A study of gas-liquid flows through random open-cell solid foams using structure-resolved simulations

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Highlights

- Digital open-cell foams with properties similar to Duocel aluminum foams are created.
- The pressure drop predictions across digital foams agree with correlations in the literature.
- The liquid distribution is marginally influenced by foam density and wettability at small *Oh* and *AB*.
- The liquid distribution is governed by the pore size other than the operating conditions.

1. Introduction

Packed bed reactors are widely used in the chemical industry to perform solid-catalyzed gas-liquid reactions. Conventional packed bed reactors are filled with catalyst pellets and are often associated with large pressure drops and liquid mal-distribution. Therefore, structured packings like foams are being investigated as an alternative to conventional catalyst pellets. Very few researchers have computationally investigated the local liquid distribution through solid open-cell foams and therefore, the impact of foam characteristics on local liquid distribution is not established. In view of the above, the objectives of the present work are to create realistic digital foams and understand the role of foam density/strut shape, wettability and pore size on the local liquid distribution and the resulting flow metrics using structure-resolved Volume-of-Fluid simulations.

2. Methods

In the present work, digital random open-cell solid foams with varying solid fraction (ε = 0.043, 0.07, and 0.099) and pores/inch (5, 10, and 20) along with strut shape corresponding to Duocel aluminum foams are generated. The digital foams are generated starting from Voronoi tessellations, which are further processed in open-source software Surface-Evolver to create open-cell foams which adhere to the Plateau's laws. One such solid foam with ε = 0.043 and 10 pores/inch is shown in Figure 1(a). The generated structure-resolved fluid domains are spatially discretized with element size of pore size/40 leading to 7.5 million elements for foams with 10 pores/inch, as it results in grid independent flow predictions. The Volume-of-Fluid (VOF) method, implemented in OpenFOAM v7, was used to simulate the gas-liquid flow dynamics through the structure-resolved fluid domains. The computational domains were initially filled with air and the liquid-phase 'water' was injected from the circular inlet located centrally on the top face [Figure 1(a)] with a constant velocity (V_L). A no-slip boundary condition along with a static three-phase contact angle

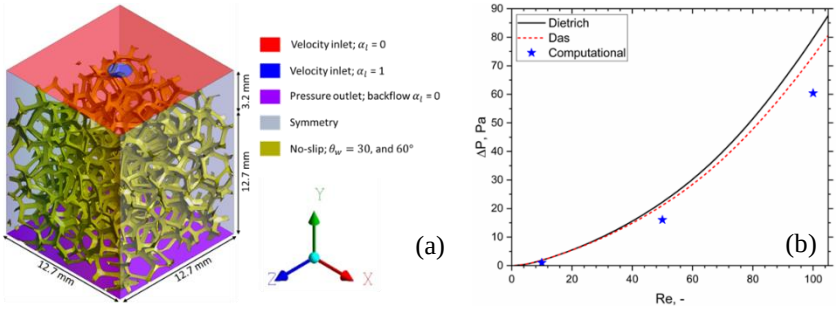
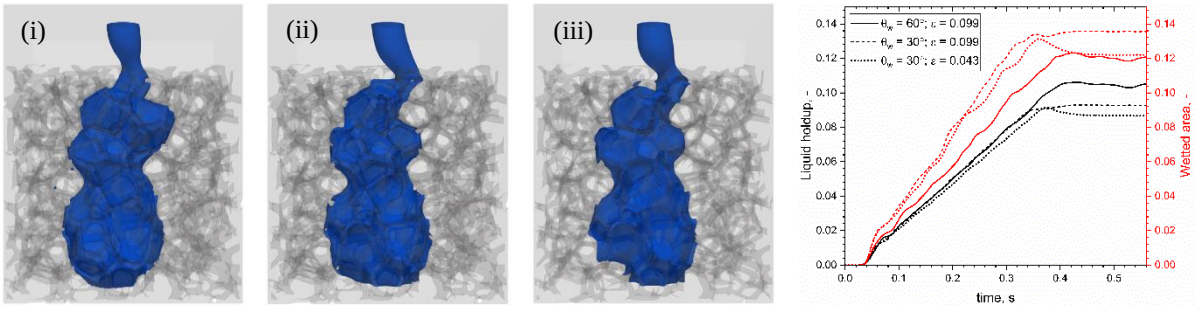


Figure 1. (a) Computational domain of open-cell foam along with boundary conditions and (b) single-phase pressure drop predictions compared with semi-empirical correlations (ε = 0.043, 10 pores/inch).

(θ_w) of 30, 60, or 90° was specified on the surface of solid foams. Please see Figure 1(a) for boundary conditions specified on remaining boundary faces.

3. Results and discussion

Before proceeding with two-phase flow simulations, single-phase flow simulations were performed and the predictions of pressure drop were compared with the semi-empirical correlations by Dietrich et al. [1] and Das et al. [2]. The difference between the predictions and estimates of the correlation was found to be between $\pm$ 4.7 to 11.16 % [see Figure 1(b)]. Two-phase simulations were performed to investigate the role of ε, θ_w, and pore size on the local liquid distribution as well as the resulting flow metrics. Figure 2(a) (i)-(iii) and (b) reveal that the local liquid distribution and the resulting flow metrics, in terms of liquid holdup and wetted area, are marginally influenced by ε as well as θ_w at a constant pore-size. To comprehend the dependency of local liquid distribution as function of ε and θ_w, we estimated the relative magnitude of governing forces with the aid of dimensionless numbers namely, Ohnesorge (*Oh*) and *AB* ($\sqrt{inertial \times capillary}/gravitational\ force$). The value of *Oh* and *AB* is 2.3 × 10^{-3} and 0.27, respectively, which indicate the dominance of gravitational force as compared to inertial, viscous, and capillary forces [3], resulting in the independency of the local liquid distribution as a function of ε and θ_w. Simulations are also being performed at large values of *Oh* and *AB* to understand the influence of ε and θ_w for flows governed by other forces and will be presented in the complete manuscript. Further, the pore size is found to substantially influence the local liquid distribution and the resulting flow metrics (results not here).



(a) (b)

Figure 2. (a) Steady-state local liquid distribution at (i) ε = 0.099, θ_w = 60; (ii) ε = 0.099, θ_w = 30; (iii) ε = 0.043, θ_w = 30 (note: water and foam is colored blue and grey, respectively. Air is transparent) and (b) effect of ε as well as θ_w on normalized liquid holdup and wetted area (10 pore/inch, V_L= 0.11 m/s, V_G= 0.167 m/s).

4. Conclusions

In the present work, digital open-cell solid foams with properties similar to Duocel aluminum foams are created. We have investigated the role of foam density, wettability as well as pore-size on the dynamics of local liquid distribution and the resulting flow metrics for a wide range of *Oh* and *AB* (a detailed quantitative analysis will be presented in the full manuscript). This work helps to understand the role of the geometrical characteristics of open-cell foams on the local hydrodynamics of packed beds and its influence on flow metrics governing the overall performance of packed beds at various conditions.

Acknowledgments

The authors acknowledge the funding received from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 899987.

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Keywords

Structure-resolved, interface-capturing, gas-liquid flow, open-cell foams