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Bubbles velocity, Taylor circulation rate and mass transfer model for slug flow in milli- and microchannels

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HIGHLIGHTS

- Simple equation for bubbles velocity prediction is proposed.
- Circulation occurs even in very short liquid slugs.
- Recirculation times in the Taylor vortices dependence on slug length is found.
- Mass transfer mathematical model for slug flow is elaborated.

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ABSTRACT

The aim of this study is to get interrelated information necessary for heat and mass transfer efficiency estimation, namely: to find simple equation for bubble velocity prediction, essential for all other model parameters; to estimate circulation rate in the Taylor vortices dependence on slug length; elaborate simplified mathematical model describing mass transfer based on the three-layer flow structure in the liquid slug. Analysis on the basis of the continuity and Navier–Stokes equations revealed that the circulation of liquid in the slugs take place, even if their length is 15 times smaller than the diameter of the capillary. By CFD-calculations was detected that although the circulation is not vanishing completely for short liquid slugs (approximately shorter than 0.7 of capillary diameter), its intensity (circulation flow rate) diminishes and dimensionless recirculation time is growing. Equation for radius of vortex center depending of slug length is proposed. It was revealed that for very short liquid slugs (shorter than 0.17 of capillary diameter) the inner circulation is less than the bypass flow rate. Effects of liquid slug length on dimensional and dimensionless recirculation times were defined. Poor difference of downward and upward flows in respect to mass transfer originates from minor differences of bubble velocity for downward and upward flows.

1. Introduction

In last two decades micro technologies and micro equipment are the objects of a great interest in a chemical engineering. Small series of the high-performance micro-heat exchangers, mixers, reactors, extractors, pumps and valves have been already developed and produced [1,2]. Such equipment has the range of cross section dimension between 10 μm and 1–3 mm. The channels with the inner hydraulic diameter less than 0.1–1 mm are usually called microchannels whereas the larger ones are called mini or milli channels.

Microreactors can be competitive in a field of fast reactions, when a process rate is limited by mass and heat transfer, and when it is necessary to take off hot spots (e.g. at the initial area of a running reactor). It is caused by unusual values of heat- and mass-transfer coefficients in microreactors that can be two times higher than in the conventional types of reactors [1].

The most useful flow regime for gas–liquid reactions is considered to be a slug flow (bubble-train or Taylor flow). Heat and mass transfer of gas–liquid flow in mini- and microchannels depends strongly on hydrodynamics. Bubble velocity influences a number of parameters like a film thickness, residence time, circulation frequency and mass transfer coefficient. Therefore it is necessary to have some convenient equation to calculate bubbles velocity in milli- or microchannels.

Kolb and Cerro [3] have investigated liquid deposited on the walls of a capillary of square cross section for Taylor downward flow. They have experimentally determined streamline patterns in liquid slugs. It was revealed, that transition to complete bypass

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Nomenclature

a, b, c, g, h, D	coefficients in Eqs. (2)–(5)
a, b	coefficients in Eq. (21a)
A_f	cross section of the film around bubble, $A_f = \pi(R^2 - R_b^2)$, m^2
A_0	cross section of the direct circulation flow in the slug, $A_0 = A_d = \pi R_0^2$, m^2
A_1	total cross section of the vortex (circulation) flow in the slug, $A_1 = \pi R_1^2$, m^2
A_r	cross section of the reverse flow in the slug, $A_r = A_1 - A_0$, m^2
C	concentration of a substance dissolved in the liquid phase, kg/m^3
d_c	diameter of capillary, m
D	diffusion coefficient, m^2/s
$\mathbf{I}$	identity matrix
$j_1, \ldots, j_{11}$	diffusion and convection fluxes of matter at the layer boundaries, kg/s m^2
k_{LG}	mass transfer coefficient from gas to liquid, m/s
k_{LS}	mass transfer coefficient from the surface of the capillary to the liquid, m/s
k_La	volumetric gas–liquid mass transfer coefficient, s^{-1}
k_sa	volumetric liquid–solid mass transfer coefficient, s^{-1}
L_b	bubble length, m
L_s	liquid slug length, m
L_c	capillary length, m
q_c	circulation flow rate, m^3/s
q_1	total (bypass and circulation) volumetric flux through the outer area $[R_0; R]$, m^3/s
q_2	volumetric flux through the inner vortex area $[0; R_0]$ (direct circulation flow), m^3/s
$(q_1 - q_3)$	volumetric flux through the outer vortex area $[R_0; R_1]$ (reverse circulation flow), m^3/s
q_3	bypass volumetric flux through the area $[R_b; R]$, i.e. through the film around vortex area, m^3/s
q_{trans}	bypass volumetric flux through the film around bubble ($q_3 = q_{\text{trans}}$, see also Eq. (29)), m^3/s
R	radius of capillary, m
R_b	radius of bubble, m
R_0	radius of point corresponding to the condition $u_z = 0$, m
R_1	radius of surface separating the transition (bypass) flow from the circulation flow, m
$\mathbf{t}$	unit vector, directed along the line
U	average velocities for real flow, m/s
U_b	average bubble velocity, m/s
U_f	average film velocity, m/s
U_s	two phase velocity (average liquid slug velocity), m/s
$u_z(r)$	relative z-velocity of liquid in the liquid slug, $u_z(r) = V(r) - U_b$, m/s
$u_f(r)$	relative z-velocity of liquid in the liquid film around bubble, $u_f(r) = V_f(r) - U_b$, m/s
$\mathbf{u}$	velocity vector, m/s
$V(r)$	absolute z-velocity of liquid in the liquid slug, m/s
$V_f(r)$	absolute z-velocity of liquid in the liquid film around bubble, m/s
w	average velocities calculated for inverted flow (bubble stopped, capillary moves), m/s
w_1, w_2, w_3, w_f	reverse, direct and bypass average velocities according to Eq. (24)
W	dimensionless slip velocity of bubble [10], $W = (U_b - U_s)/U_b$
δ	thickness of liquid film around bubbles, m
ΔC	concentration difference, kg/m^3
η	dimensionless (relative) bubble velocity of bubble, $\eta = U_b/U_s$, Eqs. (2)–(5)
θ_1, θ_2, Θ	dimensional recirculation times, s
θ_3	time of convection flow of liquid film around Taylor vortex from one bubble to the next bubble, s
θ_b	time which bubble needs to move throughout the liquid slug length, s
θ_{fb}	time of convection flow of liquid film around the bubble throughout its length, s
μ	liquid viscosity, Pa s
ρ	liquid density, kg/m^3
σ	interfacial tension, N/m
τ_1, τ_2, T	dimensionless recirculation times, see Eq. (25)
$\varphi = (q_1 - q_3)/q_3$	ratio of direct flux to bypass flux
$\psi = (q_1 - q_3 + q_2)/(q_1 - q_3)$	relative error of flow rate calculation
ω_1, ω_2, ω_3	durations of contact between layers in Taylor vortex and films, s
ω_{fb}	contact time between liquid film around the bubble and bubble side surface, s
ω_f	contact time between liquid film around the bubble and the capillary wall, s
∇	Hamilton operator
Ca	capillary number calculated by use of bubble velocity, $\text{Ca} = \mu U_b/\sigma$
Ca*	critical value of capillary number
Ca$_s$	capillary number calculated by use of liquid slug velocity, $\text{Ca}_s = \mu U_s/\sigma$
Pe	Peclet number, $\text{Pe} = U_s L_c/D$

flow occurs around Ca = 0.6 for square cross section capillaries, whereas transition from nonaxisymmetric to axisymmetric bubble was found to occur at Ca ≈ 0.1.

Thulasidas et al. [4] pointed out the strong impact of Taylor vortices in the liquid slugs on the mass and heat transfer rate. Besides, vortex center as well dividing streamline positions for channels with both circular and square cross sections are calculated and compared with experimental data [4]. The dimensionless recirculation time, defined by Thulasidas et al. [4] as the number of times a liquid slug travels its own length before a particle in the recirculation vortex will travel from one end of the slug to the other. It was shown that recirculation time in a capillary almost constant and equal to 2.0 for the range of capillary number values Ca < 0.01–0.03. For larger capillary numbers recirculation time increases dramatically and becomes infinite for completely bypass flow [4].

Tsoligkas et al. [5] used particle image velocimetry (PIV) to investigate the velocity fields within the liquid slugs and investigated the effect of hydrodynamics on reaction rates in capillary reactor (see also [6]). The rate of reaction was found to be a function of the hydrodynamics. Two distinctive cases, long slugs (longer than diameter of capillary) and short slugs (shorter are described in [6]) were studied. Long slugs had a 3-D flow field and the velocity profiles were parabolic. Short liquid slugs exhibited a 2-D flow field with a flat axial velocity profile as a function of the tube radius. Tsoligkas et al. [7] investigated dependence of reaction rate for catalytic hydrogenation of 2-butyne-1,4-diol to cis-2-butene-1,4-diol and butane-1,4-diol on the dimensionless liquid slug length as well dimensionless gas bubble length. It was concluded that ‘for short slugs, the profile of the axial velocity component across the capillary diameter was found to be flat ***resulting in***