# DEM-CFD STUDY OF FLOW IN A RANDOM PACKED BED

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**Abstract**

Most catalytic surface reactions as well as other industrial applications take advantage of fixed packed bed reactors. Designers of these reactors rely mostly on empirical formulas derived for various simplifying assumptions, e.g. uniformly distributed porosity. The made simplifications and especially the assumption of uniformly distributed porosity fail if the tube to particle diameter ratio goes under 10 and the „wall effect" becomes more significant. In such a case, the complete three-dimensional structure of the packed bed has to be considered. Thanks to ongoing improvements in numerical mathematics and computational power, the methods of computational fluid dynamics (CFD) have become a great tool for comprehensive description of the packed beds with low tube to particle diameter ratio. Three-dimensional simulations of the flow through two fixed beds differing in the type of the used particle are presented and compared with available experimental and empirical results. To generate the random fixed beds, we propose a custom approach based on the discrete element method (DEM) code implemented in open-source software Blender. Thereafter, OpenFOAM tools (snappyHexMesh, simpleFoam) are used for creation of the computational mesh and solution of the governing equations describing a single-phase flow in the packed bed.

**Keywords:** CFD, DEM, Random fixed bed, Pressure drop, OpenFOAM

# 1 Introduction

Random fixed bed reactors are widely used to perform catalytic surface reactions [1]. However, the usage of random fixed beds is not limited to the reaction engineering. Random packings are commonly applied for example in extraction and distillation columns [2]. In this work, we study the fluid flow through random fixed bed. Various flow properties are examined, especially the dependence of the bed pressure drop on (i) the fluid volumetric flow rate and (ii) the type of particles forming the fixed bed.

Generally, the random fixed beds are modelled via empirical formulas derived from various simplifying assumptions. One of the usually made simplifications is an assumptions of a uniform porosity distribution in the packed bed [3]. The assumption of uniformly distributed porosity fails if the tube to particle diameter ratio goes under 10 and the „wall effect" becomes more significant. The complete three-dimensional structure of the packed bed has to be considered for the packed beds with low tube to particle diameter ratio.

With recent advances in numerical mathematics and computational power, the methods of computational fluid dynamics (CFD) have become a great tool for comprehensive description of the packed beds that cannot be accurately described by the available empirical formulas, see e.g. [3] and references therein. In this work, we present and validate a finite volume method (FVM) based CFD model for a three-dimensional (3D) flow of an incompressible Newtonian fluid through two different types of random fixed bed. The selected bed types consist of uniformly sized spheres or Raschig rings, which are common in the chemical engineering practice.

The 3D structure of the complete bed is needed when making the CFD model. Several authors chose different approaches to the creation of such structures, e.g. the Monte-Carlo process [4] or DEM [3]. To generate the random fixed bed, we propose a custom method based on the DEM code implemented in the open-source software Blender.

The generated bed consists of randomly placed mutually touching particles. Contact points between the particles proved to be problematic for the subsequent mesh generation [5]. Automatic mesh generation programs create low quality cells near the contact points, which makes the generated finite volume mesh unusable for calculations. Different approaches to improve the overall mesh quality can be found in literature e.g. particle size reduction, size increase or flattening of the contact point [3]. In this work, we use cylinders to bridge the contact points. The applied method is similar to the one developed by Ookawara et al. [5].

The random fixed bed structure is processed via the OpenFOAM toolbox [6]. The bed geometry is meshed by the snappyHexMesh automatic mesh generator and the flow is solved using the simpleFoam solver. An overview of the used modelling approach is depicted in Fig. 1. The whole process of generating the bed structure, creating a finite volume mesh and solving the flow is fully automatic and therefore suitable for parametric studies.


**Figure 1.** Illustration of methodology

## 2 Mesh Generation

Usage of snappyHexMesh to generate a FV mesh usable for subsequent calculations requires a standard triangle language (STL) file describing the geometrical structure of the packed bed. To create such a file, we propose an algorithm for the open-source software Blender. The overall bed geometry is generated to correspond as close as possible to the experimental apparatuses used for the proposed model validation.

The model was validated using two experimental devices. Both the devices consist of a tube with inner diameter $d_t = 0.06$ m and height $h_t = 1$ m filled with random packing. One device is filled with spherical particles and the other with Raschig rings. Due to the limited available computing power, it was impossible to simulate the whole packed bed. Thus, 250 spherical particles (2.6 cm of fixed bed) and 50 Raschig rings (8.5 cm of fixed bed) were used for simulations.

We summarize the generation of the packed bed of Raschig rings in Alg. 1. The algorithm for the fixed bed consisting of spheres is similar. However, there is no need for rotation and hole creation.

```
Create cylinder with diameter d_t=0.06m, height h_t=0.1m, numOfVertices=64
Locate centre of floor plate of column at the origin of coordinates system
for i in range (1, 32):
    vertices[i].select = True
mesh.delete(type='FACE')                      # remove top face selected by vertices
                                              # to create column
for i in range (0, 49):
    Crete cylinder with diameter d_r=0.015m, height h_r=0.015m, numOfVertices=64
    location=(-.015+(random()*.03), -.015+(random()*.03), .05+i*.017)  # relocate cylinder
    rotate(10, axis=(random()*10, random()*10,random()*10))            # rotate
    for n in range (1, 32):                   # making hole to cylinder to create
                                              # Raschig ring
        vertices[n].select = True
    mesh.inset(thickness=0.25)                # inset face on the top of cylinder
    mesh.delete(type='FACE')                  # delete inner face
    for n in range (33, 64):
        vertices[n].select = True
    mesh.inset(thickness=0.25)                # inset face on the bottom of cylinder
    mesh.delete(type='FACE')                  # delete inner face
    k = 1
```

```
    while k < 64:                               # connect inset faces
        for n in range (1, 4):
            vertices[k].select = True
        mesh.edge_face_add()                    # add face between four vertices each loop
        k -= 2
    #Set properties for physics engine
    bullet.physics_type = 'RIGID_BODY'
    bullet.use_collision_bounds = True
    bullet.radius = 0.0035
    bullet.velocity_max = 10                    # for better collision detection
    bullet.collision_margin = 0.002             # detection of overlap
    bullet.form_factor = 0.001                  # low friction
Start physics engine until velocities are equal to zero for 10 seconds
```

**Algorithm 1.** Structure generation in Blender

The proposed algorithm utilizes the physics engine Bullet to simulate falling of particles to the tube. Bullet is the C++-code physics engine available in Blender and it is based on the discrete element method (DEM) [7]. DEM is a finite difference numerical method for prediction of the motion of individual and independently moving objects. The objects motion is calculated with a fixed time step. The algorithm accounts for all forces affecting each object during each time step. A simplified algorithm of the Bullet engine is given in Alg. 2 [8, 9]. DEM simulations for spheres were faster because the shape of the spherical particles is better for DEM.

**for** $i = 0$ **to** $N_p - 1$ **do**

    **#Compute theoretical position based on Newton´s second law**

    eq1 := $m_i \frac{d\boldsymbol{U}_i}{dt} = \boldsymbol{F}_i$ ; eq2 := $\boldsymbol{J}_i \frac{d\boldsymbol{\omega}_i}{dt} + \boldsymbol{\omega}_i \times \boldsymbol{J}_i \boldsymbol{\omega}_i = \boldsymbol{M}_i$

    eq3 := $\boldsymbol{U}_i = \frac{d\boldsymbol{x}_i}{dt}$ ; eq4 := $\boldsymbol{\omega}_i = \frac{d\boldsymbol{\theta}_i}{dt}$

    eq5 := $\boldsymbol{F}_i = m_i \cdot g$

    **#Collision detection**

    $\boldsymbol{F}_i = \boldsymbol{F}_i + \sum_{j=0}^{N_p-1} \boldsymbol{F}_{ij}$ **#Collision forces depend on overlap and particles velocities**

    $\boldsymbol{M}_i = \sum_{j=0}^{N_p-1} \boldsymbol{R}_j \times \boldsymbol{F}_{ij}$

    **#Right positions for next time step are compute**

t = t + Δt

**#Used variables:** $\boldsymbol{N_p}$ **number of particles in system**

**#** $\boldsymbol{m_i}$ **mass of particle**

**#** $\boldsymbol{U}_i$ **translational velocity of particle**

**#** $\boldsymbol{J}_i$ **inertia tensor**

**#** $\boldsymbol{\omega}_i$ **angular velocity of particle**

**#** $M_i$ **torques applied on particle**

**#** $\boldsymbol{R}_j$ **vector pointing from centroid to contact point**

**#** $\boldsymbol{t}$ **time**

**#** $\boldsymbol{F}_i$ **forces applied on particle**

**#** $\boldsymbol{x}_i$ **centre of particle mass position**

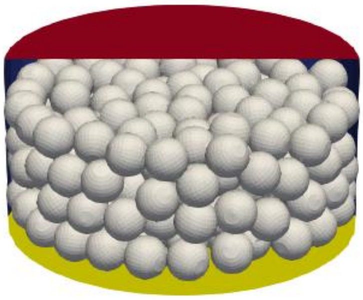
**#** $\boldsymbol{g}$ **gravity force**

**#** $\boldsymbol{F}_{ij}$ **contact force vector between particles i and j**

**Algorithm 2.** DEM scheme

The Bullet engine is set up to make 50 physics corrections for every time step and there are 4 sub-steps for every correction. After the last directly simulated particle falls into the column, we set the gravity to linearly increase to account for the weight of the rest particles and to ensure faster convergence of the geometry to the desired bed structure. Physics engine setup is validated by comparing the porosity of the artificial structure to the porosity of the experimental bed. The difference in porosities is less than 1% for both the simulated types of packing.

After the physics engine convergence, an STL file containing the generated bed structure, see Fig. 2, is exported from Blender and imported into snappyHexMesh, the OpenFOAM utility for meshing of complex geometries. The meshing process itself is fully automatic. The output of snappyHexMesh is an unstructured hex-dominated mesh conforming to the generated packed bed geometry.



**(a)** Spheres

**(b)** Raschig rings

**Figure 2.** STL surfaces generated from Blender coloured according to the patch type

# 3 CFD setup

The simpleFoam solver is used to solve the steady-state Navier-Stokes equations for an isothermal flow of an incompressible Newtonian fluid in the packed bed geometry [10].

$$\nabla \cdot \boldsymbol{U} = 0 \tag{1}$$

$$\nabla \cdot (\boldsymbol{U} \otimes \boldsymbol{U}) = -\nabla p + \nabla \cdot \boldsymbol{T}, \tag{2}$$

where $\boldsymbol{U}$ stands for velocity field, $p$ corresponds to the kinematic pressure, $\boldsymbol{T}$ is the viscous stress tensor defined as $\boldsymbol{T} = \upsilon \nabla \boldsymbol{U}$, and $\upsilon$ is the fluid kinematic viscosity. The simulated fluid properties were set up to correspond to the "fresh" water with $\upsilon = 1.3 \cdot 10^{-6}\ \mathrm{m^2\ s^{-1}}$ and density $\rho = 997\ \mathrm{kg\ m^{-3}}$. To account for potential turbulence, we used the Reynolds-averaged variant of the Navier-Stokes equations in conjunction with the k-ω SST model [11]. The system of equations needs to be completed with the suitable boundary conditions, which are given in Tab. 1. Each type of boundary (patch) is shown in different colour in Fig. 2.

| Boundary | colour in Fig. 2 | condition for $\boldsymbol{U}$ | condition for $p$ | condition for $k$ | condition for $\omega$ |
|---|---|---|---|---|---|
| Inlet | yellow | flowRateInletVelocity | zeroGradient | fixedValue | fixedValue |
| Outlet | red | inletOutlet | fixedValue | inletOutlet | inletOutlet |
| Wall | blue | noSlip | zeroGradient | zeroGradient | zeroGradient |
| Bed | white | noSlip | zeroGradient | zeroGradient | zeroGradient |

**Table 1.** Boundary condition for the set of equations

The applied boundary conditions are standard ones, possibly with the exception of the flowRateInletVelocity used at the inlet and the inletOutlet used at the outlet. The flowRateInletVelocity is a Dirichlet type boundary condition prescribing such an inlet velocity that the fluid inflow into the domain would correspond to a pre-set value of inlet flow rate $Q_i$. The inletOutlet boundary condition enforces (i) a Neuman type zero-gradient boundary condition if the fluid flows out of the computational domain or (ii) a Dirichlet type boundary condition if the velocity field in the domain would require a fluid inflow. In our case, the Dirichlet boundary condition was prescribed as $\boldsymbol{U} = (0,0,0)^{\mathrm{T}}$ to prevent the fluid from flowing into the domain through the outlet patch.

# 4 Results

## 4.1 Mesh size independence study

To determine the suitable mesh size for the simulations of flow in the fixed bed composed of spherical particles, we investigated the pressure drop over the bed for the liquid flow rate $Q_i = 0.15\ \text{dm}^3\ \text{s}^{-1}$. The pressure drop marked dp/dh is the difference in the pressure above and below the packed bed divided by the bed height.

We illustrate the results of the mesh size independence study for the spherical particles in Fig. 3. Each point is labelled by the relative difference between the current result and the value calculated on the finest tested mesh. The result obtained on 7.5 million cells differs from the result on the finest mesh by less than 0.5%. Hence, the mesh with 7.5 million cells is used for the following simulations. A similar study was performed for the case of Raschig rings and $Q_i = 0.3\ \text{dm}^3\ \text{s}^{-1}$. The mesh used for the simulations of the packed bed consisting of Raschig rings has 6.8 million cells.

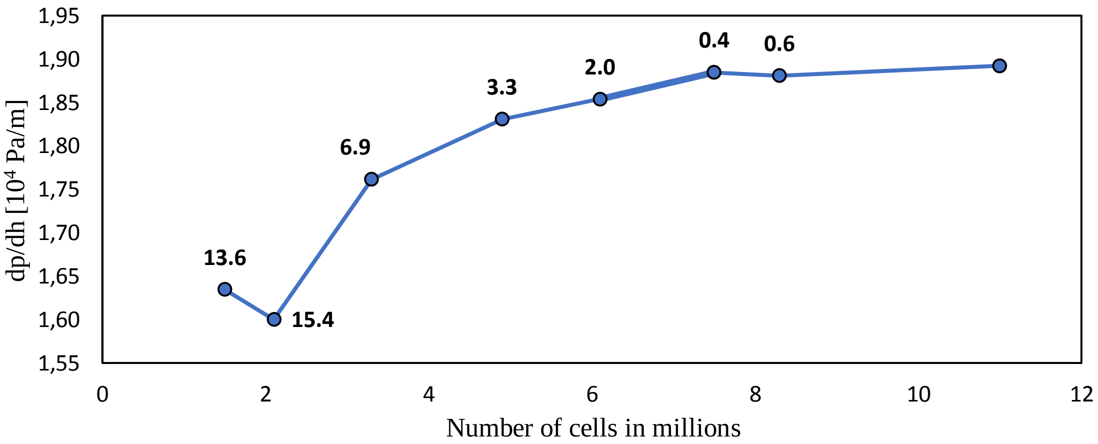
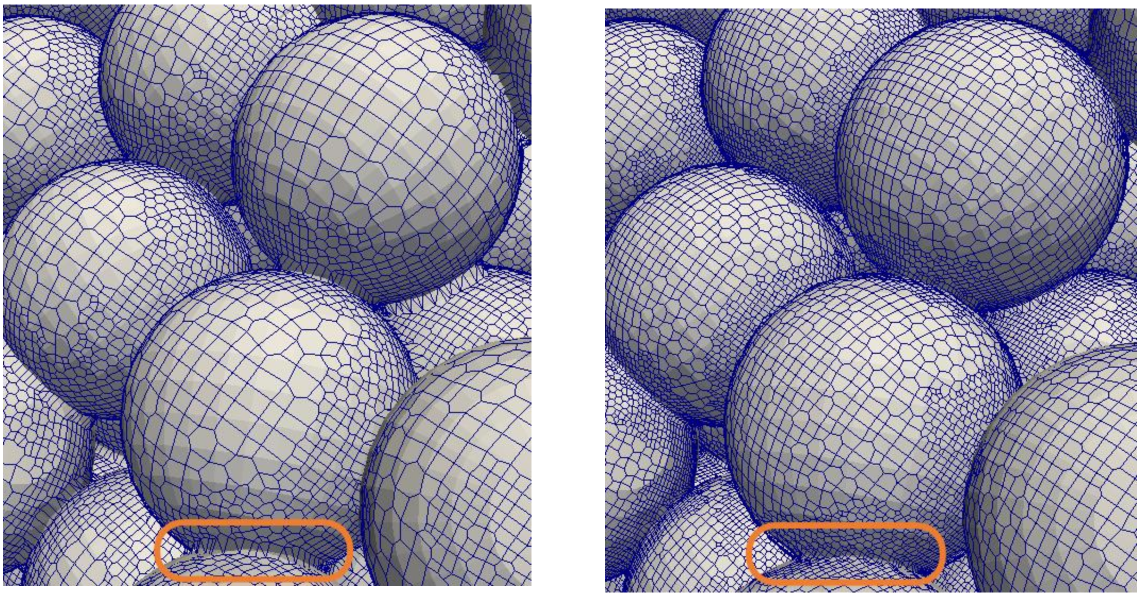



**Figure 3.** Mesh independence study for fixed bed of spheres and $Q_i = 0.15\ \text{dm}^3\ \text{s}^{-1}$

An illustrative comparison of two meshes differing in number of cells is given in Fig. 4. We show the used mesh and the mesh containing two million cells. Merging of the spheres near the contact points done to improve the overall mesh quality may be observed on both the displayed images.



**(a)** 2 million cells **(b)** 7.5 million cells

**Figure 4.** Comparison of meshes of different resolution. Area in the neighbourhood of a contact point between two spheres is highlighted to illustrate the applied bridging of contact points

## 4.2 Model validation

To validate the proposed modelling approach, we compared the estimated pressure drops to the available experimental data and empirical formulas presented in [2, 12, 13]. The results of the model validation are depicted in Fig. 5 and Fig. 6.

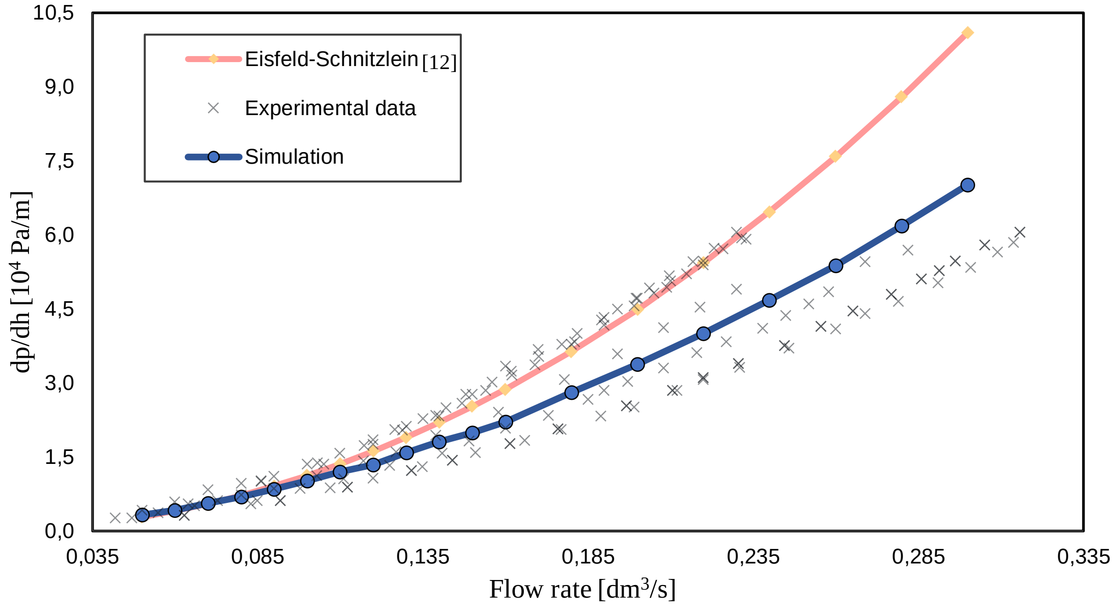



**Figure 5.** Result and validation for spherical packed bed

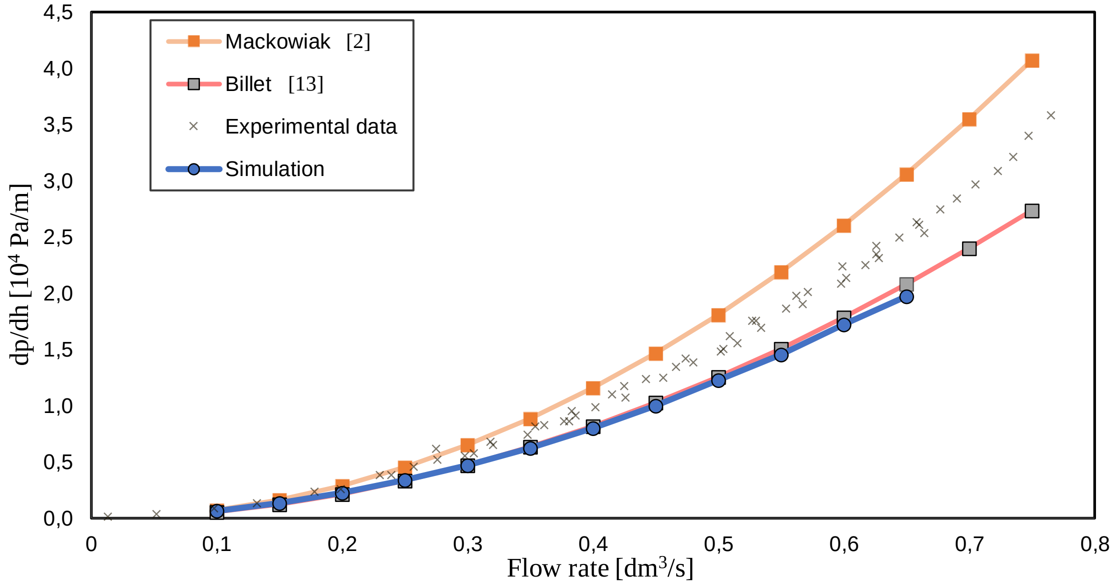



**Figure 6.** Result and validation for packed bed made of Raschig rings

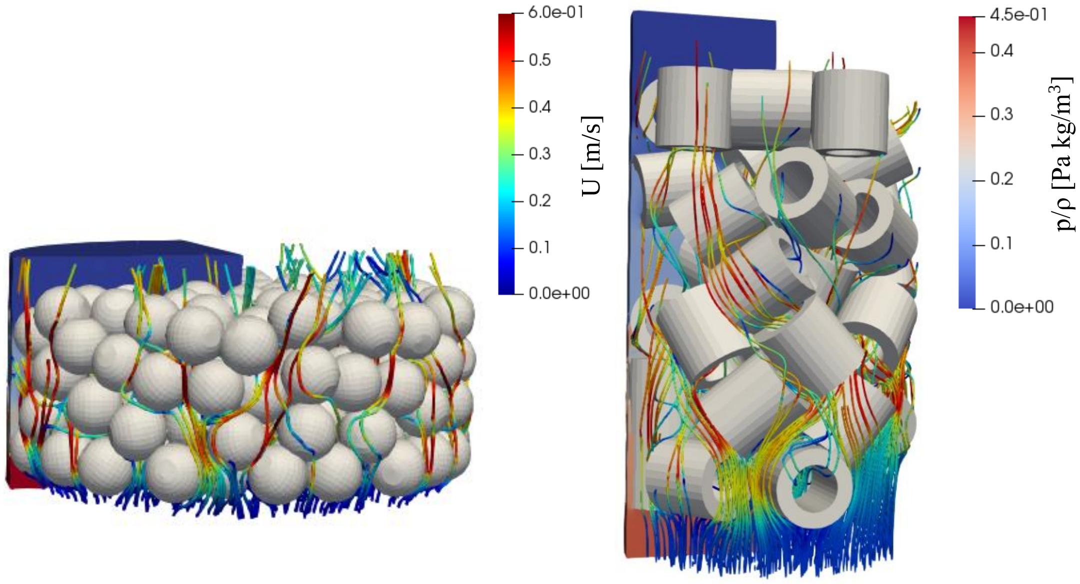
The local flow characteristics in the bed packed with Raschig rings depend on the pellets orientation. Thus, we needed to compare pressure drops computed for a single fluid flow rate and several packed beds consisting of the same number of Raschig rings but with different pellets orientation. The computed pressure drops differed at most by 3 %. Furthermore, we performed simulations on 75 Raschig rings and 400 spheres. The results differed by less than 5 % from the results computed on 50 Raschig rings and 250 spheres, respectively. Hence, we conclude that 50 Raschig rings and 250 spheres are a representative element of the studied packed beds. The computed pressure drops differed at most by 3%, which confirmed our assumption that 50 Raschig rings are a representative element of the whole packed bed.

The pressure drops estimated for the fixed bed consisting of spherical particles are in a good agreement with the experimental data. Moreover, for low fluid flow rates, the CFD results correspond to the empirical formula proposed by B. Eisfeld and K. Schnitzlein [12]. There is a difference of up to 21% between the empirical formula and CFD at higher fluid flow rates. Unfortunately, the scatter in experimental data is too big to draw any conclusions on the accuracy of the two methods.

As for the bed consisting of Raschig rings, the CFD results are consistently lower than the experimental values. However, the CFD results are in a great agreement with the Billet´s correlation [13]. The difference between the CFD results and the experimental data may be caused by an imprecisely estimated bed porosity of the experimental apparatus. The discrepancies in the bed porosity are usually caused by a destruction of some portion of the ceramic Raschig rings during the bed construction.

### 4.3 Qualitative overview of the model results

An important characteristic for the column filled with a fixed bed is the local velocity and pressure distribution in the computational domain. It is problematic to obtain the local distribution of the flow variables via standard experimental techniques. On the other hand, these data may be easily recovered from CFD simulations. An example of a qualitative result is depicted in Fig. 7. Flow rate on inlet $Q_i = 0.15\ \mathrm{dm^3\ s^{-1}}$ for the packed bed with spheres and $Q_i = 0.3\ \mathrm{dm^3\ s^{-1}}$ for the case of Raschig rings. The kinematic pressure distribution is depicted in the clips in the back of the figures. Streamlines in the front of the images in Fig. 7 show possible trajectories of the flow through fixed bed. The highest velocities occur when the fluid is passing around pellet near contact points of two pellets or near contact points of a pellet and the wall.




**(a)** Spheres **(b)** Raschig rings

**Figure 7.** Pressure field and streamlines in the simulated fixed beds.

The depicted streamlines show, within the limitations of the used Reynolds averaging, the main flow patterns in both the studied geometries. Let us note that the flow in the packed bed consisting of uniformly sized spheres is significantly more regular than the flow in the packed bed made of Raschig rings. Because of the symmetry of the spherical particles, the actual orientation of individual pellets in the packed bed does not play any role. On the other hand, for the Raschig rings the local resistance to the flow depends on the pellet orientation with respect to the main flow direction and to the orientation of its neighbours.

## 5 Conclusion

In the present work, we developed a method for generation of a random fixed bed consisting of two types of particles, spheres and Raschig rings. The generated bed geometries were used to prepare a CFD model of a single-phase flow in the complex geometry of the random packed bed. The CFD model was validated against the experimental data and available empirical relations. The differences in pressure loss between the CFD model and the validation data were less than 10% for all the studied cases, what is sufficient accuracy. In the future, we plan to generate a packed bed consisting of Pall rings and to extend the model to account for the multiphase flow.

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