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# CFD modelling of mass transfer with and without chemical reaction in the liquid–liquid slug flow microreactor

M.N. Kashid[a,b,*], D.W. Agar[a], S. Turek[b]

[a]*Institute of Reaction Engineering, University of Dortmund, 44227 Dortmund, Germany*
[b]*Institute for Applied Mathematics, University of Dortmund, 44227 Dortmund, Germany*

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**Abstract**

A finite element based computational fluid dynamics (CFD) model was developed to study the flow patterns within the slugs and mass transfer with and without superimposed chemical reaction between two consecutive slugs in the liquid–liquid slug flow capillary microreactor. Since the slug flow is a series of alternate slugs of one phase separated by the other, a single element consisting of a slug of each phase was considered. The two slugs in a single domain were distinguished by two kinematic viscosities. The effects of various operating conditions on circulation patterns, mass transfer and reaction are discussed in detail. Finally, the results are compared with data from the literature.


*Keywords:* Slug flow microreactor; Finite element CFD model; Interphase mass transfer; Chemical reaction

## 1. Introduction

Microreactors are an attractive new tool for chemical engineers due to their diverse benefits over the conventional reactors. The liquid–liquid slug flow microreactor can be seen as an alternative to suspended drop reactors for mass transfer limited and strongly exothermic reactions (Burns and Ramshaw, 2001; Dummann et al., 2003). In this reactor arrangement the phases are present as a series of alternating moving slugs, constituting a series of well-defined individual subvolumes and thus interfacial area which fulfils the basic requirement for *a priori* prediction of mass transfer rates.

Very few articles on hydrodynamics and mass transfer of liquid–liquid slug flow have been published (Burns and Ramshaw, 2001; Dummann et al., 2003; Kashid et al., 2005, 2007; Tanthapanichakoon et al., 2006; Kashid and Agar, 2007). A numerical model was developed to describe the internal flow patterns within the fluid segments by Harries et al. (2003) and the transfer of the dissolved chemical species within and across the segments for liquid–liquid slug flow. The flow was represented by two stagnant, adjacent rectangular units which are linked at both ends to form a continuous loop. The model was validated with various sets of experimental results and showed good agreement. However, this study did not show the effect of viscosity on flow patterns within the slugs and consequently its effect on the mass transfer performance. In one of our previous publications (Kashid et al., 2007), we have developed a free surface model to understand the generation of slug flow. However, to solve the complete system for mass transfer with chemical reaction using these methods requires extensive computational resources.

In the present work, a model, similar to Harries et al. (2003) but accounts effect of viscosity, has been developed to study the mass transfer with chemical reaction in the liquid–liquid slug flow. The objective was to develop a prototype model which can be used for any liquid–liquid system with fixed interface location for mass transfer with and without chemical reaction. Due to the superior experience of the in-house developed finite element code particularly for single phase flow, the model equations are implemented in the open source software FEATFLOW (www.featflow.de). The numerical model, its solution and the

* Corresponding author. Institute of Reaction Engineering, University of Dortmund, 44227 Dortmund, Germany. Tel.: +49 231 7553453.
*E-mail addresses:* kashid@bci.uni-dortmund.de, kashid@math.uni-dortmund.de (M.N. Kashid).

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results obtained are discussed in the following sections. The effects of operating conditions on flow patterns, mass transfer and chemical reaction are presented in detail. Finally, the results are compared with the experimental and numerical results of Harries et al. (2003).

## 2. Numerical model

### 2.1. Problem definition

The following assumptions were considered to be reasonable to study the mass transfer with and without chemical reaction in the liquid–liquid slug flow:

- Both liquids are Newtonian, viscous and incompressible fluids.
- No effect of mass transfer and chemical reaction on the shape and volume of the slug.
- Flow is laminar and the mass diffusivity is constant in both slugs.

An experimental snapshot and the computational domain for this problem are depicted in Fig. 1. The experimental snapshot shows well-defined slug flow consisting of alternate slugs of the two phases. This flow regime with mass transfer of single species can be schematically represented as shown in Fig. 1b. Assuming transational symmetry, the problem is reduced to a single slug unit (the pair of two slugs of two phases as shown in Fig. 1c) which can decrease the computational effort significantly. The arrows from Fig. 1c indicate that each slug exchanges mass and momentum with its two neighbours.

### 2.2. Fluid flow

The computational domain shown in Fig. 1c was considered as two-dimensional. The velocity $u$ and pressure $p$ for this problem were solved by the following Navier–Stokes equation:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot (2\mu S) + \nabla p = f$$

$$\Omega \in \mathbb{R}^2 \times [0, T], \tag{2}$$

where $\rho$ and $\mu$ are the density and dynamic viscosity respectively while $S$ is the rate deformation tensor. They are defined as follows:

$$\rho = \rho_0 f(x, y),$$

$$\mu = \mu_0 f(x, y),$$

$$S = \tfrac{1}{2}(\nabla \mathbf{u} + \nabla^{\mathrm{T}} \mathbf{u}). \tag{3}$$

Two densities and viscosities were defined to represent the two phases in the same domain. However, there is an interface between the two slugs where the transport across it is due to diffusion only. This was represented by the concept of moving boundaries. In addition to this, there is a need to connect the two sides of the domain like a strip of paper wrapped around in a continuous loop. The connection was implemented using the concept of periodic boundary, and interface boundary conditions were applied at this connection which is referred to as the interface. Thus, the interface and periodically connected interface satisfies the following condition for momentum:

$$\mu_1 \frac{\partial u_1}{\partial \mathbf{n}_1} = \mu_2 \frac{\partial u_2}{\partial \mathbf{n}_2}, \tag{4}$$

where $\mu_i$, $u_i$ and $\mathbf{n}_i$ are the dynamic viscosities, velocities and unit normal to the interface in the $i$th domain, respectively.

### 2.3. Mass transfer

The transfer of species within the two phases is governed by the general convection–diffusion equations:

$$\frac{\partial C_{11}}{\partial t} + \mathbf{u}_1 \cdot \nabla C_{11} = D_{11} \Delta C_{11}, \tag{5}$$

$$\frac{\partial C_{12}}{\partial t} + \mathbf{u}_2 \cdot \nabla C_{12} = D_{12} \Delta C_{12}, \tag{6}$$

where $C_{11}$ and $C_{12}$ are the concentration of species 1 in phases 1 and 2, respectively. The natural boundary conditions were defined at the interface to satisfy the flux continuity at the interface by the following relation:

$$D_{11} \frac{\partial C_{11}}{\partial \mathbf{n}_1} = D_{12} \frac{\partial C_{12}}{\partial \mathbf{n}_2}, \tag{7}$$

$$C_{12} = m C_{11}, \tag{8}$$

where $D_{11}$ and $D_{12}$ are the diffusivities of species 1 in phase 1 and 2, respectively. In the above formulation, the species will

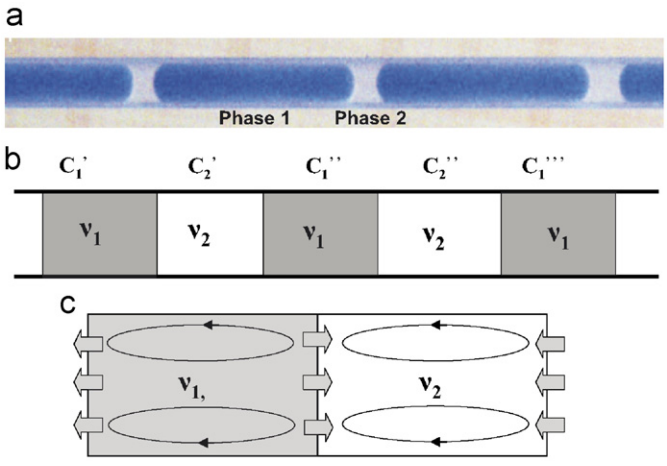


Fig. 1. Liquid–liquid slug flow: (a) experimental snapshot; (b) schematic representation of the slug flow; and (c) computational domain.