Slug Flow Capillary Microreactor Hydrodynamic Study

David Fernández Rivas[1], M. N. Kashid [2], D. W. Agar [2] and S. Turek [3]
[1] *Departamento de Ingeniería Nuclear,*
Instituto Superior de Tecnología y Ciencias Aplicadas, InSTEC,
Quinta de los Molinos, Ciudad de la Habana, Cuba
[2] *Institute of Reaction Engineering, University of Dortmund, Dortmund, Germany*
[3] *Institute for Applied Mathematics, University of Dortmund, Dortmund, Germany*

1. Introduction

Micro-fluidic applications have served as interface between the macro- and nano-world. Micro-scale systems offer many advantages such as minimal reagent consumption, complex chemical waveforms, and significantly reduced analysis and experimentation time (for example, an important concept recently introduced was μTAS, the Micro Total Analysis System for details see [14]). The absence of inertial and turbulent effects in micro-fluidic devices offers new horizons for physical, chemical and biological applications. The small dimensions give high surface-to-volume ratios, small diffusion distances and easy temperature profiling where needed, giving the opportunity to manipulate substances in ways never imagined before. Drops or slugs and their application in micro- and nano-scales are very important in various fields of present science. For instance, cell-based assays [15], models for capillary blood vessels for red cells infected with malaria [17], drug delivery targeted at specific sites in the body for a less invasive chemotherapy, miniature biosamples preparations on fully automated biochips, for DNA sampling are all known applications in medical and genomic sectors. In chemical sciences, it has been used in two-phase chemical reactions [11], [8], [7], [3], [4], and elucidation and optimization of nitration reaction demonstrated by Dumman, who concluded that the capillary micro-reactor can be used for quantitatively examining exothermic liquid-liquid reaction systems [5], fast or dangerous reactions, solvent extraction, substances separation and so on. At the micro-scales, the problems associated with the scaling-up for large scale production by simply numbering-up are reduced. This means that several micro-reactors can be used to obtain the necessary products, instead of building complicated and expensive plants. Mathematical models describing the movement of drops, or in general, multiphase flows developed so far, are not able to predict or quantify properly all the important particularities of this complex systems (capillary micro-reactors). Hence a deeper knowledge of the physical problem, say hydrodynamics transport, is essential. This task requires powerful modeling techniques. Consequently, we initiated the hydrodynamic study of drops/slug movement through capillaries. We focused on the application of a slug flow micro-reactor model to match the necessities and behavior described in [13] and [12].

2. Main results

2.1 Experimental results

Figure 1 shows the experimental setup and illustrates how two immiscible liquids (aqueous and organic) are introduced by continuously operating high-precision piston pumps to a symmetric 1200 Y-piece mixing element made of Teflon (PTFE). There is a complex flow that develops in each phase and at the interface between both phases and our objective is to gain insight of the flow pattern. In this work, the focus was on the internal circulation particularities within the slugs mainly in the aqueous phase. Particle Imaging Velocimetry (PIV) measurements were also conducted to gain insight of the internal circulation inside a slug.

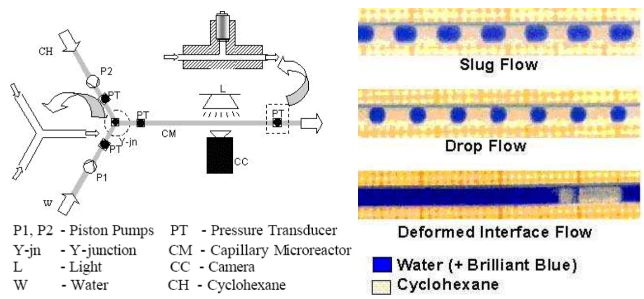

FIG.1: a) Experimental setup scheme,
b) Observed flow regimes in the capillary microreactor.

2.2 Computational modeling

The hydrodynamic flow pattern of a slug flow and the evolution of complex interfaces was determined using in-house, open-source, CFD code FEATFLOW (levelset approach). This code uses an implementation of surface tension effects in interfacial flow combining two techniques: the continuum surface force (CSF) method and a finite element discretization together with the Laplace-Beltrami operator [10], [9], [18], [16]. For the discretization of the domain, the in-house developed software DeViSoR 2.1 (Design and Visualization Software Resource) was used [2]. A structured two-dimensional coarse grid was built with an increased density of nodes closer to the wall boundaries in order to capture numerically, in a more accurate way, the complex flow in the near wall region (Fig. 2 a). The post-processing was performed with GMV software [6], and for particle tracing calculations, another in-house module, gmvpt [1], was used

Among the main numerical results we have, the velocity distributions can be plotted as color gradients or velocity vectors. Detailed information can be extracted where hydrodynamic conditions are the most complicated, for example, at the interface region, at the nose and back of the slug (Fig.1). When considering mass transfer and reactions in a micro-reactor, the transport of the species within the phases will be determined strongly on the hydrodynamic flow pattern; particle tracing results shows how species can be distributed as time passes by. Initially, a distribution of particles is placed in the back part of the slug, and as the slug moves to the right, the behaviour described above is exactly obtained (Fig. 3).

Comparing the particle tracing numerical solution with the experimental PIV measurements, it can be seen that both results are qualitatively the same and also coincide with the internal circulation expected flow pattern.

3. Conclusions

The expected physical behavior, experimental measurements and numerical results show excellent agreement. The flow pattern occurring inside a two-phase capillary micro-reactor was successfully studied both experimentally and by numerical modeling. The main hydrodynamic information extracted from the numerical code and its resemblance to the real physical system was shown. The precise control of capillary multiphase flow micro-reactors, from the hydrodynamics and chemical reaction requirements, will be possible once this model is validated and tuned.

References

[1] J. S. Acker and S. Turek, Postprocessing of FEATFLOW Data with the Particle Tracing Tool GMVPT version 1.2, Angewandte Mathematik und Numerik (LS III), Dortmund Universität, Germany, 2 (2000).

[2] C. Becker and D. Goeddeke, “DeViSoRGrid 2 User´s Manual”, Dortmund Universität, Germany, 2, (2002).

[3] Burns and Ramshaw, Lab. Chip J. (1) **1**, 10 (2001).

[4] Burns and Ramshaw, Chem. Eng. Comm. **189**, 1611 (2002) 1.

[5] Dumman et al., Catalysis Today **79-80**, 433 (2003) 1.

[6] GMV (General Mesh Viewer) user manual. Release 1.8, 1999 (see also: http: //www.xdiv.lanl.gov/XCM/gmv/GMVHome. html), 2.

[7] N. Harries, et al., Int. J. of Heat and Mass Transfer **46**, 3313 (2003) 1.

[8] S. R. Hodges, et al., J. Fluid Mech. **501**, 279 (2004) 1.

[9] S. Hysing and S. Turek, Proc. of Algoritmy **22** (2005) 2.

[10] S. Hysing, PhD Thesis, "Inst. for Applied Mathematics and Numerics", University of Dortmund (2006) 2.

[11] J. D. Tice et al., Analytica Chimica Acta 5007, **73** (2004).

[12] Kashid et al., Submitted to Journal of Computational and Applied Mathematics (2006) 1.

[13] Kashid, et al., Ind. & Eng. Chem. Res. **44 (14)**, 5003 (2005) 1.

[14] A. Manz et al., Sens. Actuators **A1**, 244 (1990) 1.

[15] J. Pihl et al., Materials Today **8**, Nr.12, 46, (2005) 1.

[16] S. Turek and C. Becker, "FEATFLOW Finite element software for the incompressible Navier-Stokes equations", User Manual Release 1.1, Preprint, Heidelberg (1998) 2.

[17] J. P. Shelby et al., Proc. Natl. Acad. Sci. USA **100**, 14618 (2003) .

[18] S. Turek, *Efficient Solvers for Incompressible Flow Problems: An Algorithmic Approach* (Springer-Verlag, Heidelberg, 1999).

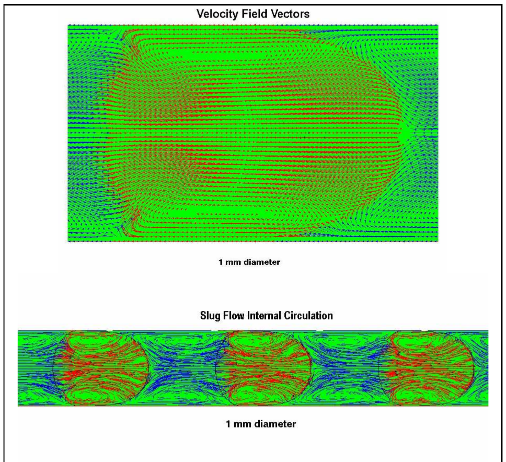

FIG.2: a) Velocity vector plot of a single slug
b) Vector plot representing the internal circulation.

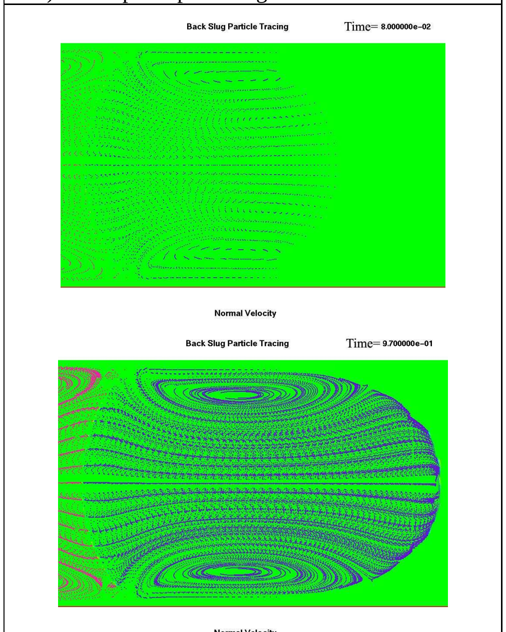

FIG.3: Particle tracing evolution at different times inside a slug.