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# Investigation of the Pressure Drop of Random Packed Bed Adsorbers

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Adsorption is one of the most often used unit operations in chemical engineering. However, due to computational limitations and time constraints simulations of adsorption processes are commonly done only with black box models or simplified porous media structures. In a new project an OpenFOAM® based CFD solver adsorpFoam, the required grid generation work flow using DEM methods for random packings and also post processing tools were created to carry out extended analyses of adsorption columns. Fully resolved packed beds were simulated to get more detailed information on gas side inhomogeneous distribution, bypass streams and near-wall effects (all these factors contribute to the total pressure drop of the packing), as well as fluid residence time distributions of random packings in columns.
The current work will summarize the first results of adsorpFoam with respect to the validation using gas flow in laboratory scale random packings: The code and the procedure have been tested for spheres, mono-dispersed cylinders and cylindrical particles with size distribution. In all cases, a good agreement of the experimental results and the CFD simulations has been achieved.
In a next stage of the project multi-component adsorption kinetics will be investigated, which are influenced by the local flow and temperature profile. Compared to common porous media CFD approaches a more realistic and reasonable residence time distribution can be achieved with this method.

## 1. Introduction

Adsorption is a well-known separation unit operation of thermal process engineering; it can be used for removal of trace substances of gaseous or liquid streams for concentrating or purifying product streams. One common application is, for example, biogas for injection into methane gas grids or the removal of dioxins from waste incinerator flue gas (Bathen and Breitbach, 2001). The common procedure for designing is using zero or one-dimensional process simulation tools (e.g. Aspen Adsim®) which are very good for fast evaluation but have no or very limited spatial resolution. The spatial resolution is needed because packings are not ideal and flow is not homogeneously distributed (Boccardo et al., 2015). That might cause bypassing gas streams, dead zones inside the packing, void zones in the packing, thermal hot spots etc. (Achenbach, 1995). This is where CFD can be applied to investigate and analyse such irregularities and calculate the effect on the separation performance of the adsorber unit (Atmakidis and Kenig, 2009). One key parameter is the correct prediction of the pressure drop of the packings – therefore it was selected as main variable for this experimental validation procedure.

## 2. Computational Fluid Dynamics (CFD)

Using computer based simulations for analysing fluid systems including fluid flow, mass transfer, heat transfer and etc. is known as Computational Fluid Dynamics or CFD (Fletcher, 1988). Compared to black box or one dimensional modelling, CFD provides a full three-dimensional spatial discretization, which lets the user have a very detailed view into the phenomena. The technique is powerful and covers a wide range of industrial and

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non-industrial applications. Although CFD has many advantages, but still it cannot be utilised without proper knowledge of the phenomena by the user. CFD is usually combined with other analysis tools and experimental tools like laboratory scale equipment to get more complete and more reliable results.

## 3. OpenFOAM®

There are two different types of CFD packages available, commercial and non-commercial. Among non-commercial packages open source codes are becoming more and more interesting, because compared to commercial codes, no license fee is necessary in using them. Since the source code is available, it provides the capacity of introducing new ideas into the software like the implementation of new models, algorithms and solvers. OpenFOAM® (OpenCFD, 2016) is one of the open source CFD codes which is published under the GNU public license - GPL (Stallman, 1993) and it has a good reputation for its extendibility and robustness. The code has been written in the programming language C++ and because of being object oriented it is easy to modify or extend.

## 4. adsorpFoam

There is no solver available in the original OpenFOAM® package which can compute adsorption. adsorpFoam (Haddadi et al., 2015) is a CFD solver developed based on OpenFOAM® for modelling adsorption phenomena. The solver is capable of multi-region, multi-species simulation with support of multi-component adsorption. The solver can handle surface adsorption and modelling of heat transfer inside solid particles. In this study we are not looking at the adsorption in packed beds therefore, the applicability of adsorpFoam for the simulation of fluid flow in the packed beds was demonstrated.

## 5. Discrete Element Method (DEM)

The Discrete Element Method (DEM) is a numerical method for modelling the movement and interaction of particles of various sizes and shapes (Norouzi et al., 2016). There are different approaches for modelling granular mediums of random shapes. One of the widely used methods is known as multi sphere approach. In this method non-spherical particles are estimated using overlapping spheres. By making the sub-spheres smaller and consequently increasing their number in one particle, the approximation of the main particle becomes more accurate but it becomes computationally more expensive. Therefore, it is important to select a suitable sub-sphere size for most accurate simulations in reasonable time.

## 6. Workflow

### 6.1 Particle type and size distribution

The simulations were performed on three different particle packings. The three types of particles and their size distributions are summarized in Table 1.

*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) |

The particle sizes and distributions were measured from particles available in the laboratory; the same particles have been used in the next stages for validation.

### 6.2 Bed geometry and packing

The bed geometry used for simulations was also measured from a setup prepared for validation experiments in the laboratory (Figure 1(a)). The bed is a cylinder which has an inner diameter of 0.032 m and a packing height of 0.13 m. Using an in house developed code, the DEM simulations for filling of the bed with the particles were done. This DEM code has the capability of creating different types of packings in different types of geometries. By using sub-sphere model in the DEM code any type of particle can be modelled. After filling the bed, the packing height was corrected to the required packing height of the experimental setup (Figure 1(b)).A built-in conversion tool in the DEM code was applied to export the surfaces of the particles as an STereoLithography(STL) file for the meshing stage (Figure 1(c)).

### 6.3 Finalizing geometry and meshing

The original empty bed geometry, including internal parts of the bed like the support grid, was created in a CAD program and then exported as STL. For performing the CFD simulations a spatial discretization is always needed, this discretization is called meshing. Inserting the packing STL file into the final bed STL, the final geometry was ready for meshing (Figure 1(d)). The boundaries were defined as shown in Figure 1d, the gas inlet is at bottom, the gas outlet is at the top. The meshing process was done using an OpenFOAM® mesh generation utility called snappyHexMesh (Figure 1(e)).

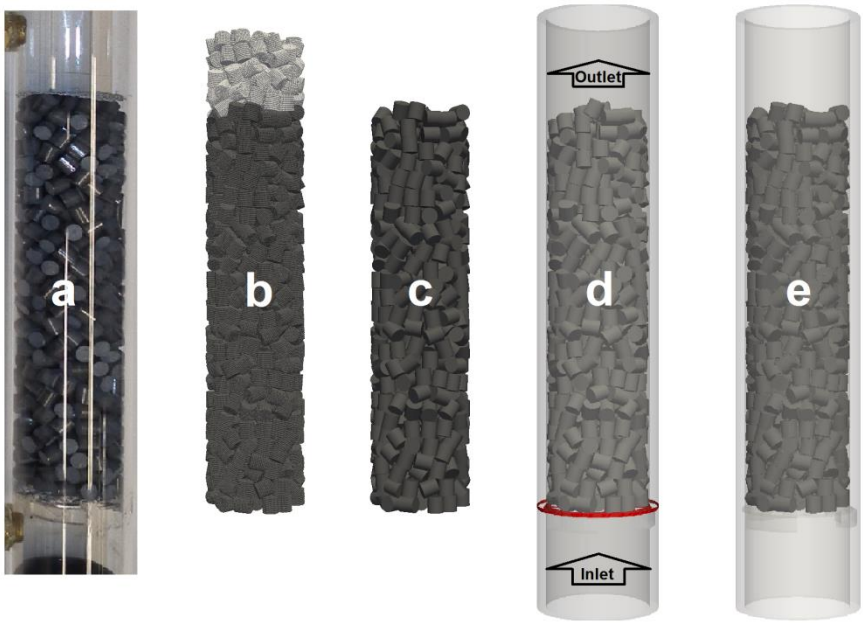


*Figure 1: Packing and mesh creation work flow*

### 6.4 Flow simulation

Using adsorpFoam and the mesh which was prepared in the last step, the flow simulations were done. As the main focus at this stage was the investigation of packings and packing quality, adsorption was not modelled in this study. The gas was air at ambient conditions (298 K, $10^5$ Pa) and the inlet gas velocity was 0.829 m/s.

### 6.5 Post processing and data evaluation

For post processing different tools were programmed. One important tool is an automation script for open source visualizing software Paraview® (Paraview, 2016) and also the code for creating cylindrical cuts and clips in the geometry. Post-processing was done in two steps. In the first step (before the fluid flow simulation), particles positions, the overall porosity and local porosity of the beds in different directions were extracted. In the second step, the flow data like pressure drop and velocity distribution in the beds were prepared for evaluation.

## 7. Validation

For checking the whole workflow process and the accuracy of the methods for all three particle types the same experimental setup was tested in the laboratory. Different properties were measured for each of the packings and compared between experiments and simulations:

- The number of particles needed for filling the bed to 0.13 m (Table 2).
- Overall porosity of the packing (Table 2).
- Packing pressure drop at different flow rates (Figure 2).

*Table 2: Comparison between simulation and experimental data (the percentage in the parenthesis shows the deviation between DEM and experiment)*

| 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 | 1,007/1,000 (Δ = 0.7 %) | 0.418/0.393 (Δ = 6.0 %) |

As it can be seen from Table 2, the number of particles is in good agreement between simulation and experiments (less than 2 % in all cases). The calculated overall porosity is also very close to the experimental values (less than 7 % error in all cases).

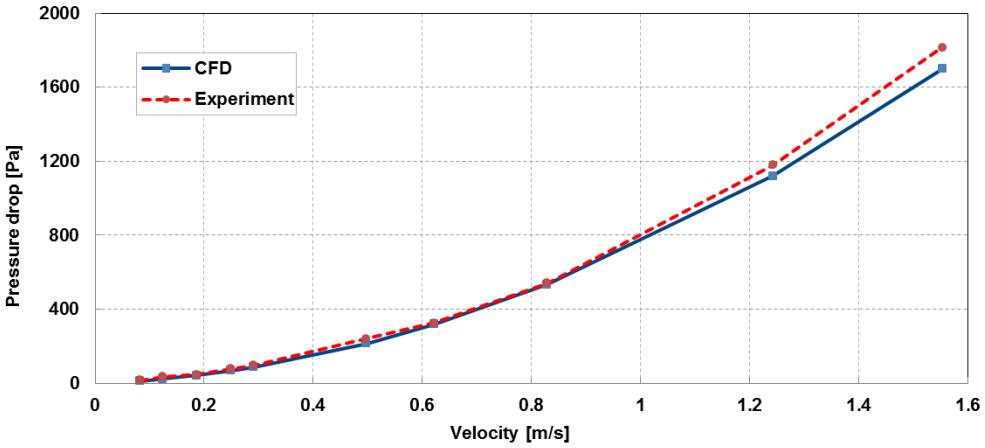


*Figure 2: Cylinder type 2 packing pressure drop at different flow rates, CFD vs. experiment (for sake of space just the one for cylinder type 1 is shown here)*

The pressure drop curves for experiments and simulations are following the same trend and are overall in reasonably good agreement (Figure 2).

## 8. Results

### 8.1 Radial porosity distribution

Figure 3 shows the porosity distribution for all three cases versus the radial coordinate of the bed. As it can be seen in Figure 3 in all packings porosity fluctuates along the bed radius and it has its highest value at the bed wall, which is expected (Achenbach, 1995). Cylinder type 2 packing (cylinders with particle size distribution) has a lower fluctuating amplitude compared to the two other packings. The same pattern can also be seen in the small figures inside Figure 3, which show the projection of the particle centres to the top plane. These particles have a more structured arrangement in the Sphere case which leads to three distinct maxima of the porosity curve with a distance of one sphere diameter (the maxima are equivalent with the circles in the top view). The non-spherical particles and the size distributions cause packing irregularities which partially smooth away the maxima due to physical constrains, except for the near wall particles.

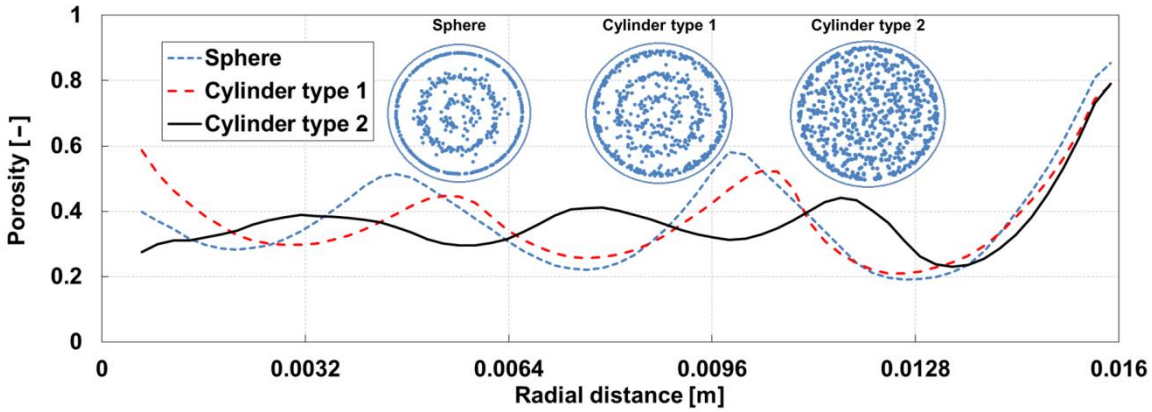


*Figure 3: Radial porosity distribution along bed radius, inserted figures show the particle centres in top view*

### 8.2 Pressure drop

As expected, there is a close to linear pressure profile along bed height. As also expected, based on porosities, the packed bed Cylinder type 2 has the highest pressure drop along the height because it has the lowest porosity.

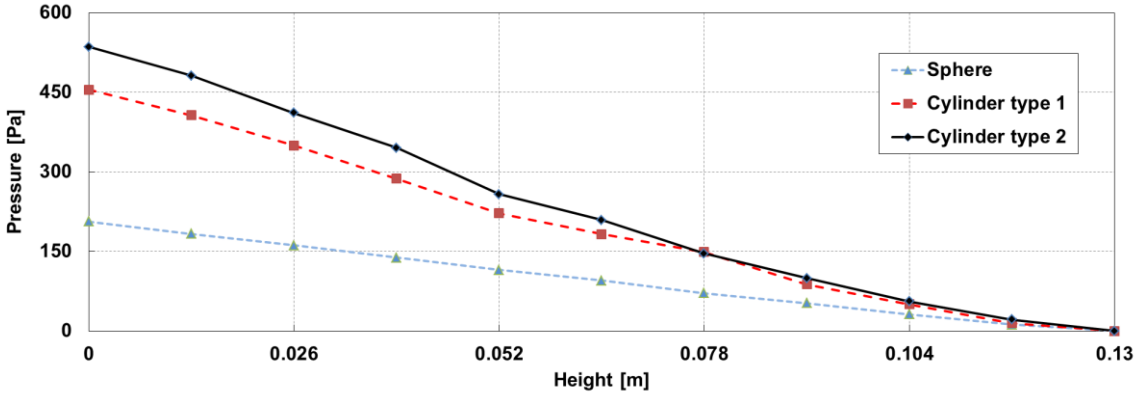


*Figure 4: Pressure drop along bed height*

### 8.3 Velocity

The radial averaged axial velocities are consistent with the porosity profile in Figure 2. In Table 3 maximum and volume averaged physical velocities for all three cases are listed. Average physical velocities are very close to each other but the maximum velocity which is occurring in the beds is the highest in the bed with particle size distribution in there (Cylinder type 2).

*Table 3: Maximum and average physical velocity for all cases*

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

Figure 5 in the left hand side shows the stream lines coloured by velocity magnitude. The streamlines indicate a quite uniform flow for the spherical packing – whereas the cylinder packings demonstrate more pronounced channelling effects close to the column wall. To confirm the positions of the channelling events, another plot has been introduced: Only cells with velocities higher than 8 times the inlet velocity (~ 6.6 m/s) are shown, the colour indicates the radial distance of the region from the column axis. This shows that most of the larger void zones (channelling events) are close to or even at the wall due to the packing irregularities caused by the cylindrical shape of the particles.

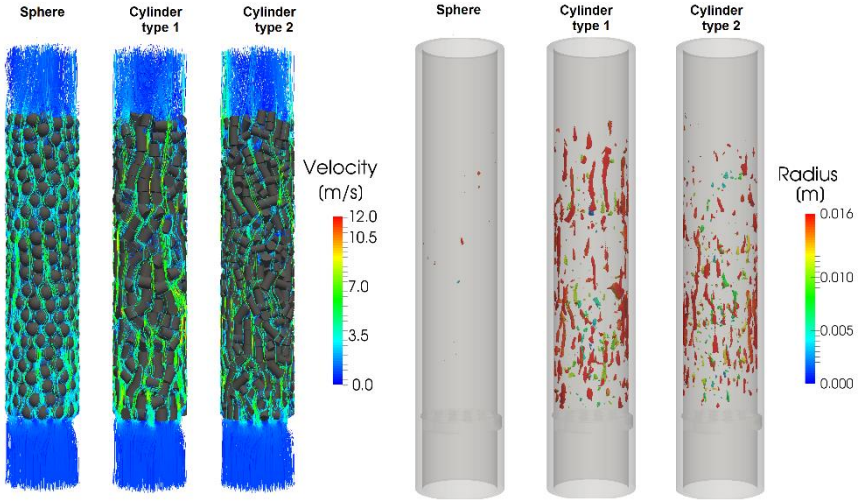


*Figure 5: Velocity streamlines (left hand side) and high velocity zones (right hand side)*

### 8.4 Residence Time Distribution (RTD)

In Figure 6 the residence time distribution for all three packed beds are shown (calculated as tracer step response at the outlet of the geometry).Since the porosities are quite close to each other, the RTD curves also

look very similar. Just the “Sphere” case has a little sharper breakthrough curve which shows that it is closer to a plug flow inside and less channeling inside the bed.

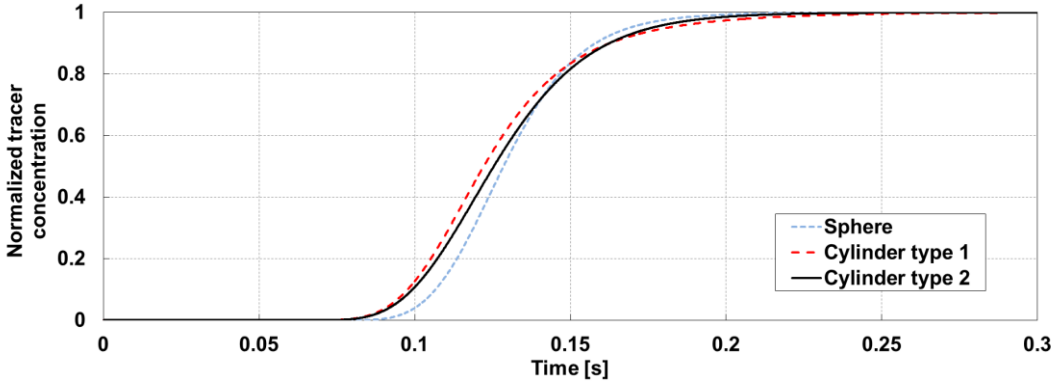


*Figure 6: Residence Time Distribution curve from transient CFD simulations for all three packed beds*

## 9. Conclusions

Three different types of packings were analysed using the work flow presented in this paper.Packing surfaces have been created by using a multi-sphere capable DEM code and extracting STL representations of the particles. They were meshed using the open source meshing tool snappyHexMesh and the packed bed gas flow was simulated using adsorpFoam, a newly developed solver based on OpenFOAM®. At this stage, just the flow was investigated and adsorption was not included in the simulations. The whole process was validated against experimental data. Data extraction was done using a customized and extended script for Paraview®. Among different types of packings investigated here, mono-sized spheres had the lowest pressure drop at the same operating conditions as the other packings consisting of cylinders. The lowest average porosity could be found fora mono-sized cylinder packed bed resulting in the highest amount of high velocity zones. The highest axial velocity was occurring in the bed with cylinders with the particle size distribution. In the next stage of project multi-component adsorption (Doung, 1998) simulations will be carried out to find out more in detail about effect of different packing types on quality of adsorption. Preliminary tests demonstrated that the new work flow is capable of handling packed columns with column diameter to particle diameter ratios of 25:1 and larger.

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