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Multiphase parallel flow stabilization in curved microchannel

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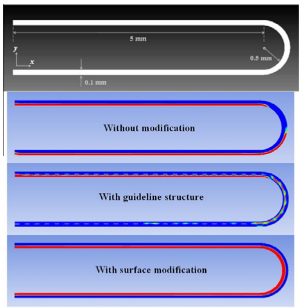
HIGHLIGHTS

- The organic–aqueous parallel flow was studied in a curved microchannel with using computational fluid dynamics.
- The effects of guideline structure and surface modification on the flow were investigated.
- The surface modification method shows good flow improvement results.

GRAPHICAL ABSTRACT



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ABSTRACT

The effect of liquid multiphase parallel flow stabilizing method (i.e. guideline structure addition and surface modification) was studied in a curved microchannel by using CFD simulation. A phase separator function can be combined within a microchannel by operating under stable parallel flow conditions. Based on our simulation conditions, the flow pattern could not be improved by using the guideline structure but the surface modification proves to be beneficial.

1. Introduction

Microreactor a process-intensifying equipment, has been applied to improve various separation and reaction systems [1–5]. An important advantage is mass and heat transport enhancement. In case of multiphase systems, the mass transfer path between phases can be decreased. The immiscible fluid systems such as organic-aqueous flows with mass transfer limitations have been studied in microreactors [6–12].

Due to large surface-to-volume ratio, surface effects become important. Therefore, multiphase flow with many interfaces in microstructures shows different flow patterns from typical size systems. Two common patterns of liquid multiphase flow, parallel and slug flows, have been studied. In this work, parallel flow is focused because it can provide phase separation at the outlets. Therefore, the requirement of a post-treatment unit can be reduced. This microdevice with phase separation is expected to be used in design of continuous flow integrated microsystems. In order to stabilize parallel flow pattern in a microdevice, guideline structure addition [13–15] and surface modification [16–18] have been proposed for liquid multiphase systems. In our previous

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Nomenclature

Ca	Capillary number
d_H	Hydraulic or equivalent diameter
De	Dean number
F	Surface tension force
n	Surface normal
$\hat{n}$	Unit surface normal
$\hat{n}_w$	Unit vector normal to the wall
$\hat{t}_w$	Unit vector tangential to the wall
p	Pressure
R	Curve radius
Re	Reynolds number
t	Time
u	Superficial velocity
v	Velocity
Greek letters	
α	Volume fraction
κ	Curvature
μ	Viscosity
θ_w	Contact angle at the wall
ρ	Density
σ	Surface tension coefficient

studies, the effects of guideline structure and surface modification were investigated in straight glass microchannels [19,20]. The results show that the parallel flow pattern could be improved by these two techniques.

Computational fluid dynamics (CFD) is a useful method to study fluid flow. Several works have applied this technique to study flows in microdevices especially slug flow [21–23] because it can provide detailed flow field information. Glatzel et al. [24] studied the performance of four CFD software programs, CFD-ACE+, CFX, Flow-3D and FLUENT by simulating four different microfluidic applications in 3D.

A straight microchannel has been studied in a number of works. In practice, a serpentine channel is widely used because of its compactness. It can provide high heat and mass transport and narrow residence time distributions [25,26]. In this work, the effect of parallel flow stabilizing method, i.e. guideline structure addition and surface modification, was studied in the curved microchannel by using ANSYS FLUENT, a well-known commercial CFD program.

2. Numerical simulation

Three-dimensional geometrical models were generated by GAMBIT and the simulations were performed with FLUENT 12.0 [27]. The interface was tracked by using the volume of fluid (VOF) method. The immiscible liquids were considered as isothermal incompressible Newtonian fluids. The conservation equations for momentum and mass can be written as:

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v}\right) = -\nabla p + \mu\nabla^2\vec{v} + \vec{F} \tag{1}$$

$$(\nabla\cdot\vec{v}) = 0 \tag{2}$$

where $\vec{v}$, p and $\vec{F}$ are the velocity, pressure and surface tension force, respectively.

The physical properties ρ and μ are density and viscosity respectively which were calculated by averaging based on the individual fluid volume fraction in each control volume. The interface between the phases was identified by the continuity equation for the volume fraction (α) which can be expressed as:

$$\frac{\partial\alpha}{\partial t} + \vec{v}\cdot\nabla\alpha = 0 \tag{3}$$

The surface tension effect was included using the continuum surface force (CSF) model proposed by Brackbill et al. [28] in the VOF calculation. The calculated surface tension force was added as an additional source term in the momentum conservation equation. The force for two phases is modelled as:

$$F_{\mathrm{vol}} = \sigma\frac{\rho\kappa\nabla\alpha}{\frac{1}{2}(\rho_1+\rho_2)} \tag{4}$$

where σ and κ are the surface tension coefficient and the curvature which was computed from the divergence of the unit surface normal:

$$\kappa = \nabla\cdot\hat{n} \tag{5}$$

where,

$$\hat{n} = n/|n| \tag{6}$$

and the surface normal defined as the gradient of the volume fraction:

$$n = \nabla\alpha \tag{7}$$

The surface normal in the cell next to the wall is corrected by including the wall adhesion effect and can be written as:

$$\hat{n} = \hat{n}_w\cos\theta_w + \hat{t}_w\sin\theta_w \tag{8}$$

where $\hat{n}_w$ and $\hat{t}_w$ are the unit vectors normal and tangential to the wall, respectively and θ_w is the contact angle at the wall.

Our simulation approach was validated by comparison with the previously published work [29]. Two phase liquid flows were simulated in the 156,000 cell T-shaped microchannel model. Water and kerosene with the surface tension of 0.045 N/m were fed as aqueous and organic phases, respectively. The contact angle of kerosene in water on PMMA calculated using Young's equation was 77.48°. The simulation results showed slug and parallel flow patterns at low and high flow rates, respectively, which agree well with the previous study. The measured water slug lengths were compared with the experimental and 78° contact angle simulated results in Fig. 4 of the literature. At a water flow rate of 10 mL/h, the simulated slug lengths were 1.77, 1.38 and 1.15 mm when kerosene was fed at 20, 40 and 60 mL/h, respectively. These results were between the published experimental and simulation results.

The microchannel 3D model was created based on a standard product of Institute of Microchemical Technology Co., Ltd. (IMT). The channel width, height and curvature radius are 100, 40 μm and 0.5 mm, respectively. In order to study the effect of curvature on the parallel flow pattern, microchannels with curve radius of 1 and 3 mm were also created. The microchannel model with microtexture called guideline structure was generated to study the structure effect on flow characteristics. The guideline wall and interval lengths were 100 μm as in the straight microchannels in our previous work [19]. Without guideline structure, the 0.5, 1 and 3 mm curvature radius microchannels were meshed to 50,000, 60,000 and 90,000 cells, respectively. For the guided microchannel case, the model has 51,776 cells. Fig. 1 shows the model outline and meshed model parts of microchannel with guideline structure. The meshed parts in Fig. 1(b)–(e) were enlarged from the rectangle areas in Fig. 1(a). In Fig. 1(e), the black lines are wall grids and white lines are interior grids. Water and toluene were fed