IMPLEMENTATION OF A FLEXIBLE AND MODULAR VOLUME OF FLUID MULTIPHASE FRAMEWORK FOR NON-ISOTHERMAL INCOMPRESSIBLE FLOWS

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In this work we discuss the development of a flexible and modular numerical framework for the simulation of thermocapillary flows implemented within the open source toolbox OpenFOAM®. In non-isothermal systems, surface tension gradients may occur as a consequence of a non uniform temperature distribution along a free liquid-liquid or liquid-gas interface. Such flows, which do not require gravity, pressure gradients or other body forces, are generally referred to as Marangoni convection, after the Italian physicist who originally studied this phenomenon. The study of such flows and related effects has extensive engineering applications in variety of different fields, such as crystal growth from the melt, metal welding and the processing of both organic and metal alloys. It also has important implications in the study of multilayer non-isothermal configurations, as well as microdroplet migration and coalescence phenomena.

The present framework has its roots in the Volume of Fluid Method (VOF) and related variants such as the Continuum Surface Force (CSF) approach [1]. Such strategies are conveniently tuned and adapted to the typical numerical environment provided by OpenFOAM®. Tangential interfacial stresses, generated in the fluid by the gradients of surface tension, are modelled via an additional body force term added to the momentum equation. Such a term can be cast in compact form as [2]:

$$Ma_F = \left[\sigma_T\left(\mathbf{I}-\mathbf{nn}\right)\cdot\nabla T\right]\left\|\nabla\alpha\right\| \tag{1}$$

where $\sigma_T = -\,\partial\sigma/\partial T$ represents the temperature derivative of the interfacial tension, $\mathbf{I}$ and $\mathbf{n}$ are the second order unit tensor and the normal unit vector at the interface, respectively, ∇T is the temperature gradient and α the volume fraction. An energy transport equation is also solved in order to determine the temperature field evolution, which in turn influences the flow field through the Marangoni forces herein considered.

The solver was first tested using a 2-D configuration of two layers of immiscible fluids separated by an interface at mid-height as shown in Fig. 1a. We impose two constant different temperatures (T_1 and T_2) at the lateral walls; gravity and external pressure gradient are considered negligible. Fig. 1b shows the streamlines and temperature contours for a Marangoni number $\mathrm{Ma} = 10^5$, defined as the ratio of the surface tension gradient driven stresses and viscous stresses:

$$\mathrm{Ma} = \frac{\sigma_T (T_2 - T_1) L}{\mu D} \tag{2}$$

where L is the length between the walls, D is the thermal diffusivity and μ the dynamic viscosity.

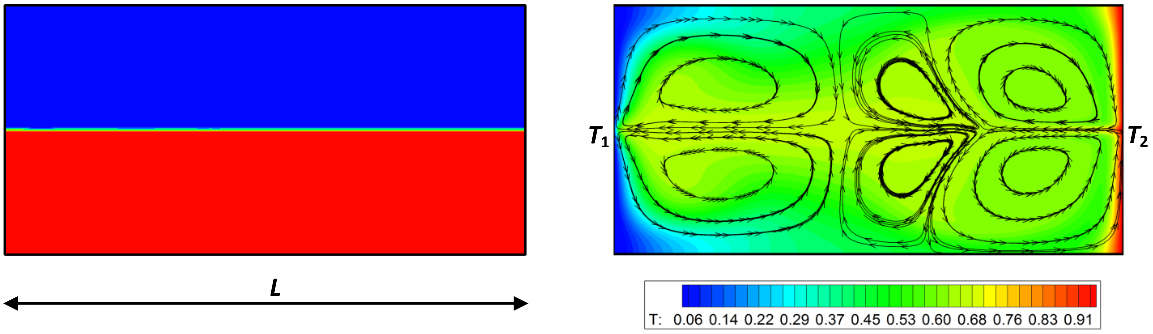

Figure 1: a) Initial configuration of the system showing the two layers of immiscible fluids. b) Example of streamlines and contour plot of the normalised temperature (Ma = 10^5).

We compared our numerical simulations using a well-established code [2] and good agreement was found in terms of velocity and temperature fields.

The second case investigated was the thermocapillary migration of a droplet for finite Marangoni numbers under a reduced gravity environment [3,4,5]. A droplet is placed in a closed box and a linear thermal gradient imposed to replicate the experiments of Hadland *et al.* [5]. Our findings are in a very good agreement with the experiments for the whole range of Marangoni numbers considered.

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