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RESEARCH PAPER

Progress in computational microfluidics using TransAT

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Abstract The paper reports on the progress made in predicting single- and multi-phase microfluidics flows using the computational multi-fluid flow dynamics (CMFD) code TransAT. In the multi-phase context, the code uses either the level-set approach or the phase-field variant as the "Interface Tracking Methods". The solver incorporates phase-change capabilities, triple-line dynamics models, Marangoni effects, electro-wetting and a micro-film sub-grid scale model for lubrication. Subtle microfluidics problems like droplet generation or surface tension-driven flows are shown to be within reach of modern CMFD techniques using interface tracking, with relatively fast CPU response times. In most of the cases presented here, the comparison between CMFD and experiments is rather satisfactory.

1 Introduction

Microfluidics flows are multi-faceted in terms of physics and as such they represent a perfect class of multiscale, multiphysics examples: these flows are associated with free-surface motion evolving as falling films, spreading and de-wetting of liquids on solid or liquid substrates, chemical reaction of binary mixtures, micro-bubbles and droplet motion, phase change or transition. The control of such micro-flow systems (using pressure, Marangoni, electro-wetting or acoustics) is central to future technological advances in emerging technologies, like biological reactors, microreactors, biochannel arrays, or lab-on-a-chip devices. The role of CMFD may be critical in this challenging enterprise, since the technique has proven to be highly effective in predicting small-scale multi-phase flows and has successfully integrated the free-surface dynamics capability. CMFD is an excellent exploration tool capable of virtually informing about tiny flow details, regardless of the system size, which are otherwise impossible to detect (in time or space) by available measurement and visualization technologies. CMFD has the capability to deliver simulated data about mixed fluids of all natures, passive or reactive, acid or basic, proteins, DNA and reagents, etc.

The main issue is to arrive at a CMFD tool capable of dealing with the various physical facets at once; a sort of multi-scale, multi-physics computational strategy. Considerable progress has been made towards efficient and accurate numerical methods for small-scale multiphase flows and many have been integrated into commercially available codes that can be used to simulate microfluidics flows. For a comprehensive review of the state-of-the-art, we refer the reader to the excellent review by Wörner (2012).

Here, we will discuss various examples relevant to microfluidics computed using our CMFD platform TransAT. Section 2 introduces the modeling concepts and numerical approaches in TransAT and their applicability to various flow problems. The following sections discuss a selection of single and multiphase microfluidics flow problems, with variable degree of complexity and requiring physical models for free surfaces, conjugate heat transfer, phase change and phase separation, Marangoni effects, and dynamic contact angle effects. Section 3 shows the validity of continuum models with no-slip boundary conditions for common microfluidics applications. In Sects. 4 and 5, we show examples of two-phase flow simulations in the

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