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Particle-resolved Simulations of Local Liquid Spreading in Packed Beds

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1. Introduction

Packed bed reactors (PBR) are widely used for processes involving solid-catalysed gas-liquid reactions (e.g. trickle bed reactors used for hydrodesulphurization of liquid fuels) or gas clean-up processes (e.g. absorption columns). The overall performance of gas-liquid packed beds or trickle beds is influenced by the local liquid distribution which is a strong function of particle characteristics (e.g. wettability, shape, size, etc.), physical properties of the liquid phase and the operating conditions (e.g. gas/liquid flow rates, etc.). While CFD models based on the Eulerian multiphase approach are developed and used to predict the effects of the aforementioned parameters of the local liquid distribution, the predictions of these models depend on the contributions of different interphase coupling forces and also on the capillary force. It is not understood how the magnitude of such interphase coupling and capillary forces depend on particle size, surface wetting characteristics, particle shape, etc. In the present work, we report particle-resolved two-phase flow simulations performed to understand the effect of particle wettability and size on the local liquid spreading in packed beds.

2. Methods

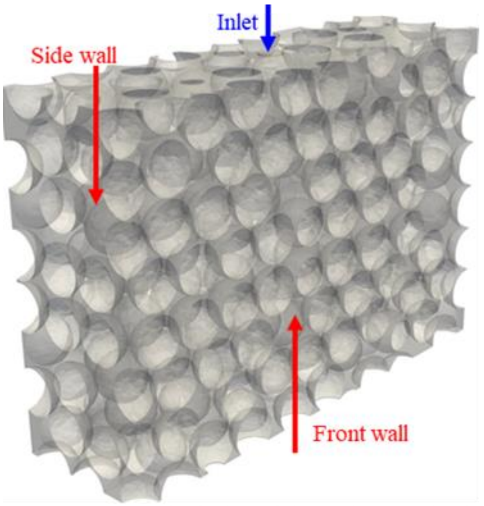


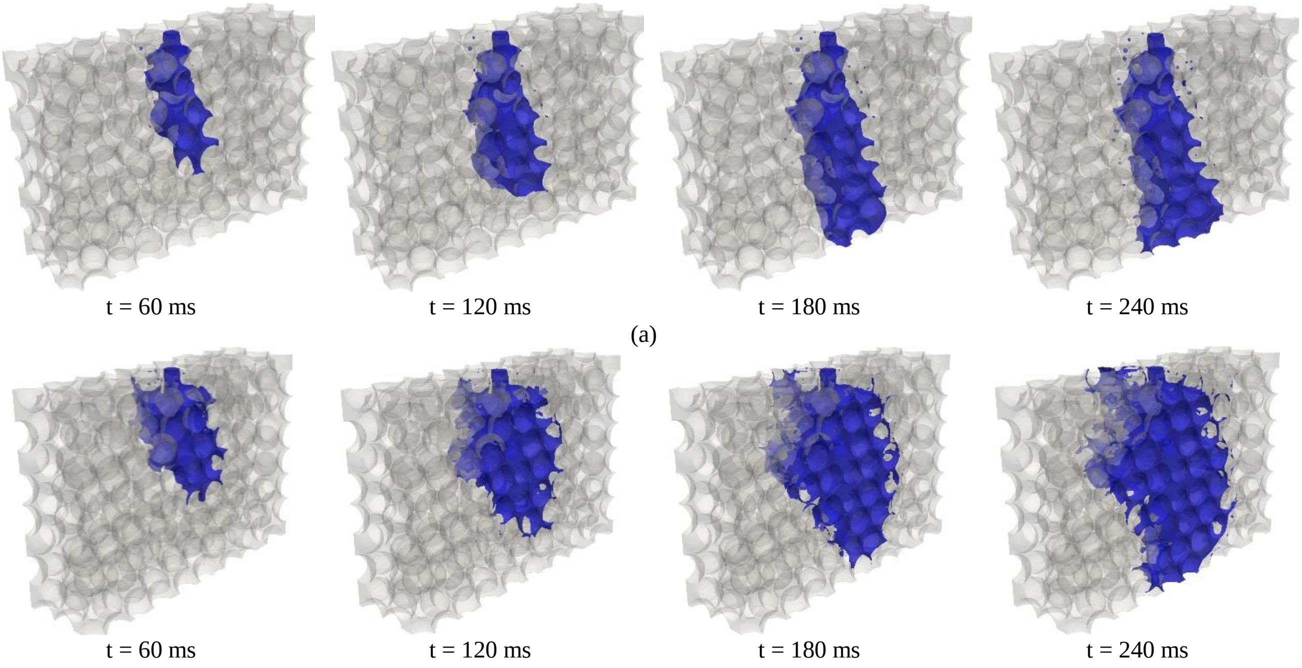
Figure 1. Spherical particle pack created using rigid body simulation

A small portion of the random-filled packed bed was created by mimicking the process of filling a box randomly with 440 uniformly-sized spherical particles (d_p = 4 mm) under the influence of gravity by performing rigid body simulations using open-source software 'Blender' (see Fig.1). The particle-particle contact regions were difficult to mesh due to the sharp intersection angles formed in these regions. In order to resolve the difficulties in meshing, the particles were shrunk by 1 % (volumetrically) avoiding contact regions. It is well established in the literature that the reduction in particle volume by 1% does not change the hydrodynamics significantly. The near-wall regions of the domain were trimmed to avoid large void spaces present near the wall resulting in a pack with dimension 10 d_p ×3 d_p ×8 d_p. The void space was meshed using tetrahedral elements of size d_p/40 resulting in 32 million elements for the domain shown in Fig. 1. With above-mentioned methodology, similar packed-bed domains with varying particle size were created (the details will be provided in the full manuscript).

The Volume of Fluid (VOF) method implemented in the open-source CFD code OpenFOAM Version 19.06 was used to simulate the interface-resolved two-phase flow through packed-beds. Water and air were considered as the liquid and gas phases, respectively. The domain was assumed to be completely occupied by the gas phase and water was injected locally through a small inlet at the top (see Fig.1) with a constant injection velocity of 0.1 m/s. A no-slip boundary condition was specified at the particle surfaces and the outlet was maintained at atmospheric pressure by using the constant pressure boundary condition. The particle surface wettability was changed by specifying different values of three-phase static contact angle ($\theta = 0,\ 50$ and $90°$). The front and the back walls of the domain were specified with no-slip boundary condition along with $\theta = 90°$, rendering it neutrally-wet. While the symmetry boundary condition was applied on the side walls. The iso-advector interface reconstruction algorithm was used to minimize interface smearing.

The simulations were performed using the super-computing facility of RRZE, FAU-Erlangen and took approximately 1.2 hr/ms of computing time using 800 cores.

3. Results and discussion



t = 60 ms t = 120 ms t = 180 ms t = 240 ms

(a)

t = 60 ms t = 120 ms t = 180 ms t = 240 ms

(b)

Figure 2. Dynamics of liquid spreading for a three-phase static contact angle (θ) of (a) 50° and (b) 0°, the iso-volume of liquid-phase with volume fraction greater than 0.5 are shown in the figures.

Fig. 2 shows the effect of particle surface wettability on the local liquid spreading. It is evident that as the surface wettability changes from weekly water-wet to strongly water-wet, the liquid spread in the lateral direction increases. The increase in the lateral spread of liquid is due to the increase in the capillary force as it is the driving force in the lateral direction whereas the viscous force is the driving force in the direction of flow. Further simulations on the effect of particle size and wettability on the dynamics of liquid spreading are in progress and the results will be provided in the full manuscript.

4. Conclusions

In the present work, we have created a small section of randomly packed bed of varying size using the rigid body simulation methodology and have performed particle-resolved simulations of two-phase gas-liquid flow using the Volume of Fluid simulations. This work helps to understand the dynamics of liquid spreading in packed beds and how particle characteristics (wetting and size) influence the liquid distribution. The methodology can be extended to other commonly used particle shapes.