Evaluation of Recirculation Time in Bubble Train Flow by Using Direct Numerical Simulation

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ABSTRACT: In this research, hydrodynamics of the Bubble Train Flows (BTF) in circular capillaries has been investigated by Direct Numerical Simulation (DNS). The Volume of Fluid Based (VOF) interface tracking method and streamwise direction periodic boundary conditions has been applied. The results show that there exists an appropriate agreement between DNS and experimental correlation results. The recirculation time as an important parameter, which affects the mass transfer of gas-liquid slug flow through the capillaries channel, has been calculated. The effects of different parameters such as capillary length, capillary diameter, unit cell length, and surface tension on recirculation time have been investigated. Afterwards, the DNS based correlation has been proposed for BTF recirculation time in a circular capillary.

KEYWORDS: Recirculation time; Bubble Train Flows (BTF); Direct Numerical Simulation (DNS); Volume Of Fluid (VOF); Circular Capillaries.

INTRODUCTION
Monolith reactors are increasingly considered for multiphase catalytic reactions such as hydrogenations [1], hydrodesulphurization [2], oxidations [3], bioremediation [4] and Fischer–Tropsch synthesis [5]. These reactors have shown many advantages over conventional reactors such as high catalytic surface concentration, high mass transfer rate, low pressure drop, and ease of scale up. In monoliths, the predominant flow pattern is a Bubble-Train Flow (BTF) of elongated bubbles. BTF regime is an unsteady periodic flow of identical bubbles in regular sequence form. In this flow regime the bubbles, which are separated by liquid slugs, fill almost the entire channel cross-section and travel with the same axial velocity. Optimization of mass transfer in monolith reactors requires profound understanding of the principle transport processes. The mass transfer from Taylor bubble to surrounding liquid slug takes place by two different modes. The first mode is the mass transfer to liquid film, flowing down the sides of the bubble, and the second one is the mass transfer from the two bubble capes to liquid slug. This mode of mass transfer is strongly influenced by radial mixing of the liquid moving as a slug [6].

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Radial mixing in bubble train flow in capillaries is affected by the length and frequency of bubbles. Some researchers reported that the length and frequency of bubbles plays a crucial role in heat and mass transfer enhancement in BTF regime. Horvath et al. calculated the radial mixing in slug flow through circular pipes by the bulk controlled reaction rates, measured in tubes with immobilized enzyme on the inner wall [7]. They reported that the radial mass transport in BTF regime increases rapidly with decreasing the liquid slug length. The experimental data reveals the remarkable effects of liquid slug and gas bubble hydrodynamics on mass transport in BTF regime.

The parameter that can be used as an index of radial mixing in BTF regime is recirculation time [8]. The estimation of recirculation time in BTF regime needs the detailed knowledge of its hydrodynamics. At this point, numerical simulations provide a beneficial tool to explore the hydrodynamics characteristics of the multiphase regime. Due to increase in computational power, multi-phase Direct Numerical Simulation (DNS) become feasible. In this approach the flow filed is obtained by solving the Navier-Stocks equation and appropriate interface capturing technique. There are different tracking methods for simulation of multiphase flow; some researchers used these methods to simulate Taylor bubble, such as VOF [9], Level set [10], and marker point [11]. Among these methods, Volume Of Fluid (VOF) is the most widely used method.

In literature, the hydrodynamics of BTF regime was simulated both in entire capillary length and in a single unit cell. Modeling of BTF regime in entire capillary length is very difficult and needs a high computational cost. Some researchers have modeled the BTF regime in entire capillary length [12-16]. Modeling of BTF regime by this method requires only the superficial velocities of two phases as an input and the void fraction, the bubble velocity are calculated as a part of the solution. However, when using such an approach, a long computational domain is required to obtain fully developed BTF regime [17]. Moreover, it needs a refined computational grid in order to capture flow features accurately.

Some researchers have modeled fully developed BTF regime in a single unit cell where liquid flows over the stationary bubble and the moving channel wall [18-22]. This approach not only can reduce the computational complexity significantly, but also requires flow parameters such as the slug length, void fraction and the bubble velocity as input parameters. In this approach mixture velocity was specified at the inlet and fully developed boundary condition at the outlet. The wall velocity has been guessed initially and then iteratively updated until the bubble no longer moved in axial direction, so this method also needs a large computational effort.

Another approach to model BTF regime is combination of the above methods, in which one unit cell is considered and a bubble moves through this cell [23-26]. In this approach the periodic boundary conditions are used in the streamwise direction. The use of periodic boundary conditions requires a special treatment of the pressure term in momentum equations. To this aim, a reduced pressure is defined and the buoyancy force and the axial pressure gradient appear as source terms in the Navier–Stokes equation. With these source terms the bubble moves up and after elapsing enough run time the bubble shape eventually becomes steady. This approach has been used for simulating the hydrodynamics of BTF regime in a circular capillary in this study.

On the grounds of this fact that the mass transfer in BTF regime is strongly affected by the recirculation time in liquid slug, in this work DNS has been used for calculating the recirculation time. In this paper we investigate, to our knowledge for the first time, the effects of parameters such as capillary length, capillary diameter, unit cell length, and surface tension on recirculation time in laminar BTF through circular capillary. Based on the results of DNS a predictive correlation has been proposed for BTF recirculation time in a circular capillary.

**MATHEMATICAL MODELING**

**Hydrodynamics**

Fig. 1 shows the computational set-up for two dimensional axisymmetric simulation of laminar bubble train flow. The coordinate system is defined by taking y as axial direction and x as the radial direction. The gravity vector points in the negative y-direction. The boundary conditions used in this study have been shown in Fig. 1. In order to simulate bubble train flow, the approach of Gidersa et al. [23] has been used.

Two phase computations and interface tracking in this work are based on the VOF method. In the VOF model,