Computational Microfluidics for Miniaturized Bio-Diagnostics Devices using the Multiphysics code "TransAT"

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ABSTRACT

In this paper we have presented new developments achieved on the computational microfluidics front using the dedicated code TransAT. In particular, we have shown how it behaves for the prediction of the Marangoni effects within the Interface Tracking Concept, which can be used in controlling the dynamics of micro-droplets in bio-chips. We have also presented first results of a sub-grid scale ultra-thin film model, capable to mimic the wettability of inner surfaces allowing for a realistic representation of what might be expected in arterial microbubble delivery in gas embolotherapy.

Keywords: Microfluidics, Thin fim, Marangoni, effects

1 INTRODUCTION

Microfluidic devices are now used for such diverse applications as DNA microarrays, drug screening, sensors, and in clinical and forensic analysis. Typical microfluidics flows feature free-surface motion evolving (sometimes) in porous media or as falling films, spreading and dewetting of (complex) liquids on solid or liquid substrates, chemical reaction of binary mixtures, micro-bubbles and beads control and manipulation, phase change or transition. The control of such micro-flow systems is central to future technological advances in emerging technologies, like biological reactors, microreactors, biochannel arrays, and labs-on-chip. It is expected that robust, accurate and fast response computational microfluidics solutions will play a key role in the development in this new business segment. In practical microfluidics applications the flow involves phenomena acting at different time and length scales. At each level of the scale cascade, the physics of the flow is amenable to numerical prediction by scale-specific strategies.

In this paper will present our recent computation results obtained with our CFD code TransAT, in which interfacial flows are treated using the Level Set method. As bio-chips may comprise various components, a new fully automatized version has been developed for microfluidics applications, using IST (Immersed Surfaces Technology) to map complex geometries into a rectangular Cartesian grid. Since IST forces the grid to remain Cartesian and equidistant, high-order schemes (up to 3rd order for flux convection and 3rd order WENO schemes for free surface flows) can maintain their high degree of accuracy. Further, to better resolve boundary-layer regions, near wall flow areas are treated by another new feature, namely the BMR (Block-based Mesh Refinement), in which sub-scale refined blocks are placed around each component. The combination IST/BMR can save up to 70% grid cells in 3D. In this paper we discuss simulation examples treated with this approach (see details in [1]). We will particularly focus on the role played by the Marangoni effects in controlling the dynamics of micro-droplets in bio-chips, and the way ultra-thin film can be predicted using a sub-grid scale model.

2 PREDICITING INTERFACIAL MICROFLUIDCS FLOWS

Interfacial flows refer to multi-phase flow problems that involve two or more immiscible fluids separated by sharp interfaces which evolve in time. Typically, when the fluid on one side of the interface is a gas that exerts shear (tangential) stress upon the interface, the latter is referred to as a free surface. Interface tracking methods (ITM) are schemes capable to locate the interface, not by following the interface in a Lagrangian sense (e.g., by following marker points on the interface), but by capturing the interface by keeping track, in an Eulerian sense (the grid is fixed), of the evolution of an appropriate field such as a level-set function or a volume-fraction field. Examples and classifications are provided in [2]. Application of ITM's to microfluidics flows requires particular attention to the way surface forces and triple-line dynamics are handled.

2.1 Mathematical Formulation

ITMs are based on solving a single-fluid set of conservation equations with variable material properties and surface forces. The coupled fluid and heat transfer equations in incompressible flow conditions take the form

$$\nabla . \mathbf{u} = 0 \tag{1}$$

$$\partial_t(\rho \mathbf{u}) + \nabla .\left(\rho \mathbf{u}\mathbf{u} + pI\right) = \nabla .\mu\left(\nabla \mathbf{u}\right) + F_s + F_g + F_w \tag{2}$$

$$\partial_t(\rho CpT) + \nabla .\left(\rho CpT\,\mathbf{u}\right) = \nabla .\lambda\left(\nabla T\right) + Q''' \tag{3}$$

where $\mathbf{u}$ is the velocity vector, ρ is the density, p is the pressure, $\mathbf{I}$ is the identity matrix, and μ is the dynamic viscosity. The source terms in (2) represent body forces (F_g), surface tension (F_s) defined by

$$F_s = \gamma\,\kappa\,\mathbf{n}\,\delta(\phi) + (\nabla_s \gamma)\,\delta(\phi); \quad \kappa = -\nabla\phi / |\nabla\phi| \qquad (4)$$

where **n** stands for the normal vector to the interface, κ for the surface curvature, γ for the surface tension coefficient of the fluid, δ for a smoothed delta function centered at the interface, and ϕ for the phase indicator function (e.g. level sets, or volume of fluid). The second term in the above expression refers to the Marangoni forces, expressing heat-induced variation of the surface tension coefficient. The contact–line wall contribution (F_w) is defined next by (8). In (3), T is the temperature, Cp is the heat capacity, λ is the heat conductivity, and Q''' is the volumetric heat source. In the Level Set method the interface between two immiscible fluids ϕ represents a continuous distance-to-the-interface function that is set to zero on the interface, is positive on one side and negative on the other. The location of the physical interface is thus associated with the zero level. Material properties, body and surface forces in (2) are locally dependent on ϕ, whose equation reads:

$$\partial_t(\phi) + \mathbf{u}.\nabla\phi = \dot{m} / \rho |\nabla\phi|, \qquad (5)$$

In (5) above $\dot{m}$ stands for the heat/mass transfer rate, which can be either directly determined using the energy jump across the interface, or modeled using heat transfer correlations [2]. If the mass transfer rate is forced to be active only at the triple line then the source term in (2) is applied only in the cell containing the triple line. Note that, if the mass transfer rate per unit length is known, it is converted to a rate per unit area based on the contact line length and the area of the cell. Material properties (density, the viscosity, heat capacity, thermal conductivity) are updated locally based on ϕ and distributed across the interface using a smooth Heaviside function H(ϕ):

$$\rho, \mu, Cp, \kappa = \rho, \mu, Cp, \kappa|_L \; H + \rho, \mu, Cp, \kappa|_G \; (1 - H) \qquad (6)$$

The level set function ceases to be the signed distance from the interface after advecting (5). To restore its normal distribution near the interface, a re-distancing equation is solved during a time period τ:

$$\partial_\tau(d) = \mathrm{sgn}(d_0)\left[1 - |\nabla d|\right]; \quad d_0(x,t) = \phi^n(x,t) \qquad (7)$$

where **sgn(x)** is the Signum function. The expression above is solved after each advection step of (4), using the 3rd or 5th order WENO schemes. Details about alleviating the mass conservation issue in this approach can be found in [2, 3].

The numerical treatment of wetting dynamics is based on the physical forces associated with triple lines. A triple line force is included in the momentum equation, which could then provide a physically adequate description of wetting dynamics, eliminating the need for any particular boundary condition specifying the contact angle. The triple line force is based on interfacial free energy; accordingly, it contains only two parameters: the interfacial tension between the fluids and the equilibrium contact angle θ_{eq}:

$$F_w = \gamma\left(\cos(\theta_{eq}) - \cos(\theta_{dy})\right) l_t\, \vec{b}, \qquad (8)$$

where θ_{dy} is the instantaneous dynamic contact angle, l_t is the length of the triple line in the cell, and $\vec{b}$ is the unit vector normal to the triple line and parallel to the wall surface. The triple line force is obtained by considerations similar to the derivation of Young's Law and can be referred to as the unbalanced Young force [4]. In the case of the static contact angle treatment, the wall value of the level set is calculated such that the contact angle is always equal to the equilibrium contact angle specified.

2.2 TransAT© Microfluidics Flow solver

The Microfluidics code TransAT© [5] is a multi-physics, finite-volume code based on solving multi-fluid Navier-Stokes equations on structured multi-block meshes. MPI parallel based algorithm is used in connection with multi-blocking. Grid arrangement is collocated and can thus handle more easily curvilinear skewed grids. The solver is pressure based, corrected using the Karki-Patankar technique for weak compressible flows. The Navier-Stokes and level set equations are solved using the 3rd order Runge-Kutta explicit scheme for time integration. The convective fluxes are discretized with TVD-bounded high-order schemes [6]. The diffusive fluxes are differenced using a 2ndorder central scheme. Multiphase flows are tackled using Level Sets [3] and VOF for both laminar and turbulent flows. TransAT deals with phase change, surface tension and triple-line dynamics, Marangoni effects, and micro-film sub-grid scale modeling for lubrication.

3 MICROFLUIDCS FLOW EXAMPLES

3.1 Flows Driven by Marangoni Effects

The problem has been borrowed from [7]. Computations were performed in 2D, and the physical model applied is described in Sec. 2.1. The domain size is Lx = 5.0mm and Ly = 1.5mm. A semi-circular droplet with a diameter of d_0 = 1.5mm is initially placed on the lower wall. The initial temperature is set to 20°C and the fluid is at rest. The temperature driving force is represented by a deficit set between west and east walls of 50°K. The contact angle is 90°. The variation of γ is set linearly, according to

$$\gamma = \gamma_{Tw}\left(T_{crit} - T\right) / \left(T_{crit} - T_{weber}\right) \qquad (9)$$

where γ_{Tw} is the surface tension coefficient value at T_{weber} known a-priori, and T_{crit} is the critical temperature. The fluid properties used are listed in Table 1.

Properties	Water	Silicon
γ_{Tw} N/m	0.0728	0.0210
T_{weber} °K	293.0	293.0
T_{crit} °K	327.83	305.83

Table 1: Fluid properties used for our simulations.

Qualitative results are shown in Figs. 1 and 2 for silicon oil and water. The drop is seen to react to the imposed temperature gradient rather vigorously. For water the droplet travels in the negative direction (according to our nomenclature), while for silicon it travels in the positive direction; in both cases the drop is displaced at least one half radius from its initial position. The receding (water) and advancing (silicon) phenomena observed here are very interesting, and corroborate with the results of [7]. This is explained by the properties of the fluids. The velocities of the drops obtained are also in line with the data of [7]: for Silicone oil: $V_d = 0.025$ m/s, and for water: $V_d = -0.25$ m/s.

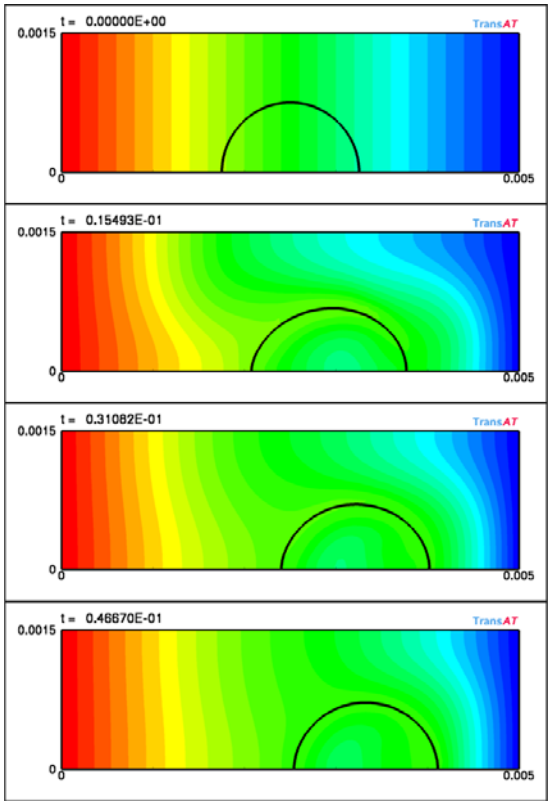

Figure 1: Marangoni driven drop (Silicon).

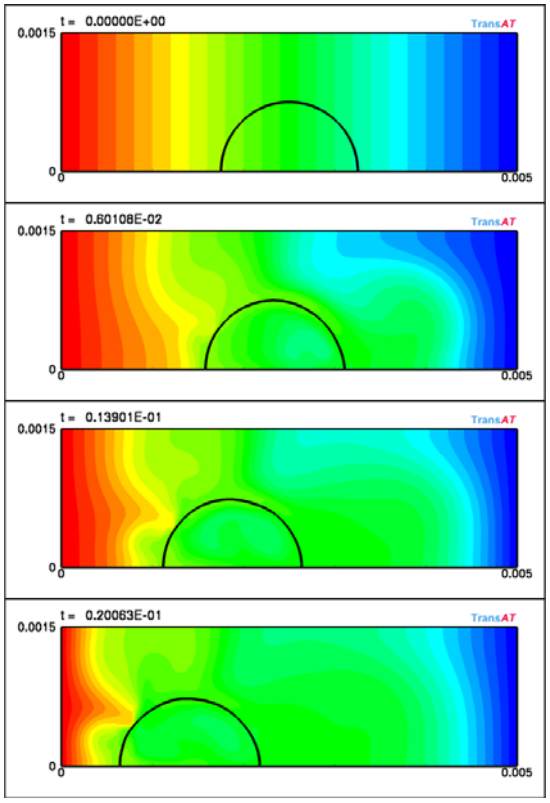

Figure 2: Marangoni driven drop (Water).

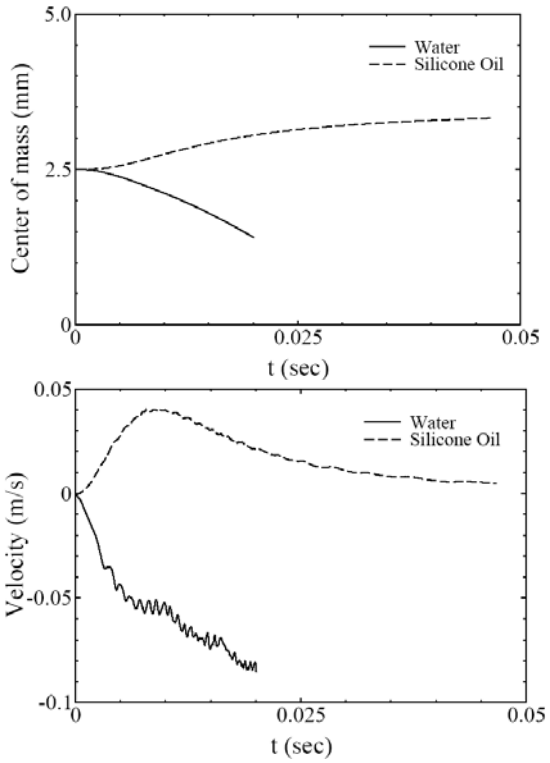

Figure 3: Center of mass displacement (a) and velocity (b).

The drop center-of-mass displacement and velocity are compared in Fig. 3 for both fluids. The plot shows how the center of mass moves recedes (from the initial center of mass 2.5mm) for water and advances for silicon, up to 2.95mm. In [7] the authors report that water moves to the higher temperature side only for 90° contact angle, which has not been checked in our simulation campaign. The drop velocities compared in the 2nd panel of Fig. 3 show clearly the difference between the motion of the two fluids; while the speed rises rapidly for the initial 10ms then decays for silicon, it grow from the start (in the - direction) for water, without marking an inflexion as for silicon oil.

3.2 Thin-film Confined Flows

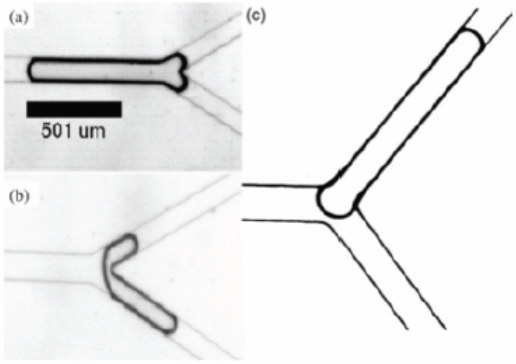

Figure 4: (a) Lodging state, (b) lodging state, (c) bubble lodged in one of the branches [8].

Cardiovascular gas bubbles in arteriole bifurcations have been experimentally addressed to understand the dynamics of their lodging mechanism [8]. The research is motivated by novel gas embolotherapy techniques for the potential treatment of cancer by tumor infarction. To solve such problems, one should resort to detailed multiphysics, interfacial flow simulation. The presence of the junction singular-point controls the bubble dynamics and rupture. In the junction a thin film is formed preventing bubble breakup. This can be predicted only with high-fidelity simulations using with a sub-grid scale model for thin film treatment, and contact angle treatment for wetting.

Present CMFD technology without multiscale treatment will fail to deliver accurate and physical sound results. The bubble will separate producing a non-physical solution (i.e. numerical dry-out) whereas wetting should sustain) as the bubble enters in the junction. Multiscale simulation of thin film flow is necessary here, requiring SGS thin-film models and wetting capabilities. The ultra-thin film SGS model implemented in TransAT for this class of flow is based on a modified model of the Taylor [9] thin-film theory, which originally proposes to model the height of a thin film as a function of the fluid Capillary number $Ca = \mu U / \gamma$; i.e. $\delta / r = 1.337 Ca^{2/3}$, where r stand for the pipe radius, and U for the speed of the bubbles inside the tube.

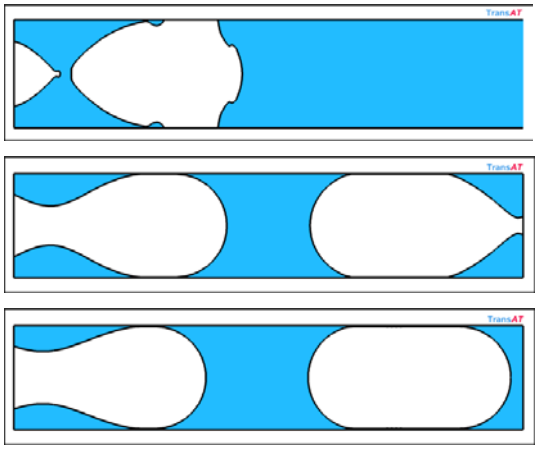

Figure 5: (a) Numerical dry out, (b) Imposed water film thickness of 5micron, (c) 10micron.

The results depicted in Fig. 5 clearly show that without such a SGS thin-film model, numerical dry-out will occur (panel a). Our SGS model is able to take into account the effect of lubrication by imposing a liquid film thickness, thus allowing for a smooth transport of the bubbles at low Capillary number (1mm diameter channel containing air and water, for Capillary number: Ca = 1.5463E-03). Note that the inflow liquid and gas velocities are 0.111 and 0.066 m/s, respectively

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