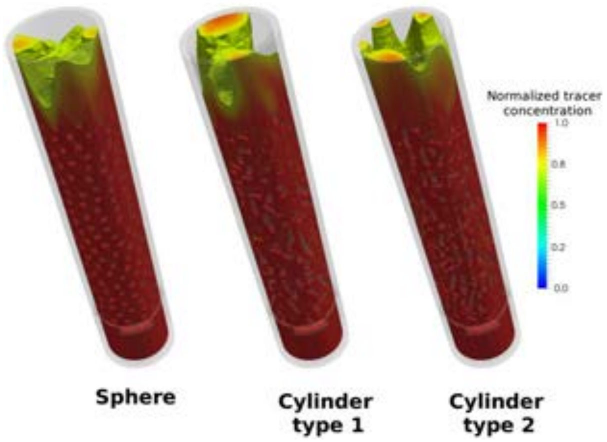

Figure 19: Tracer iso volumes (normalized concentration higher than 0.5) coloured with Normalized tracer concentration at t = 135 ms**.**

CONCLUSION

In this study the effects of particle type on the packing and packing properties were investigated. For this purpose three different types of particles (spheres, mono-disperse cylinders and particle size distribution particles) were packed into the same bed geometry up to the same height using a custom DEM code and simulated with a new solver developed based on the OpenFOAM® platform for simulation of adsorption phenomena. Experiments with similar types of particles in a bed with the same dimensions as simulated were performed to confirm the validity of the creation and analysis of the packings. Overall porosity of the beds, particle counts and also pressure drop of the beds at different inlet velocities were compared between experiments and simulations and good agreement was observed. In the next step the simulated packings were investigated in more detail to get a better and deeper understanding of their behaviour. Various parameters were investigated, pressure drop, particles angles, velocities and residence time distributions in the beds. Among investigated beds, the bed filled with spherical particles had the best flow distribution (less axial dispersion) and also the least pressure drop and the mono-disperse cylinders packed bed was the second for flow distribution and pressure drop. Residence time distributions were very similar for all three beds except a little sharper breakthrough for the spheres packed bed which also shows less axial dispersion for this packed bed.

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