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Pressure drop in monolith reactors ☆

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Abstract

A theoretical model for the computation of pressure drop in bubble-train flow inside capillaries of square cross-section was developed. The model is based on three contributions: hydrostatics, viscous pressure drop, and capillary pressure drop. Capillary pressure drop is related to the shape of the fronts and ends of the bubbles. The model does not include entrance or exit effects, has no adjustable parameters, and agrees very well with available experimental data.

For a given set of flow parameters, bubble velocity and liquid slug average velocity are computed as a function of gas and liquid superficial velocities. The length of the unit cell determines the number of bubbles inside the capillary for a given flow situation. The model requires experimental information of average bubble lengths to compute the length of a unit cell consisting of a bubble and a liquid slug.

The three pressure contributions for a unit capillary length are linear functions of the number of bubbles inside the capillary. The length of the bubbles in bubble-train flows is a critical parameter in the computation of pressure drop.

Keywords: Pressure drop; Bubble-train flow; Monolith reactors

1. Introduction

A theoretical model for pressure drop during bubble-train flow inside monoliths is presented. This model is based on first principles and has no adjustable parameters, except for the experimental determination of bubble lengths.

The velocity of bubbles inside the capillaries of circular or square cross-section is a complex function of fluid properties, and gas and liquid superficial velocities. Bubbles move faster than the sum of the superficial velocities of gas and liquid phases. The average speed of liquid in the slugs is identical to the sum of vapor and liquid superficial velocities. A part of the liquid in the slugs is overtaken by the bubbles, leaving behind a film of liquid in contact with the capillary walls. Speed determines the size and shape of the bubbles. The faster the bubbles move, the smaller their cross-section and thicker the film left behind. Flow patterns in liquid slugs for slugs of different lengths have a large effect on pressure drop, mass transfer and reaction rates. It is important to establish the role of liquid slug and bubble lengths, when describing the flow of a train of bubbles.

A pressure drop model developed by Grolman et al. [2] includes hydrostatics and viscous forces, but neglects the contribution of capillary forces acting on the front and back of the bubbles. Their model correctly accounts for a pressure drop contribution other

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than viscous and hydrostatic and proportional to the number of bubbles inside a capillary, but assumes that the additional pressure drop was determined by entrance and exit effects. Grolman et al. [2] matched experimental and theoretical values of pressure drop by introducing an empirical term proportional to the velocity of the bubbles.

In our model, pressure drop in bubble-train flow is determined by three contributions: (1) hydrostatic pressure inside the liquid slugs, (2) pressure drop due to viscous forces inside the liquid slugs, and (3) pressure drop measurable by capillary forces at the liquid–gas interface. The role of capillary forces in pressure drop during the flow of single bubbles was first analyzed by Bretherton [1] who estimated the shape of the front and back end of bubbles, and using the normal stress condition established the following equation for pressure drop across a single bubble.

2. Pressure drop computations

The differential pressure between the ends of capillaries in bubble-train flows is the result of three contributions: hydrostatics, viscous losses in the liquid slugs, and the contribution due to the difference in shape between the front and back ends of the bubble. Neglecting the hydrostatic contribution of the gas

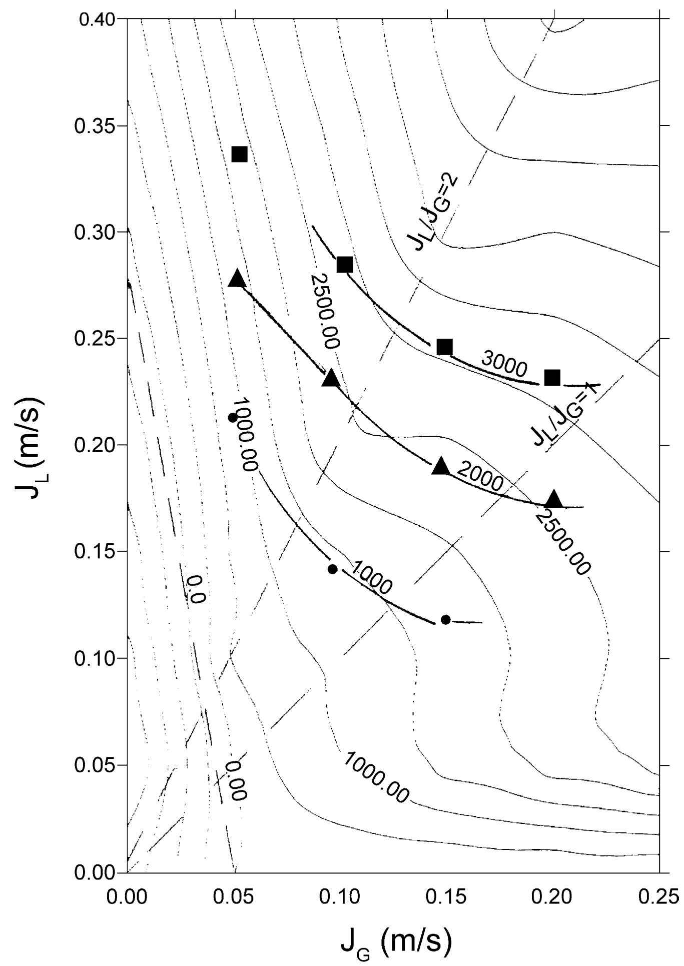

Fig. 1. Pressure drop, in Pa, inside a 30 cm/400 CPSI monolith (square channels).

bubbles, the hydrostatic pressure field inside the capillary is a function of the number and length of liquid slugs. Hydrostatic pressure always acts in the direction of gravity, regardless of the direction of flow. In upward flow, hydrostatics must be added to the other pressure drop contributions. In downward flow, hydrostatics acts in the direction opposite to the viscous and capillary effects. This characteristic was successfully used by Grolman et al. (1995) to describe the region of unstable flow at small velocities in downward bubble-train flows.

Thulasidas et al. [3] demonstrated that velocity profiles in liquid slugs in bubble-train flows inside capillaries follow very closely the velocity profiles predicted by Poiseuille flow. Thus, the average velocity of the liquid inside the capillary, v_{1s}, was used to compute the viscous pressure drop.

Finally, the contribution to pressure drop due to the difference in shape between the front and back ends of the bubble was developed by Bretherton [1]. The shape of the bubbles merely reflects the pressure field determined by viscous and inertial forces in the liquid surrounding the bubble cap. Flow patterns in the liquid slugs are best described as Poiseuille flows in capillaries, except for the region near the bubble ends. At the front of the bubble, a part of the liquid in the liquid slug is drawn into the film surrounding the bubble. The rest of the liquid turns around and conforms a toroidal circulating pattern in a coordinate system moving with the bubble.

To obtain the overall pressure drop, the three pressure contributions are added with the provision of a minus sign in front of the hydrostatic term for down-flow conditions or a plus sign for up-flow conditions. A pressure drop contour map as a function of J_L and J_G, using the results from Woehl [4] is shown in Fig. 1. The region above the straight line labeled $J_L/J_G = 2$ and the region below the straight line labeled $J_L/J_G = 0.5$ indicate the regions where there is no experimental information on bubble length. Within the range of liquid to gas ratio where bubble lengths can be predicted using an empirical correlation, theoretical pressure drops are close to experimental data. Three of the contour lines ($DP = 1, 2$, and 3 kPa) from the experimental data of Woehl [4] were sketched on top of the contour map of theoretical values. Agreement between theory and experiments is remarkable considering the fact that there are no adjustable parameters in our theoretical model. The physical properties of parameters used in the computations were standard values of density, viscosity, and surface tension, not taking into account variations due to impurities always present in experimental fluids.

There is a fairly good correlation between capillary pressure drop and bubble velocity, which itself explains the linear correlation used by Grolman et al. [2]. Except for the points outside the range of experimentally determined bubble lengths, most of the points fall within 10–20% of a straight line with slope $c = 5625\,\mathrm{Pa/m/s}$. Although this number is approximately three times larger than the constant determined by Grolman et al. [2], it is easy to see why one would be tempted to develop an empirical correlation where the additional pressure drop is a linear function of bubble velocity.

3. Conclusions

Within the range of liquid to gas flow ratios where experimental data on bubble lengths are available, computed pressure drop agrees very well with experimental data. The theoretical model applies at its best for single capillaries. The experimental data of Grolman et al. [2] was measured in capillary bundles where other effects associated with flow distribution may be present. This is a faithful model of the phenomena involved in pressure drop in capillaries during bubble-train flow. This model has no adjustable parameters and takes into account the three main contributing phenomena. It predicts reasonably well the area of unstable flow, that is the flow around the pressure gradient reversal in down-flow, and it predicts the trend that takes place with changes in bubble and liquid slug length. Careful experiments and rigorous control of physical properties — such as interfacial tension — during experiments will help to improve agreement between experiments and computations.

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