CAMURE-11 11th International Symposium on Catalysis in Multiphase Reactors
ISMR-10 10th International Symposium on Multifunctional Reactors
MILANO, ITALY - 21-24 March, 2021

Particle-resolved Simulations of Turbulent Flow through Packed Bed Reactors: Comparison of Flow Simulations using RANS, LES and DNS Approaches

Aniket S. Ambekar[1], Christoph Schwarzmeier[2], Ulrich Rüde[2,3], Vivek V. Buwa[1]*
1 Department of Chemical Engineering, Indian Institute of Technology Delhi, New Delhi 110016, India
2 Chair for System Simulation, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany
3 Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique, 31057 Toulouse, France
**Corresponding author E-Mail: vvbuwa@iitd.ac.in*

1. Introduction

Packed bed reactors with varying particle size and shape (e.g. spheres, cylinders and particles with external or internal shaping) and structured/intensified reactors packed with catalytic foams, monoliths and high-performance packings are used in industry to perform different commercially important solid-catalyzed gas-phase reactions. These reactions include methanol or dimethyl ether synthesis, methane-steam reforming, water-gas shift reactions and many more. The particle-scale (local) flow depends strongly on the particle shape or the local catalytic structure. It influences particle-scale heat and mass transfer processes and the overall reactor performance in terms of pressure drop, conversion and product selectivity. Thus, in order to improve the reactor performance, it is crucial to gain an understanding of this local flow. For this purpose, particle-resolved computational fluid dynamics (CFD) simulations are being increasingly used to evaluate the effects of particle shape and local catalytic structures on the pressure drop characteristics, as well as on the heat and mass transfer limitations. Owing to the very high Reynolds numbers used in commercial reactors, such particle-resolved CFD simulations are often performed by solving the Reynolds-averaged Navier-Stokes (RANS) equations with appropriate turbulence models, e.g., different variants of two-equation eddy viscosity models or the Reynolds stress transport models. In order to use such particle-resolved CFD simulations based on the RANS approach with confidence, it is necessary to evaluate the accuracy of the predictions of different turbulence models by comparison with results obtained from Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES). The DNS of single-phase flow in packed beds at moderate Reynolds numbers is itself challenging due to computational costs. Therefore, we perform our DNS with a software framework that is suitable for massively parallel CFD simulations based on the lattice Boltzmann method (LBM). The objectives of the present work are (a) to perform a fully-resolved 3D DNS of turbulent flow in the particle-resolved geometry of a packed bed using the LBM to simulate the velocity field and turbulence characteristics accurately and (b) to investigate the accuracy of RANS simulations with different turbulence models and LES by comparison with DNS results.

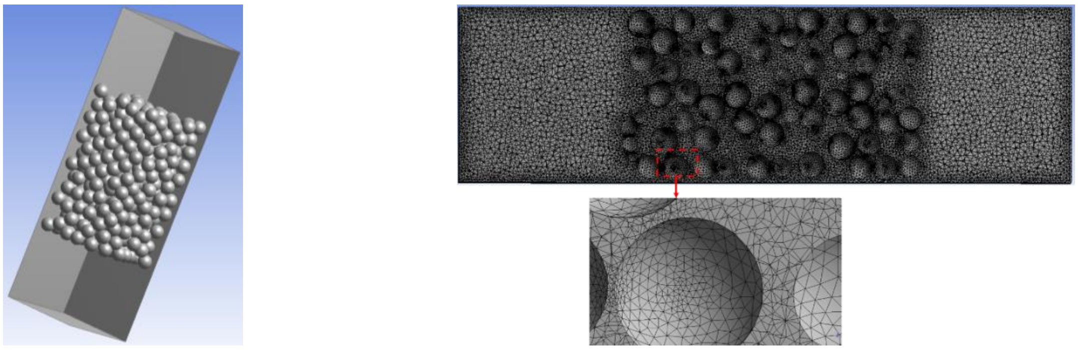
2. Methods

We use the open-source CFD toolbox OpenFOAM (v1906) to perform particle-resolved RANS simulations and LES of turbulent flow in a packed bed. These simulations are based on the finite volume method (FVM) and various commonly used turbulence models, such as the SST k-ω, the k-ε and the Reynolds stress model are applied. The fully resolved LBM-based unsteady DNS is performed with the open-source software framework waLBerla[1], which is specifically designed for multi-physics simulations on massively parallel computers. Further details of the model equations and their numerical solutions will be provided in the full manuscript. A small portion of the packed bed with void fraction $\emptyset = 0.51$ is shown in Fig. 1(a). It is created by mimicking the process of random filling of a box with 128 uniformly-sized particles (particle diameter d_p = 4 mm) under the influence of gravity using a rigid particle dynamics simulation. These particles contact each

---

[1] https://www.walberla.net

other at a single point of contact. Since it is challenging to create a mesh for the sharp angles close to these contact points, the particles are shrunk volumetrically by 1%. A typical mesh with 22 million elements that is used to simulate laminar flow with the RANS approach is shown in Fig. 1(b). The mesh required for simulations of turbulent flow using the RANS models consists of 5 boundary layers at the particle surfaces. The thickness of the mesh's first boundary layer is adjusted to meet the specific requirement of y^+ for different turbulence models. The computational grid used for the LBM-based DNS consists of a cubical lattice resolved up to the size of the Kolmogorov length scale.

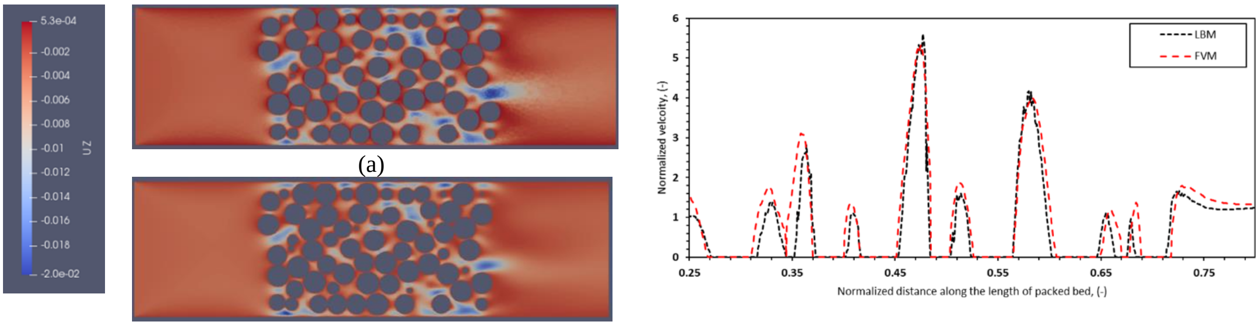


(a) (b)

Figure 1. (a) Randomly packed bed with spherical particles created using rigid particle dynamics simulations and (b) central plane of the bed showing the computational grid that consists of tetrahedral elements.

3. Results and discussion

Initial simulations were performed under laminar flow conditions with particle Reynolds number $Re_p = \rho v d_p/(\emptyset\mu) = 10$. A comparison of the simulated velocity fields at a central plane is shown in Fig. 2(a) and (b). It can be seen that the velocity fields predicted by the RANS and LBM simulations agree qualitatively well. A quantitative comparison of the velocity, normalized by the maximum velocity in the respective cases, is shown in Fig. 2(c) and a good quantitative agreement can be observed. A comparison of the velocity and pressure distributions predicted by RANS simulations, LES and DNS for turbulent flow conditions will be presented in the full manuscript. The accuracy of different turbulence models to predict velocity and pressure distributions in packed beds will be validated with the corresponding DNS.



(a)

(b) (c)

Figure 2. Steady-state velocity field at a central plane predicted using (a) RANS and (b) LBM simulations. The corresponding velocity profiles along the center-line of the domain at $Re_p = 10$ are shown in (c).

4. Conclusions

In the present work, we generate a small section of a randomly packed bed consisting of spherical particles with rigid particle dynamics simulations. We perform particle-resolved simulations of turbulent flow. The DNS are based on the LBM and performed with the software framework waLBerla. The RANS simulations and LES are based on the FVM and performed using the CFD toolbox OpenFOAM. Our results help us to evaluate the accuracy of different turbulence models to predict velocity and pressure distributions in packed beds. These insights allow us to use CFD simulations with turbulence models reliably to analyze transport limitations and the reaction performance of packed bed reactors.