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Recirculation time and liquid slug mass transfer in co-current upward and downward Taylor flow

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ABSTRACT

In this paper we investigate the recirculation time (τ) in the liquid slug of laminar Taylor flow theoretically and numerically. Theoretically, we develop a correlation for τ in rectangular channels, which depends on the aspect ratio and the ratio (ψ) between the bubble velocity and the total superficial velocity. This correlation suggests that τ is – for a given value of ψ – larger in upward than in downward Taylor flow because of buoyancy. The evaluation of τ from direct numerical simulations of Taylor flow confirms this result. The lower value of τ suggests that the sequential mass transfer between the gas bubble, the liquid slug and the channel wall is more efficient in downward than in upward flow. Numerical investigations of the overall wall-to-bulk mass transfer, which also contains the contribution through the liquid film between the bubble and the channel wall, show, however, that upward Taylor flow is slightly more efficient than downward Taylor flow. This indicates that for heterogeneously catalyzed gas–liquid reactions in monolith reactors a general statement whether mass transfer in upward or downward Taylor flow is more efficient is not reasonable, since the overall mass transfer depends on a large number of hydrodynamic and physical–chemical parameters.

1. Introduction

Bubble train flow or Taylor flow constitutes an attractive flow pattern for catalytic multiphase monolith reactors [1,2] because of its excellent mass transfer properties. It consists of a sequence of bubbles that almost fill the cross-section of a narrow channel and are separated by liquid slugs. Recent reaction studies [3,4] have shown that Taylor flow is superior as compared to other two-phase flow patterns.

For heterogeneously catalyzed chemical reactions in Taylor flow, the mass transfer of chemical species from the gas bubble to the solid wall takes place by two parallel paths. Each path consists of two steps in series. The first path is given by the mass transfer from the lateral sides of the bubble into the liquid film surrounding the bubble body (step 1), and by the mass transfer from the liquid film toward the solid wall (step 2). The second path consists of the mass transfer from the front and rear cap of the bubble to the liquid slug (step 1) and from the liquid slug toward the solid wall (step 2). The mass transfer of this second path is strongly affected by the recirculation in the liquid slug. The intensity of this recirculation can be quantified by the time needed for the liquid to move from one end of the slug to the other end, T_L. A second characteristic time scale is the time needed by the liquid slug to travel a distance of its own length. This time is given by $T_s \equiv L_s/U_B$, where L_s is the length of the liquid slug and U_B is the bubble velocity. Thulasidas et al. [5] defined the ratio of both times as the non-dimensional recirculation time

$$\tau \equiv \frac{T_L}{T_S} = \frac{T_L U_B}{L_S} \quad (1)$$

Multiphase monolith reactors can be operated in co-current upward or co-current downward flow. Recent experimental investigations of Taylor flow in a square mini-channel suggest that mass transfer between the slug and the channel wall may be more efficient in upward than in downward flow [6]. This is attributed to the lower recirculation time.

In this paper we perform, to our knowledge for the first time, a theoretical analysis of the recirculation time in laminar Taylor flow in rectangular channels. Based on this analysis we develop in Section 2 a predictive correlation which indicates that the recirculation time in Taylor flow is larger in upward than in downward flow because of buoyancy. In Section 3 we confirm this result for a square channel by evaluations of the recirculation time from direct numerical simulation (DNS) results. In this section, we also discuss results of new numerical investigations on the

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wall-to-bulk mass transfer in co-current upward and downward Taylor flow at similar values of the total superficial velocity. In Section 4 we present the conclusions.

2. Theoretical analysis of recirculation time in Taylor flow

The evaluation of the time T_L requires the knowledge of the velocity field within the liquid slug. Here, we assume that the liquid slug is sufficiently long to form a fully developed Poiseuille profile. According to Thulasidas et al. [5] this assumption is valid when the liquid slug length is larger than about 1.5 times the hydraulic diameter of the channel, D_h. Neglecting end effects in the liquid slug close to the front of the trailing and the rear of the leading bubble, we introduce the approximation

$$T_L = \frac{L_S}{\langle V_{Po}\rangle_{A_0}} \tag{2}$$

Here,

$$\langle V_{Po}\rangle_{A_0} = \frac{\iint_{A_0} V_{Po}\,dA}{\iint_{A_0} dA} = \frac{1}{A_0}\iint_{A_0} V_{Po}\,dA \tag{3}$$

is the mean velocity in the channel cross-section area A_0, where the Poiseuille velocity profile in the moving frame of reference, V_{Po}, is positive. Then, the non-dimensional recirculation time is given by

$$\tau \equiv \frac{T_L}{T_S} = \frac{U_B}{\langle V_{Po}\rangle_{A_0}} = \frac{\iint_{A_0} dA}{\iint_{A_0}(V_{Po}/U_B)dA} \tag{4}$$

2.1. Circular channel

In a circular channel with radius R, the Poiseuille velocity profile in the frame of reference moving with the bubble is given by

$$V_{Po}^{cir}(r) = U_{L,max}^{cir}\left(1-\frac{r^2}{R^2}\right) - U_B = C_{Po}^{cir}U_{L,mean}^{cir}\left(1-\frac{r^2}{R^2}\right) - U_B \tag{5}$$

where $C_{Po}^{cir} = U_{L,max}^{cir}/U_{L,mean}^{cir} = 2$. In an incompressible Taylor flow, the mean velocity in the liquid slug is equal to the total superficial velocity J, so that $U_{L,mean} = J$. A recirculation pattern in the liquid slug occurs for $U_B < U_{L,max}$ or $\psi \equiv U_B/J < C_{Po}$, i.e. in a circular channel for $\psi < 2$. From Eq. (5) one obtains for the radial position r_0, where the velocity V_{Po}^{cir} is zero, the result

$$\frac{r_0}{R} = \sqrt{1-\frac{\psi}{2}} \tag{6}$$

With $A_0 = \pi r_0^2$ and $dA = 2\pi r\,dr$ Thulasidas et al. [5] obtained from Eq. (4) the relation

$$\tau_{cir} = \frac{U_B r_0^2}{2\int_0^{r_0} V_{Po}^{cir}(r)r\,dr} \tag{7}$$

Introducing Eqs. (5) and (6) in Eq. (7) and performing the integration yields

$$\tau_{cir}(\psi) = \left(\frac{1}{\psi}-\frac{1}{2}\right)^{-1} = \frac{C_{Po}^{cir}}{\phi^{-1}-1} \tag{8}$$

where $\phi \equiv C_{Po}^{cir}/\psi$. The velocity ratio ψ is in the range $1 \le \psi < 2$ so that the minimal recirculation time in a circular channel is 2 while it becomes infinity for $\psi \to 2$. From Eq. (6) we obtain for the non-dimensional area where $V_{Po}^{cir} \ge U_B$ the result

$$\frac{A_0}{A_{ch}} = \frac{\pi r_0^2}{\pi R^2} = \frac{2-\psi}{2} \tag{9}$$

In Taylor flow, the cross-sectional regions with bypass flow (close to the walls) and recirculation flow (in the channel center) are separated by the "dividing streamline" [5]. The position of the dividing streamline is obtained from the condition that the total axial flow rate within the recirculation area is zero in the moving frame of reference. For a circular channel this requirement is equivalent to the condition

$$2\pi\int_{r_1}^{R} V(r)r\,dr = \pi R^2(U_B - J) \tag{10}$$

given in [5] which yields

$$\frac{r_1}{R} = \sqrt{2-\psi} \tag{11}$$

Thus, in a circular channel the non-dimensional cross-sectional recirculation area is $A_1/A_{ch} = 2-\psi$ and it is $A_1/A_0 = 2$ for any value of ψ.

2.2. Rectangular channel

We consider a rectangular channel with dimensions $2a$ and $2b$ as displayed in Fig. 1. The cross-sectional area of the channel is $A_{th} = 4ab$ and its aspect ratio is $\alpha \equiv b/a \le 1$. The origin of the coordinate system is located in the channel center so that $-a \le z \le a$ and $-b \le y \le b$. In the moving frame of reference, the laminar Poiseuille velocity profile for this channel is given by [7]

$$V_{Po}^{rec}(y,z) = \frac{64}{\pi^3}J\frac{\sum_{n=1,3,5}^{\infty}(-1)^{(n-1)/2}/n^3[1-\cosh((n\pi/2a)y)/\cosh(n\pi b/2a)]\cos((n\pi/2a)z)}{1-(192a/\pi^5 b)\sum_{n=1,3,5}^{\infty}(1/n^5)\tanh(n\pi b/2a)} - U_B \tag{12}$$

Since for this velocity profile an analytical evaluation of the recirculation time according to Eq. (4) is not practicable, we adopt the approximation

$$V_{Po}^{rec}(Y,Z) = C_{Po}^{rec}J(1-Y^n)(1-Z^m) - U_B \tag{13}$$

first proposed by Purday [8]. Here, it is $Y \equiv y/b$, $Z \equiv z/a$ and

$$C_{Po}^{rec} = \frac{U_{L,max}^{rec}}{U_{L,mean}^{rec}} = \frac{m+1}{m}\frac{n+1}{n} \tag{14}$$

The values of n and m depend on the aspect ratio. Here, we adopt the following correlations proposed by Natarajan and Lakshmanan [9]

$$n = \begin{cases} 2 & \text{for} \quad 0 \le \alpha \le 1/3 \\ 2+0.3(\alpha-1/3) & \text{for} \quad 1/3 \le \alpha \le 1 \end{cases} \tag{15}$$

$$m = 1.7 + 0.5\alpha^{-1.4} \tag{16}$$

For this velocity profile, a Taylor flow with recirculation pattern in the liquid slug occurs for $1 \le \psi < C_{Po}^{rec}$ or $1/C_{Po}^{rec} \le \phi < 1$, respectively.

In the sequel, we will utilize the curves $Z_\lambda = Z(Y, C_{Po}^{rec}, \lambda)$ where the ratio $\lambda \equiv V_{Po}^{rec}/U_B$ is constant. Here, λ is in the range

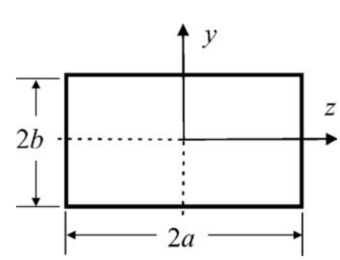

Fig. 1. Sketch of rectangular channel with dimensions and co-ordinate system.