DEM-CFD Study of Flow in a Random Packed Bed

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Introduction

Most catalytic surface reactions as well as other industrial applications take advantage of fixed packed bed reactors [6, 3]. Designers of these reactors rely mostly on empirical formulas derived for various simplifying assumptions, e.g. uniformly distributed porosity [2]. 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“ [1] 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, see Fig. 1. 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.

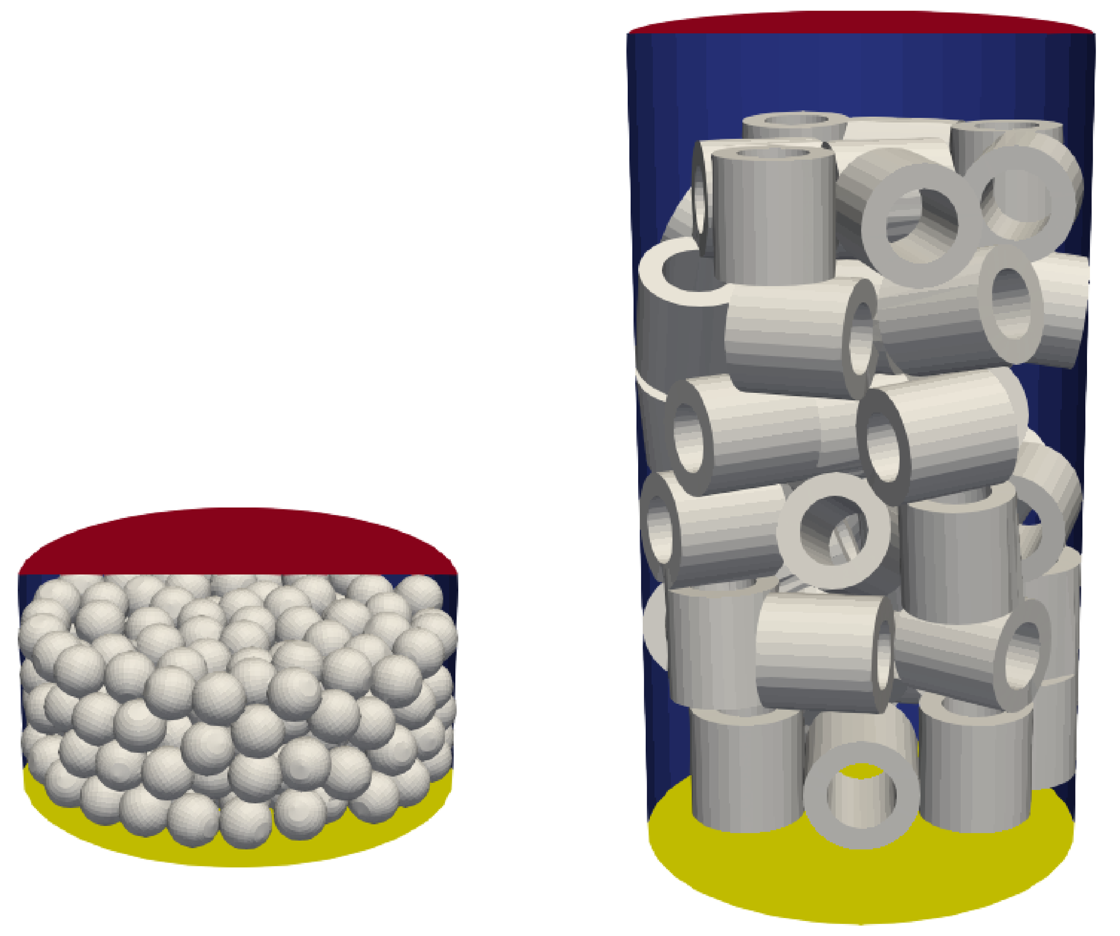

Figure 1 : Illustration of studied packings consisting of different type of the used particle. Colors are used to point out different boundaries

Packed bed geometry generation algorithm (Raschig rings)

Require: Number of vertices in one cylinder *numOfVertices* = 64 and number of Raschig rings in geometry *numOfRings* = 50

Create cylinder with diameter d_t = 0.06m, height h_t = 0.1m and number of vertices *numOfVertices*
for $i = 1$ **to** $\frac{numOfVertices}{2}$ **do**
  vertices[*i*].select=True
end for
mesh.delete(type='FACE') {remove top face selected by vertices to create column}
for $i = 1$ **to** *numOfRings* **do**
  Create cylinder with diameter d_t = 0.015m, height h_t = 0.015m and number of vertices *numOfVertices*
  $location = (-0.015 + (random() * 0.03), -0.015 + (random() * 0.03), 0.05 + i * 0.017)$ {relocate cylinder}
  $rotate(10, axis = (random() * 10, random() * 10, random() * 10)$ {rotate}
  for $n = 1$ **to** $\frac{numOfVertices}{2}$ {making hole to cylinder to create Raschig ring} **do**
    vertices[*n*].select=True
  end for
  mesh.inset(thickness=0.25) {inset face on the top of cylinder}
  mesh.delete(type='FACE') {delete inner face}
  for $n = \frac{numOfVertices}{2} + 1$ **to** *numOfVertices* **do**
    vertices[*n*].select=True
  end for
  mesh.inset(thickness=0.25) {inset face on the bottom of cylinder}
  mesh.delete(type='FACE') {delete inner face}
end for
{Set properties for physics engine}
bullet.physicsType='RIGID BODY'
bullet.useCollisionBounds = True
bullet.radius = 0.0035
bullet.velocityMax = 10 {for better collision detection}
bullet.collisionMargin = 0.002 {detection of overlap}
bullet.formFactor = 0.001 {low friction}
Start physics engine until velocities are equal to zero for 10 seconds
return Geometry representation of the random packed bed consisting of Raschig rings suitable for the snappyHexMesh utility

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Simulation set up

To estimate the pressure loss over the packed bed, we need to solve a set of isothermal, turbulent, steady-state Navier-Stokes equations for an incompressible Newtonian fluid [5],

$$\nabla \cdot (\overline{\mathbf{U}} \otimes \overline{\mathbf{U}}) - \nabla \cdot (\overline{\mathbb{T}} + \mathbb{T}') = -\nabla \overline{p}$$
$$\nabla \cdot \overline{\mathbf{U}} = 0\,,$$

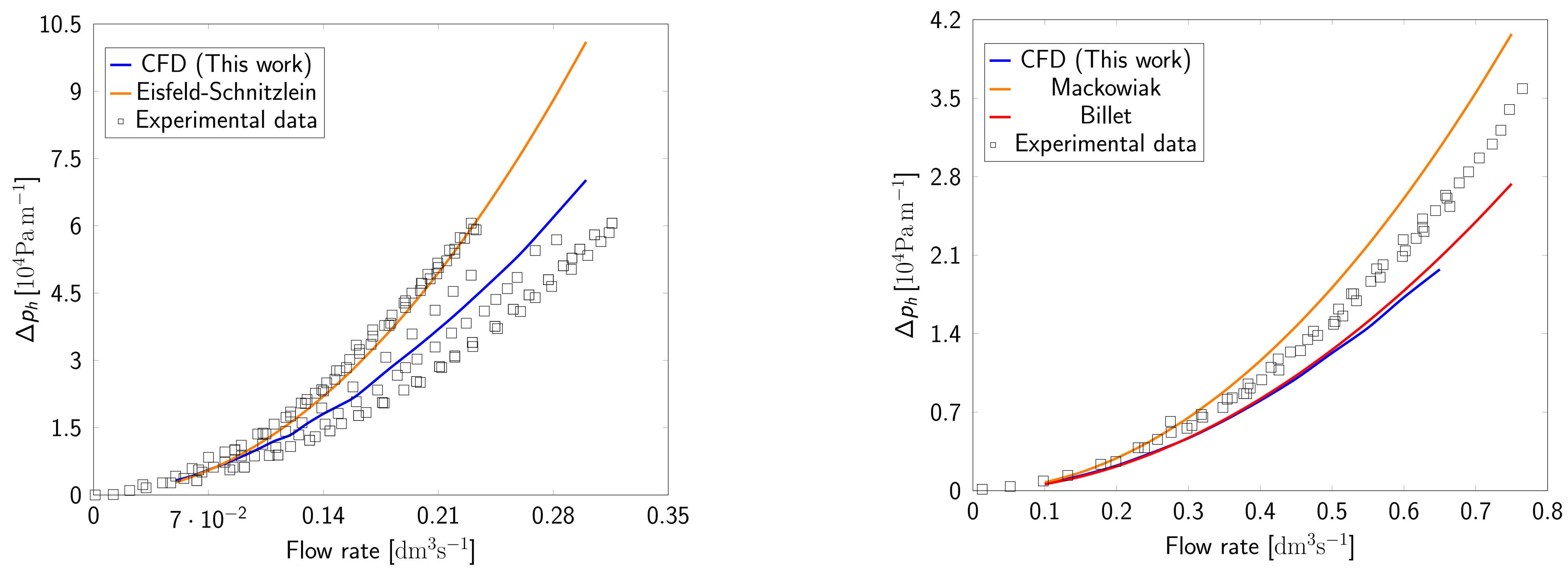
where $\mathbb{T}'$ is the Reynolds stress tensor. In this work we used the k-ω SST model [4] for the closure of the problem.

The flow governing equations together with the equations for the turbulence variables k and ω were solved via the simpleFoam solver from the OpenFOAM toolbox . The used finite volume (FV) mesh was created using the snappyHexMesh software, which is available in the OpenFOAM installation. The needed representation of a packing geometry in STL format was prepared via SuperPak type packing geometry generation algorithm implemented in the Blender software. The applied boundary conditions are listed in Tab. 1. As initial guess, we prescribed $\mathbf{U} = (0,0,0)^{\mathrm{T}}$, $p = 0$, $k = 0$, $\omega = 0$ in the whole solution domain.

Boundary	Colour in Fig. 1	$\mathbf{U}$	p	k	ω
Inlet	yellow	flowRateInletVelocity	zeroGradient	fixedValue	fixedValue
Outlet	red	inletOutlet	fixedValue	inletOutlet	inletOutlet
Wals & Bed	blue & gray	noSlip	zeroGradient	zeroGradient	zeroGradient

Table 1 : Applied boundary conditions. InletOutlet boundary condition is used for simulation stabilization.

Model validation



(a) Spheres (b) Raschig rings

Figure 2 : Result and validation for different types of packed bed

Results

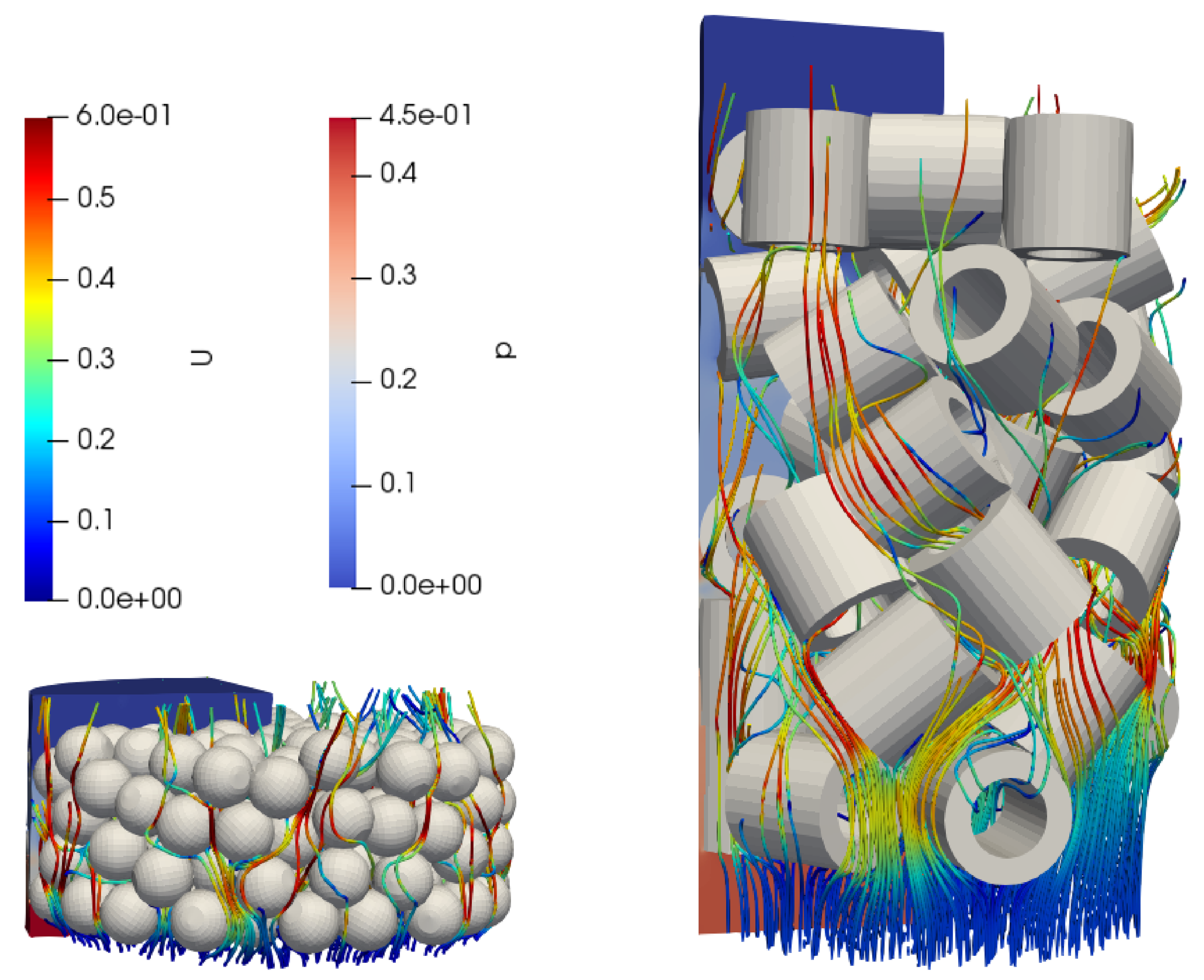


Figure 3 : Pressure field and stream lines in the simulated fixed beds

The kinematic pressure distribution is depicted in the clips in the back of the figures. Stream lines in the front of the images in Fig. 3 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.

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