ANALYZING MICROFLUIDIC DEVICES USING NUMERICAL MODELING

Cătălin MĂRCULESCU[1], Cătălin Mihai BĂLAN[1], Andrei AVRAM[1] and Marioara AVRAM[2]

The present microfluidic study is emphasizing the flow behavior of two immiscible fluids within a Y shape micro-bifurcation with two inlets and one outlet, in order to create a test case for designing a microfluidic device using numerical modeling. We report here a numerical investigation on the interface shape dynamics manifested for different heights of the microchannel. After choosing the proper geometry, experiments were performed on the proposed geometry. The experimental data were compared with numerical simulations performed with commercial computational code FLUENT™. The numerical flow patterns are found to be in good agreement with the experimental manifestations.

Keywords: CFD, droplet behavior, immiscible fluids, interfacial tension.

1. Introduction

Through the current study, we propose to emphasize the flow behavior of two well-known Newtonian immiscible fluids within a Y shape micro-bifurcation with two inlets and one outlet. The main purpose of the study was to create a test case for early stage designing of a microfluidic device using numerical modeling. We report here a numerical investigation on the interface shape dynamics manifested for different heights of the microchannel.

The test geometries were two microchannels with a "Y" shape that presented a squared cross-section of 300x370 μm (G1) and 300x300 μm (G2), respectively. They had two separate inlets for each fluid and one outlet. An important feature from the physical characterization of the working fluids is represented by the interfacial tension, value measured with a goniometer and taken into consideration in the numerical model.

The numerical results were compared with experimental investigation, performed with a special design setup based on an optical microscopic device (a CCD camera was coupled at the objective of an inverted microscope). Using this setup, direct visualizations and quantitative observations were obtained.

[1] Principal Researchers, Laboratory of Micro and Nano Fluidics L10, National Institute for R&D in Microtechnologies IMT-Bucharest, Romania, e-mail: catalin.marculescu@imt.ro
[2] Senior Researcher, National Institute for R&D in Microtechnologies IMT-Bucharest, Romania

2. Numerical considerations

In this paper the 3D numerical solutions of investigated micro-flows are computed (for proper boundary and initial conditions) with the commercial numerical code FLUENT™. FLUENT™ is a complex specialized program dedicated exclusively to CFD (Computational Fluid Dynamics); it is based on finite volumes method to solve the corresponding PDE (Partial Differential Equations) and is using the pre-processor GAMBIT to construct the mesh geometry.

Two immiscible Newtonian fluids (oil and water, respectively) were chosen to study the droplet formation. The main material characteristics of the two fluids are the following: $\eta_{\text{oil}} = 0{,}11\,\text{Pas}$, $\rho_{\text{oil}} = 874\text{kg/m}^3$, $\eta_{\text{water}} = 0{,}001\text{Pas}$, $\rho_{\text{water}} = 1000\text{kg/m}^3$. This initial data, along with the interfacial (surface) tension at the interface of the two fluids, $\sigma = 0.059N/m$, was used as inputs for the numerical simulations. This initial approach consists in a study case with the variation of the microchannel depth and maintaining the flow rate ratio constant for both cases: 10:1, considering the flow rate ratio between Inlet 1 and Inlet 2.

Considering that our flow domain consists of two immiscible fluids, a special numerical method is required. The VOF (Volume of Fluid) method was used to solve the Navier-Stokes equations, the governing equations in this case. This method utilizes a fixed grid of finite elements to calculate the interface position of the two immiscible fluids. The motion equations are computed for each of the two fluids, and the volumetric concentration of the two fluids is being calculated in each cell of the mesh, at each time moment. The VOF model is robust and relatively simple to implement in specialized numerical codes for Navier -Stokes equation solvers. It allows the computation of large interface deformations. The main disadvantage is the poor discretization of the interface, the computations providing an interval of possible locations with the width dependent of the mesh resolution.

The flow domain has been discretized using a structured mesh for both geometries containing 1.286.823 hexahedral finite elements for G1 and 1.043.370 for G2, respectively (Fig. 1.). For the investigated cases a 3D model with pressure based solver, implicit and unsteady flow scheme was used. The computed solution presents a precision of 10^{-10}.

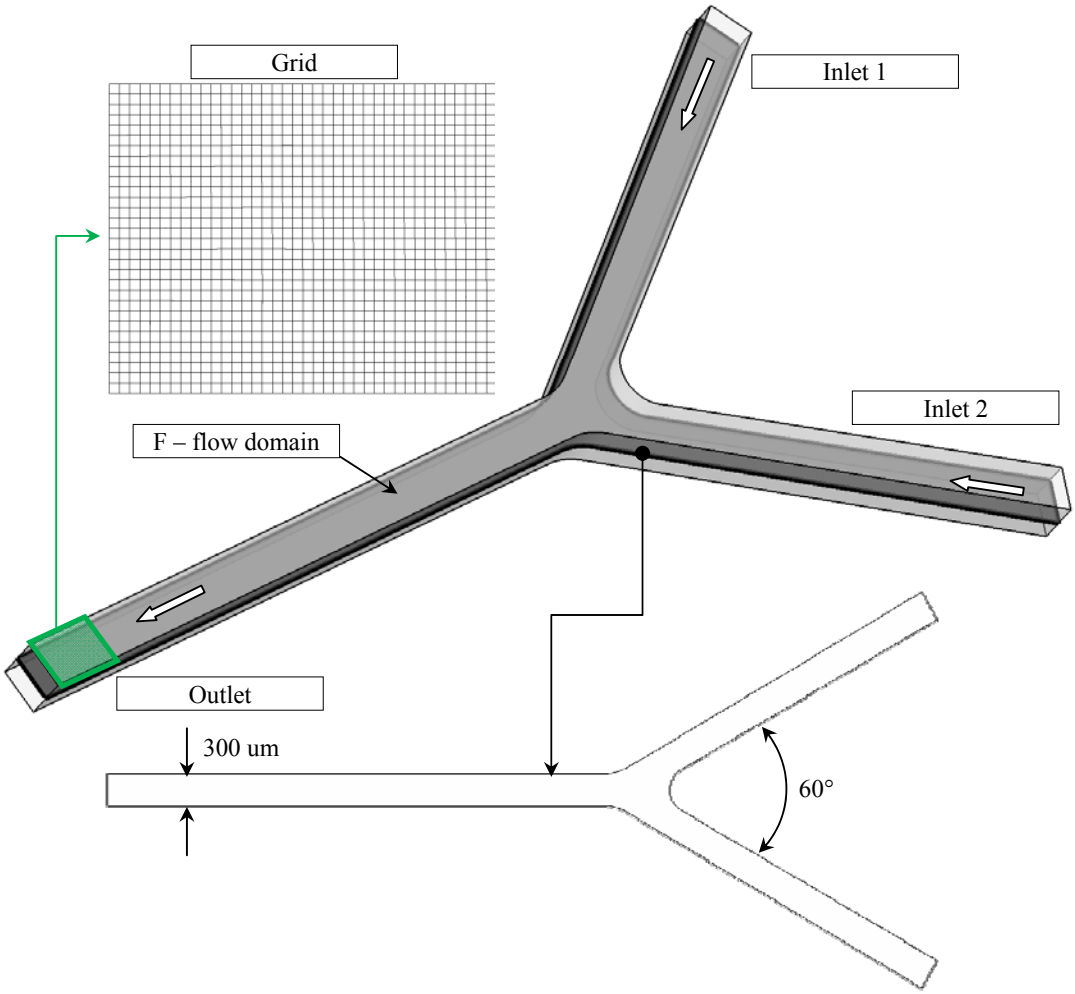

Fig. 1. Geometry description and detail on flow domain discretization

3. Theoretical considerations

The motion equation for a domain F (occupied by the two fluids) is the following:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\nabla)\mathbf{v}\right) = \rho\mathbf{b} - \nabla p + \nabla(2\eta\mathbf{D}) + \sigma_S k\mathbf{n}\delta(\phi), \tag{1}$$

where ρ is the fluid density, $\mathbf{v}$ – the mean velocity, $\mathbf{b}$– the body force, p – pressure, η – fluid viscosity, $\mathbf{D}$ – strain rate tensor, σ_S – surface tension, $\phi(\mathbf{x}, t) = 0$ is the interface defining equation, with $\phi < 0$ for fluid A (water) and $\phi > 0$ for

fluid B (mineral oil),$k = \nabla \mathbf{n}$ - the double of the medium curvature of the separation surface, in the point characterized by the normal **n** and:

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \tag{2}$$

The interface is considered to be a material surface, which implies the validity of the following condition:

$$\frac{\partial \phi}{\partial t} + (\mathbf{v}\nabla)\phi = 0, \tag{3}$$

The relation (1) states that the pressure jump is compensated by the superficial tension, considered constant on the separation surface:

$$[\mathbf{T}]\mathbf{n} = \sigma_S k \mathbf{n}, \tag{4}$$

For a generalized Newtonian fluid, the relation (4) reduces to:

$$p_A - p_B = \sigma_S k, \tag{5}$$

With the material constants known, the equations (1) and (3), along the continuity equation$\nabla \mathbf{v} = 0$, are solved simultaneously at each time step for the velocity and pressure fields computations in the D domain and also the interface equation $\phi = 0$ [1-2].

The superficial tension is a tendency measure of a fluid surface to reach a minimum area. In general, the term “superficial tension” is used for a liquid-gas interface (free surface) and “interfacial tension” for liquid-liquid interface, respectively.

From the thermodynamic point of view, the superficial tension is interpreted as an increase of the Helmholtz or Gibbs system energy when infinitesimal reversible increase of the considered interface area occurs, at constant temperature and volume or pressure. From mechanically point of view, the superficial tension is the contraction force on length unit that acts at the interface, on a parallel direction with it; therefore, the superficial tension can be measured as the necessary force to increase infinitesimally the interface area. For isotropic interfaces, this specific force is independent from the surface direction and orientation. At equilibrium, the two approaches, thermo-dynamical and mechanical, are equivalent (when the interface has enough time to reach the equilibrium state, in other words, at low Deborah numbers or with the lack of elasticity). In this case, we refer to static superficial tension.

When the interface does not reaches the equilibrium state, the superficial tension is called "dynamical", only the mechanical formulation remains valid [3-5]. The non-equilibrium state can be determined by the large relaxation times of some interfacial processes.

One of the most important relations for the interface phenomena study is the Young-Laplace equation that expresses the equilibrium between the superficial tension and the pressure tension (mass tension respectively), establishing the link between the superficial tension value ($\sigma_S = ct$) and the pressure difference along the interface (also called capillary pressure) [6]:

$$\Delta p = \sigma_S \left(\frac{1}{R_1} + \frac{1}{R_2}\right), \tag{6}$$

where Δp is the pressure difference, σ_S is the superficial/interfacial tension, R_1 and R_2 being the surface curvature radius, see (5).

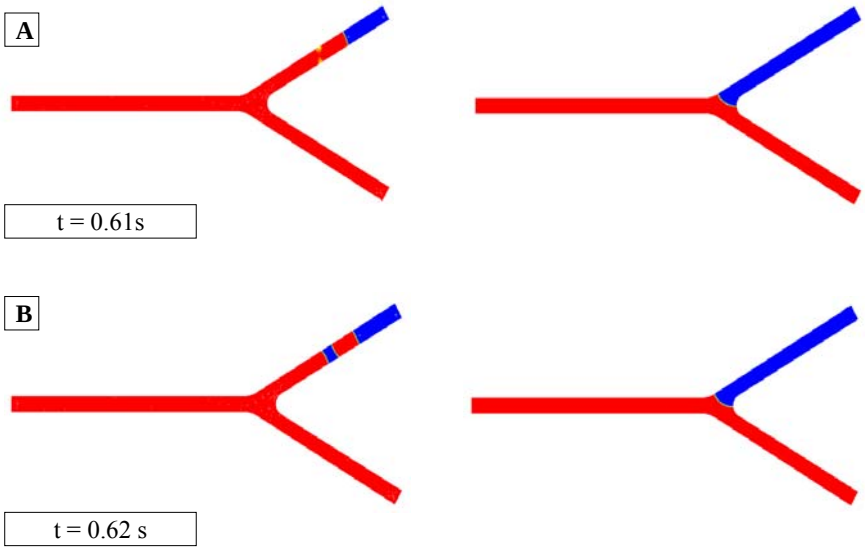

Fig. 2. 2D interface representation for the two investigated cases, G1 (left side) and G2 (right side) at two different time moments : A) t = 0,61 s; B) t= 0,62 s.

4. Results and discussions

As being an early stage study we first compared two numerical models in order to choose the correct prediction and model for design introduction in the

microfabrication process. The comparison was performed using 2D interface representations of the different moments in time. For these particular cases two time moments were chosen as representative: t_1 = 0,61 s and t_2 = 0,62 s. At t_1 for case using the G1 geometry (370 μm in depth) the flow behavior is crucially modified by a water droplet appearance in the oil injecting branch (Fig. 2). This phenomenon normally appears after the junction. Also in the second case the phenomenon is much faster, even though the entry velocities are the same for both cases. Considering this, we choose the G2 geometry for comparison with experimental results.

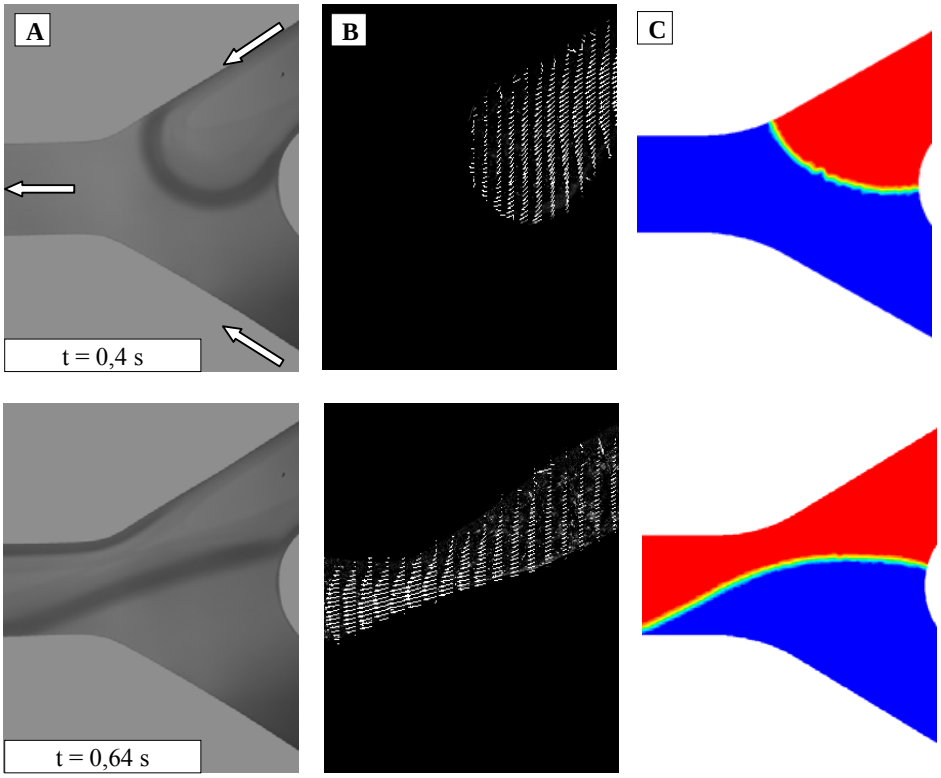

Fig. 3. A) Experimental visualizations of droplet formation; B) Quantitative representations of the flow field inside the water droplet obtained with the micro-PIV measuring system; C) Numerical representations of the interface.

The numerical results for G2 were compared to the experimental investigation, consisting of direct visualizations and quantitative observations (Fig. 3.). The results are in good agreement, considering the approximations of the numerical model, in order to reduce the total convergence time. Also the direct visualizations with the micro-PIV system are not performed in a single median

plane, but in a series of very close planes with a spread of a few microns. This led to the optical deformation of the interface curvature, therefore to differences to the numerical predictions.

6. Conclusions

The main purpose of the study was to create a test case for early stage designing of a microfluidic device using numerical modeling. We reported here a numerical investigation on the interface shape dynamics manifested for different heights of the microchannel. The results pointed out that the ratio between the channel width and depth must be at least equal to one.

The numerical flow patterns were found to be in good agreement with the experimental manifestations.

Acknowledgements

This work is funded by the SOP-IEC, O.2.1.2, Project (Microfluidic Factory for "Assisted Self-Assembly" of Nanosystems), No.209, ID 665.

R E F E R E N C E S

[1]. *J. Ferziger, M. Peric.* "Computational methods for fluid dynamics". Springer-Verlag, Berlin, 1999.

[2]. *R. Scardovelli, S. Zaleski.* "Direct numerical simulation of free surface and interfacial flow". Annu. Rev. Fluid Mech. **vol. 31**, 1999, pp. 567-603.

[3]. *G. Faour, M. Grimaldi, J. Richou, A. Bois,* "Real-time pendant drop tensiometer using image processing with interfacial area and interfacial tension control capabilities". Journal of Colloid and Interface Science, **vol. 181**, 1996, pp. 385-392.

[4]. *E.M. Freer, H. Wong, C.J. Radke*. "Oscillating drop/bubble tensiometry: effect of viscous forces on the measurement of interfacial tension". Journal of Colloid and Interface Science. **vol. 282,** 2005, pp. 128-132.

[5]. *B. Stueckrad, W.J. Hiller, T.A. Kowalewski*, "Measurement of dynamic surface tension by the oscillating droplet method". Experiments in Fluids. **vol. 15,** 1993, pp. 332-340.

[6]. *M. Pasandideh-Fard, P. Chen, J. Mostanghimi, A.W. Neumann*. "The generalized Laplace equation of capillarity. I. Thermodynamic and hydrostatic considerations of the fundamental equation for interfaces". Advances in Colloid and Interface Science, **vol. 63**, 1996, pp. 151-178.