Volume-of-Fluid Simulations of Particle-Scale Liquid Spreading in Trickle Beds

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Highlights

- 2D Volume-of-Fluid simulations of particle-scale liquid spreading in trickle beds
- Understanding the effects of particle size/shape, packing structure, particle wetting properties and liquid properties on local liquid spreading
- Evaluation of the closures used in Eulerian multiphase models for simulations of liquid spreading in large-scale trickle beds

1. Introduction

Gas-liquid packed bed reactors, in particular, trickle bed reactors are widely used in the chemical process industry to carry out the solid-catalyzed gas-liquid reactions. One of the foremost commercially important application is the hydrodesulphurization of petroleum feed stocks. With emission norms getting more and more stringent, it has become important to improve the performance of hydroprocessing reactors to produce better quality fuel with sulphur content less than 10 ppm (e.g. ultra low sulphur diesel). Over last two decades, significant efforts were made to develop the computational models to predict the local liquid distribution in trickle beds. The present state of literature shows that the predictive abilities of Eulerian multiphase models, used to simulate local liquid distribution in large-scale trickle beds, overwhelmingly depend on the closure models used to estimate the interphase momentum exchange terms, capillary pressure force and mechanical dispersion force. It is not clear from the existing models how the magnitude of aforementioned parameters depend on the particle size and shape, bed voidage, packing structure, particle wetting characteristics, and liquid properties. The development of improved closures is limited by the understanding of the particle-scale liquid spreading behavior.

In the present work, we have performed Volume-of-Fluid (VOF) simulations to understand the effects of particle size and shape, bed voidage, packing structure, particle wetting characteristics, and liquid properties on the particle-scale liquid spreading behavior.

2. Methods

The VOF method, implemented in commercial flow solver ANSYS FLUENT (v 14) was used to simulate the local liquid spreading behavior. 2D beds of size $31.5d_p$ x $44d_p$ packed with spherical particles of different sizes (d_p = 2, 4, 8 mm) and different shapes (spheres, cylinders and trilobes) were considered for the simulations (see Figure 1). The liquid was introduced through the middle inlet (with length of $5d_p$) as shown in Figure 1. The liquid superficial velocity was varied from 0.01 to 0.1 m/s, the gas superficial velocity was varied from 0 to 0.5 m/s. A pressure outlet boundary condition with zero gauge pressure was specified at the outlet. The side walls of the solution domain were specified as no slip walls. Initial simulations were performed with air and water as the working fluids. The effect of particle wetting characteristics was investigated by specifying limiting static contact angles i.e. 1° and 179° representing hydrophilic and hydrophobic surfaces. An unstructured mesh, with total number of tetrahedral elements in the range of 0.3 to 1 million was used for the 2D simulations. Simulations were performed using the "PADAM" supercomputing facility of IIT

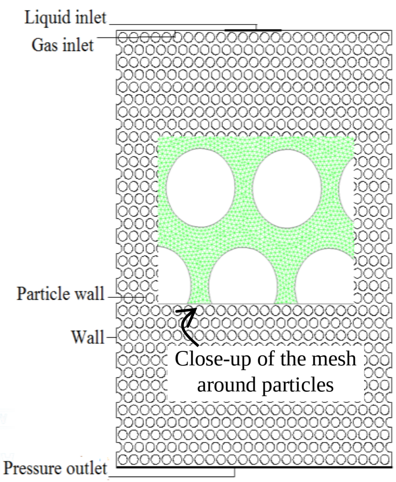
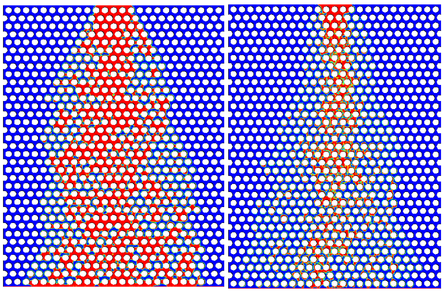


Figure 1: Solution domain and boundary conditions

Delhi. A typical transient simulation with 0.5 million cells and a time-step of 1×10^{-5} s took about 7 days for simulating ~ 5 s of real time liquid spreading, with simulations performed with 24-48 cores in parallel. Further details of the governing equations, boundary conditions and numerics will be provided in the full length manuscript.

3. Results and discussion

Preliminary simulations were performed to examine the effect of grid resolution. It was found that the predicted pressure drop across the bed and the overall liquid holdup in the bed changed considerably with the increase in total number of cells from 0.15 to 0.3 and then from 0.3 to 0.5 million. However, the predictions were found to be independent of the grid resolution for grids with total number of elements greater than 0.5 million cells. Therefore, all subsequent simulations were performed using a grid resolution corresponding to 0.5 million cells. The effect of particle size (d_p = 2, 4, 8 mm) on the liquid spreading is shown in Figure 2. The liquid spreading and also the overall liquid hold up was found to decrease with increase in the particle diameter. This trend agreed well with the measurements available on laboratory-scale trickle beds. The effect of particle shape (sphere, trilobe) is shown in Figure 3 (compare Figure 2(a) and Figure 3). The effect of particle wetting characteristics is shown in Figure 4. The liquid spreading was found to increase for trilobe-shaped particles in comparison to that of the spherical particles. Further, it was also found to increase with increase in the contact angle. The effects of particle wettability, liquid properties (surface tension and viscosity) on the liquid spreading will be discussed in the full manuscript. The predictions of different closures used to calculate the interphase momentum exchange terms, capillary pressure force and mechanical dispersion force will be analyzed and compared with the predictions of the particle-scale liquid spreading obtained using the VOF simulations. The results will be presented in the full manuscript.



(a) (b)

Figure 2: Effect of particle size on local liquid spreading with static contact angle 1^0 for (a) d_p = 4 mm and (b) d_p = 8 mm (bed voidage= 0.5, U_L=0.1 m/s, U_G=0 m/s)

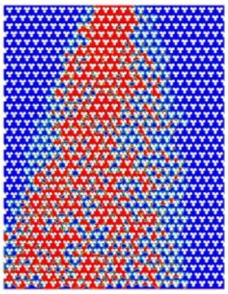
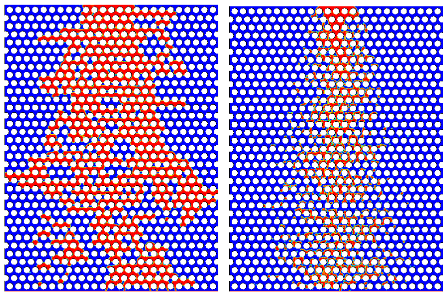


Figure 3: Effect of particle shape on local liquid spreading for trilobe-shaped particles (U_L=0.1 m/s, U_G=0 m/s). The dimensions of these trilobes correspond to spherical particles with (d_p = 4 mm) (also see Figure 2(a))



(a) (b)

Figure 4: Effect of particle shape on local liquid spreading with static contact angle 179^0 for (a) d_p = 4 mm and (b) d_p = 8 mm (bed voidage= 0.5, U_L=0.1 m/s, U_G=0 m/s)

4. Conclusions

In the present work, VOF simulations of the particle-scale liquid spreading in trickle beds were performed to understand the effects of the particle size and shape, particle surface wettability and liquid properties (surface tension and viscosity) on the local liquid spreading. The particle-scale simulation data is being used to analyze different interphase momentum exchange terms, capillary pressure force and mechanical dispersion that are used in the Eulerian models. The present contribution will be useful to understand the particle-scale liquid spreading process. Such an understanding and simulation data will be very useful to improve the closures used in the Eulerian models.

Keywords
Liquid distribution, Volume of fluid simulation, computational fluid dynamics, trickle bed, particle