

Implementation of a Flexible and Modular Multiphase Framework for the Analysis of Surface-Tension-Driven Flows Based on a LS-VOF Approach

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Abstract: The mathematical modelling and numerical simulation of multi-phase flows are both a demanding and highly complex exercise. In typical problems with industrial relevance, the fluids are often in non-isothermal conditions and interfacial phenomena are a relevant part of the problem. A number of effects due to the presence of temperature differences must be adequately taken into account to make the results of numerical simulations consistent and realistic. Moreover, in general, gradients of surface tension at the interface separating two liquids are a source of numerical issues that can delay (and even prevent completely in some circumstances) the convergence of the solution algorithm. Here, we propose a fundamental and concerted approach for the simulation of the typical dynamics resulting from the presence of a dispersed phase in an external matrix in non-isothermal conditions based on the modular computer-aided design, modelling, and simulations capabilities of the OpenFOAM environment. The resulting framework is tested against the migration of a droplet induced by thermocapillary effects in the absence of gravity. The simulations are fully three-dimensional and based on an adaptive mesh refinement (AMR) strategy. We describe in detail the countermeasures taken to circumvent the problematic issues associated with the simulation of this kind of flows.

1 Introduction

The motion of gas bubbles and liquid droplets in fluid media is a widespread phenomenon in nature and a subject of great relevance to many engineering and materials processing applications.

A drop or a bubble can move under the influence of different driving forces of distinct nature. As an example, a falling rain drop or a bubble rising in a denser liquid are put in motion because of the gravity force exerted on it by Earth. Other body forces such as magnetic and ultrasonic fields can also be used to induce or “control” the motion of droplets in some specific circumstances (see for instance,

Nguyen et al (2006), Brunet et al. (2010)). Even in the absence of body forces, a similar phenomenon can be induced by another fundamental mechanism, the so-called *thermal Marangoni (or thermocapillary) effect*. This process, which occurs every time a gradient of temperature or concentration is present at the interface separating two fluid phases, becomes particularly important in all those situations where body forces (such as gravity) do not play a major role, *e.g.* in the microgravity environment provided by orbiting platforms, or when either the densities of the fluid pair are similar and/or the typical size of the dispersed phase is very *small* (*e.g.* atomised droplets).

The first pioneering study on the thermocapillary migration of droplets was conducted in the late 50's by Young et al. (1959), who, under some limiting assumptions (perfectly spherical drop of radius R moving in an indefinite liquid under Stokes flow conditions) derived a landmark solution (in analytical form) of the governing equations. With such approach, velocity and temperature fields were considered to be fully established at every moment of time, while neglecting the inertia and convective effects. Under this approximation the temperature field can be inferred independently of the flow field and this greatly simplifies the derivation of an analytical solution to the problem, yielding a precise relationship between the asymptotic (steady) droplet migration velocity and the properties of the considered fluids and characteristics of the driving force.

Over subsequent years, especially because of the advent of space programs and the possibility to execute experiments in the field of fluids and materials in space (sounding rockets, Space Shuttle and most recently the International Space Station, see, *e.g.*, Lappa, 2004), the subject gained an increasing popularity, with this kind of research extending to multidisciplinary fields.

Balasubramanian and Subramanian (2000) extended the analytical study of Young et al. (1959) to the case in which the Reynolds number tends to infinity. They analysed the steady migration of a spherical drop in a continuous phase when subjected to a temperature gradient under conditions such that inertial terms in the momentum equation and convective-transport terms in the energy equation dominate over the corresponding molecular-transport terms (*i.e.* $Ma \rightarrow \infty$ and $Re \rightarrow \infty$ for which they were able to derive analytical solutions partially based on the earlier mathematical model of Harper and Moore (1968)). The migration velocity of the drop was obtained by these authors in the framework of a potential-flow theory by equating the rate at which work is done by the thermocapillary stress to the rate of viscous dissipation of energy; the method of matched asymptotic expansions was employed to solve the conjugate heat-transfer problem in the two phases (characterised by the presence of thin thermal boundary layers both outside and within the drop). In physical terms, they found that in the limit of $Ma \rightarrow \infty$, the velocity of a drop is proportional to the square of the temperature gradient and the cube of the radius of the drop, whereas in the opposite limit ($Ma \rightarrow 0$), both dependences are linear.

Beyond theoretical studies, a number of experimental works have also appeared over the last two decades (see, *e.g.*, Wozniak (1991), Balasubramanian et al. (1996) and Hadland et al. (1999) for experiments in weightless conditions). More

recently, attempts have been made to approach the problem directly in the framework of moving boundary methods such as Volume of Fluid (VOF) or Level Set (LS) techniques, by which the typical simplifications of past analytical approaches can be removed and the typical difficulties (and cost) of microgravity-based experimentation avoided.

Despite valuable numerical advances over the years (Haj-Hariri et al., 1997; Tryggvason et al., 2001; Lappa, 2005a; Yin et al., 2012, Ma et al., 1999; Zhao et al., 2011; Brady et al., 2010), the numerical simulation of droplet migrating under the influence of surface-tension gradients at finite values of the Reynolds and Marangoni numbers can still be regarded as an “open task”. In the present chapter, we lay the general foundation of a possible theoretical and mathematical treatment of the subject based on the modular capabilities of the OpenFOAM environment. Starting from an already existing algorithm (Yamamoto et al., 2016) we undertake all the necessary steps to expand the range of treatable physical effects as necessary. Furthermore, the code is validated against the analytical solution of Young et al. (1959) and used to study the impact of the geometrical configuration on the drop migration pattern.

2 Mathematical Formulation

The ingredients of our overall conceptual architecture are provided and discussed with a step-by-step approach with the declared intention to define the involved sub-models as simply as possible and build and grow the framework “organically” by progressive integration of components and parts. The class of such sub-parts or sub-models (well known or partially of a prototypical nature as we will see later in this chapter) is highly diverse including typical moving boundary methods and energy transport models in synergy with non-dimensional and asymptotic analyses.

2.1 Governing Equations

We consider the Marangoni migration of a liquid drop surrounded by an immiscible liquid under the effect of a constant temperature gradient $\nabla_{\infty} T$. The most common way to describe such flow is based on the consideration of two distinct phases, each with its set of governing equations, and appropriate interface stress jump conditions to guarantee proper phase coupling (see e.g., Tryggvason et al., 2011). However, the problem can be also approached in terms of “interface capturing methods”, such as the Level Set or the Volume of Fluid. These techniques are based on a different strategy known as “single-fluid” or “one-fluid” approach (see, e.g., Lappa, 2005b and references therein). The underlying idea is that the

system might be considered as if composed by one single fluid with variable material properties (undergoing discontinuities across the fluid-fluid boundaries). In terms of momentum, the presence of the interfacial stresses is accounted by adding “extra” forces to the transport equation.

More precisely, if we assume that the effect of the gravity and any other external body force is negligible, the conservation of momentum can be written as:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \mathbf{f}_\sigma \quad (1)$$

where t represents time, ρ , μ are the fluid density and viscosity, respectively, p is the pressure and \mathbf{u} the velocity vector. The last term \mathbf{f}_σ is a force accounting for the capillary ($\mathbf{f}_{\sigma,n}$) and thermocapillary ($\mathbf{f}_{\sigma,\tau}$) forces at the interface:

$$\mathbf{f}_\sigma = \mathbf{f}_{\sigma,n} + \mathbf{f}_{\sigma,\tau} = \sigma(T_0) k \mathbf{n} \delta_s + \nabla_{\square} \sigma(T) \delta_s \quad (2)$$

Here, k and \mathbf{n} are the curvature and normal unit vector at the interface, respectively, \mathbf{I} is the identity tensor and the operator $\nabla_{\square} = (\mathbf{I} - \mathbf{n}\mathbf{n})\nabla$ accounts for the projection of the surface tension gradient along the direction tangent to the interface. The term δ_s represents a function which can be shown to be coincident with the canonical Dirac δ -function (Lappa, 2005b). Since the interfacial tension depends on the temperature T , we have explicitly included the related dependence in Eq. 2. Closure of the mathematical model requires consideration of the conservation of mass for incompressible flows (Eq. 3) and the temperature transport equation (Eq. 4)

$$\nabla \cdot \mathbf{u} = 0 \quad (3)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (\kappa \nabla T) \quad (4)$$

where c_p is the specific heat and κ the thermal conductivity coefficient of the fluid. Following common practice for this kind of problems (see, e.g., Yin, 2012), all material properties are assumed to be constant in each phase and are evaluated at a suitable reference temperature. The dependence on temperature, however, is retained for the surface tension σ via a linear relationship:

$$\sigma(T) = \sigma_0 + \sigma_T (T - T_0) \quad (5)$$

where $\sigma_T = -\partial\sigma(T)/\partial T$ is negative for most known fluids (Balasubramanian and Subramanian, 2001) and T_0 is the reference temperature.

2.2 The Simplified LS-VOF Method

Our solver relies on a simplified coupled LS-VOF code (based on the hybrid formulation originally developed by Albadawi et al. (2013), see also Sussman and Puckett (2000)) implemented into the framework of OpenFOAM (Yamamoto et al., 2016) as an extension of the standard VOF solver “interFoam”. The simplified coupled LS-VOF for an isothermal system is based on the solution of the Eqs. 6-10. The equation for the volume fraction reads:

$$\frac{\partial\alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) + \nabla \cdot (\alpha(1-\alpha) \mathbf{u}_c) = 0 \quad (6)$$

where α is the volume fraction and \mathbf{u}_c is an artificial “compressive velocity” (Berberović et al., 2009). Although, there was a consistent improvement in terms of accuracy and reduction of the so-called “parasite” currents with respect to the original two-phase solver, we had to take additional countermeasures to fix typical “algorithm stability” issues at the interface (where Marangoni stresses of thermal nature are produced). This was accomplished by “proper” smoothing both the level set and volume of fluid phase functions, as further described in Sect. 2.3.

The resulting time-marching procedure can be outlined as follows: in order to calculate the level set function φ , first we calculate the field $\varphi_0 = (2\alpha - 1)\Gamma$ where $\Gamma = 0.75\Delta x$ and Δx is the grid resolution (see Albadawi et al., 2013). Subsequently, a re-initialisation equation is solved (see, e.g., Sussman and Fatemi, 1999):

$$\frac{\partial\varphi}{\partial\tau} = \text{Sgn}(\varphi_0)(1 - |\nabla\varphi|) \quad (7)$$

with the initial condition $\varphi(\mathbf{x}, 0) = \varphi_0(\mathbf{x})$ and where $\text{Sgn}(\varphi_0) = \varphi_0/|\varphi_0|$. Once the scalar field φ is known at each point, it is possible to evaluate the curvature at the interface

$$k(\varphi) = -\nabla \cdot \mathbf{n}(\varphi) \quad (8)$$

with $\mathbf{n}(\varphi) = \nabla\varphi/|\nabla\varphi|$ being the unit vector perpendicular to the interface. Finally, the term described by Eq. 2 is evaluated leading to the momentum equation cast in compact form as

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right] + \sigma k(\varphi)\eta(\varphi)\nabla\varphi + \sigma_T\nabla_{\perp}T|\nabla\alpha| \quad (9)$$

where

$$\eta(\varphi) = \begin{cases} 0 & \text{if } |\varphi| > \varepsilon \\ \frac{1}{2\varepsilon}\left(1 + \cos\left(\frac{\pi\varphi}{\varepsilon}\right)\right) & \text{if } |\varphi| \leq \varepsilon \end{cases} \quad (10)$$

and $2\varepsilon = 3\Delta x$.

The reader is referred to Lappa (2005b) for additional information about the mathematical manipulations required to turn the surface force seen in Eqs. 1-2 into a corresponding volume force spread over a region of finite thickness, which no longer relies on the use of the Dirac function. Additional details on the dependences on φ and α present in Eq. 9 are provided in Sect. 2.3.

2.3 Implementation of the thermal Marangoni migration method in OpenFOAM

We used properly mollified variables to increase algorithm stability and avoid unphysical effects at the interface. More precisely, the smoothing was applied to each ‘‘relevant variable’’ χ (various variables required by the LS and VOF implementation in different parts of the solver, as needed) using a ‘‘pure diffusive’’ evolution equation $\chi_{mol}^{n+1} = \chi_{mol}^n + (\nabla^2\chi_{mol}^n)\Delta\tau$ where τ is an artificial or fictitious time, to be solved with the initial condition for a prefixed number of cycles n (the condition $n = 0$ corresponding to the recovery of the original non-smoothed function). $\Delta\tau$ is defined according to the following well-known numerical stability criterion (see e.g. Fletcher (1991))

$$\Delta\tau = \frac{0.5^2}{(1/\Delta x)^2 + (1/\Delta y)^2 + (1/\Delta z)^2} \quad (11)$$

We used mollified quantities to evaluate the new curvature at each time step, i.e.

$$k_{\varphi_{mol}} = -\nabla \cdot \mathbf{n}_{\varphi_{mol}} = -\nabla \cdot \frac{\nabla \varphi_{mol}}{|\nabla \varphi_{mol}|} \quad (12)$$

where φ_{mol} is the smoothed version of φ .

As discussed in Sect. 2.1, accounting for surface-tension effects requires two additional source terms in the momentum equation (see Eq. 2). In the framework of an optimisation strategy based on a trial-and-error approach, we could obtain the best results using the mollified level set function to determine the unit vector perpendicular to the interface (and the corresponding tangent unit vector) and retaining a non-mollified volume fraction in the gradient appearing in the expression of the thermal contribution (see Eq. 13). The level set function was also used accordingly to determine the curvature.

$$\mathbf{f}_{\sigma, \tau} = \sigma_T \nabla_{\square} T |\nabla \alpha| = \sigma_T (\mathbf{I} - \mathbf{n}_{\varphi_{mol}} \mathbf{n}_{\varphi_{mol}}) \nabla T |\nabla \alpha| \quad (13)$$

The portion of code in which we have included the thermocapillary force is shown in Fig. 1.

```
fvVectorMatrix UEqn
(
    fvm::ddt(rho, U)
  + fvm::ddt(rhoPhi, U)
  + turbulence->divDevRhoReff(rho, U)
  + ddtSigma*TangentialGradT*mag(fvc::grad(alpha))
  ==
    sources(rho, U)
);
```

Fig. 1 Snippet of code from the UEqn.H file. The line highlighted in boldface represents the stresses due to the thermocapillary effect, where **ddtSigma** represents the interfacial tension coefficient σ_T , **TangentialGradT** is the projection $\nabla_{\square} T$ of the temperature gradient (implemented in the code as **gradT - (gradT & nMoll)*nMoll** where **gradT** is the temperature gradient and **nMoll** corresponds to $\mathbf{n}_{\varphi_{mol}}$) and the last term is the magnitude of the gradient of the volume fraction $|\nabla \alpha|$

Following common practice in the literature (Brackbill et al., 1992), the smoothing philosophy has also been applied to the fluid properties (assumed to be constant in each phase) in order to prevent the algorithm from developing spurious oscillations due to the discontinuity established at the liquid-liquid interface. In our hybrid implementation we decided to rely on a standard VOF approach expressing each property as

$$\gamma = \alpha_{mol} \gamma_1 + (1 - \alpha_{mol}) \gamma_2 \quad (14)$$

Special care has also been devoted to the solution of the energy equation. Some mathematical manipulations were indeed necessary to increase algorithm stability and its related ability to reproduce available test cases in the literature (as discussed later in this chapter). We rearranged the equation as follows: by introducing the thermal diffusivity $D = \kappa / \rho c_p$ and considering that all the fluid material properties can in general change across the interface, after some algebraic manipulations we obtained the following equivalent expression for the energy equation:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \nabla \cdot (D \nabla T) + \frac{1}{\rho c_p} \nabla \kappa \cdot \nabla T - \nabla D \cdot \nabla T \quad (15)$$

The snippet of code displayed in Fig. 2 shows the corresponding implementation.

```
fvScalarMatrix TEqn
(
    fvm::ddt(T)
  + fvm::ddt(phi, T)
  - fvm::laplacian(D, T)
  - 1.0/(rho*cp)*(fvc::grad(k) & fvc::grad(T))
  + fvc::grad(D) & fvc::grad(T)
);
```

Fig. 2 Implementation of the temperature equation. The name of the variables have direct correspondence to the symbolism adopted in Eq. 15

The different macro steps in which our algorithm has been articulated can be finally sketched as follows:

1. Solve the re-initialization equation (Eq. 7);
2. The volume fraction equation is solved using MULES algorithm (which is essentially an explicit method, see e.g., the OpenFOAM user guide, 2008) to guarantee the boundedness of the scalar field α ;
3. Solve the temperature equation;
4. Computation of the thermal Marangoni force $\mathbf{f}_{\sigma, \tau}$;
5. Calculation of the velocity and pressure field using a projection method (PISO algorithm);
6. Back to step 1

Before the validation and discussion of the results in the next section, we list here the independent non-dimensional parameters governing the physics of the flow under discussion. These are: the fluid properties ratios $\tilde{\rho} = \rho_d / \rho_m$,

$\tilde{\mu} = \mu_d / \mu_m$, $\tilde{c}_p = c_{p,d} / c_{p,m}$ and $\tilde{k} = k_d / k_m$, the capillary number $Ca = \sigma_T (\nabla_\infty T) R / \sigma_0$, the Marangoni number $Ma = \sigma_T (\nabla_\infty T) R^2 / \alpha_m \mu_m$ and either the Reynolds number $Re = \rho_m \sigma_T (\nabla_\infty T) R^2 / \mu_m^2$ or the Prandtl number $Pr = \mu_m / \rho_m \alpha_m$, since $Ma = Re Pr$. The subscripts “*m*” and “*d*” stand for matrix and drop, respectively.

3 Solver validation

As indicated at the end of Sect. 2, our overall framework has been built via the integration of self-contained modules, which could be individually tested. However, because it is crucial that the entire numerical architecture is tested as a single integrated unit, we considered available solutions in the literature for comparison. In order to validate our code, in particular, we focused on the thermocapillary motion of a perfectly spherical Newtonian droplet of radius R in a constant temperature gradient $\nabla_\infty T$ embedded in an unconfined Newtonian matrix in the limiting case of $(Ma, Re) \rightarrow 0$ and negligible buoyancy effects. As discussed in the introduction, in such a case an analytical solution exists for the velocity of the droplet (Young et al., 1959) (YGB theory), which in dimensional form reads:

$$U_{YGB} = \frac{2|\sigma_T|(\nabla_\infty T)R/\mu_m}{\left(2 + \frac{k_d}{k_m}\right)\left(2 + 3\frac{\mu_d}{\mu_m}\right)} \quad (16)$$

where the temperature gradient $\nabla_\infty T$ is defined as $\nabla_\infty T = (T_{hot} - T_{cold})/H$, where H is the height of the channel along the direction of the motion (between the hot wall and cold wall) and T_{hot} and T_{cold} correspond to the temperature at the hot wall and cold wall, respectively (cf. Figure 3a). In our simulations we assumed conditions corresponding to the following set of (non-dimensional) characteristic numbers $Pr = 0.1$, $Re = 1.0 \times 10^{-4}$, $Ma = 1.0 \times 10^{-5}$ and $Ca = 2.0 \times 10^{-1}$ (with the capillary number being sufficiently small to guarantee negligible deformations, see e.g., Zhao et al. (2011)). For simplicity, we also considered the fluid material parameters to be the same for both fluids (i.e. unit fluid property ratios). Assuming the radius of the droplet to be $R = 0.5$ cm, we fixed the size of the external container to $(6 \times 4.5 \times 4.5)$ cm³ (shown in Fig. 3a), corresponding to a confinement ratio $C = R/L = 0.22$, where L represents the distance between the centre of the drop and the wall. This size is intended to mimic the effective geometry of the container used in microgravity experiments by Hadland et al., (1999). As shown in Fig. 3b, a structured mesh with $85 \times 64 \times 64$ elements adaptively refined in the re-

gion of the drop is employed. For the boundary conditions, we have applied no-slip conditions for the velocity and "zeroGradient" for the pressure at each wall of the container (a reference pressure "pRefValue = 0" has been set at the centre of the "cold" wall). For the temperature, we set constant values at the two "cold" and "hot" sides, and adiabatic ("zeroGradient") conditions in the rest of the domain.

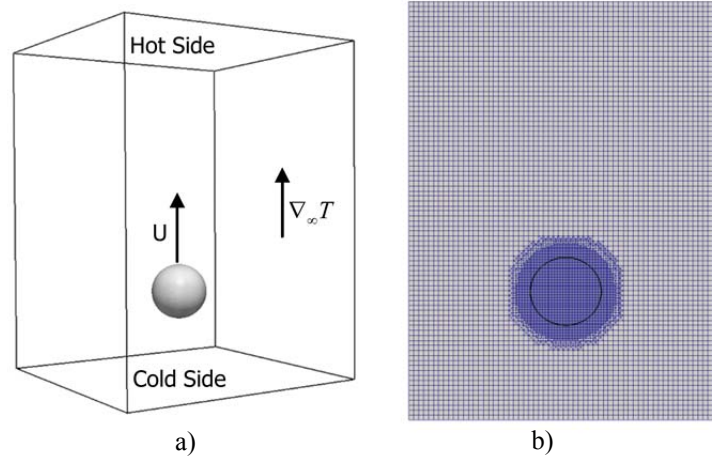


Fig. 3 a) Initial conditions used for the simulation. At the initial instant the droplet is at rest. The velocity arrow has been included to show the migration direction when a temperature gradient $\nabla_{\infty}T$ is imposed. b) Particular of the mesh in a plane parallel to the motion of the droplet. Note the area of refinement in the region of the droplet.

All simulations were executed applying two ($n = 2$) cycles of smoothing for the Level Set function φ .

Fig. 4 shows a snapshot of the flow pattern and the temperature distribution in a plane parallel to the direction of migration in the case of $C = 0.22$. As expected, a toroidal roll is formed by the thermocapillary effect. The intersection of such a roll with the considered visualisation plane clearly shows regions of recirculating fluid surrounding the droplet. As time increases such vortices move with the droplet.

Fig. 5 shows the dimensionless migration velocity as a function of the dimensionless time $t' = \mu_m / \sigma_T (\nabla_{\infty}T)$ for the same case. As evident in this figure, after a given transient, the droplet reaches a steady state where its (final) migration velocity is in excellent agreement with the predictions of the YGB theory.

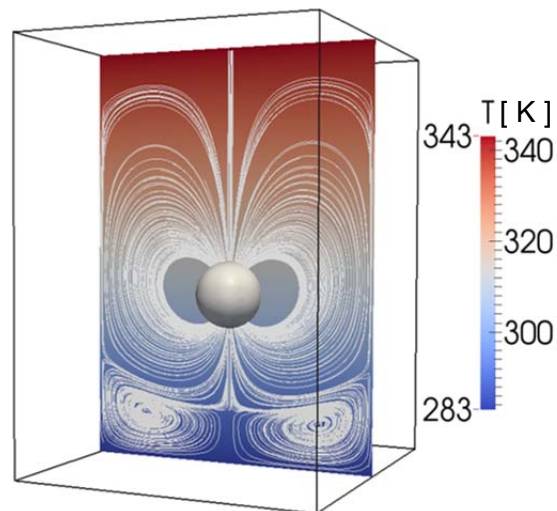


Fig. 4 Snapshot of flow pattern and temperature field in a plane parallel to the direction of migration at instant $t' = 10$. The droplet is moving from the bottom (cold side) toward the top (hot side).

We also studied the effect of the geometric “confinement” considering narrower containers with $C = R/L > 0.22$. We found that the migration velocity decreases non-trivially with the degree of confinement. More specifically, when the height of the geometry is halved ($C = 0.44$), the resulting steady state migration velocity is about 12% smaller than the limit predicted by the YGB theory. Such results, summarised in Fig. 5, clearly indicate that some care should be taken in the choice of the geometry if wall effects are not intended to be a relevant aspect of the analysis.

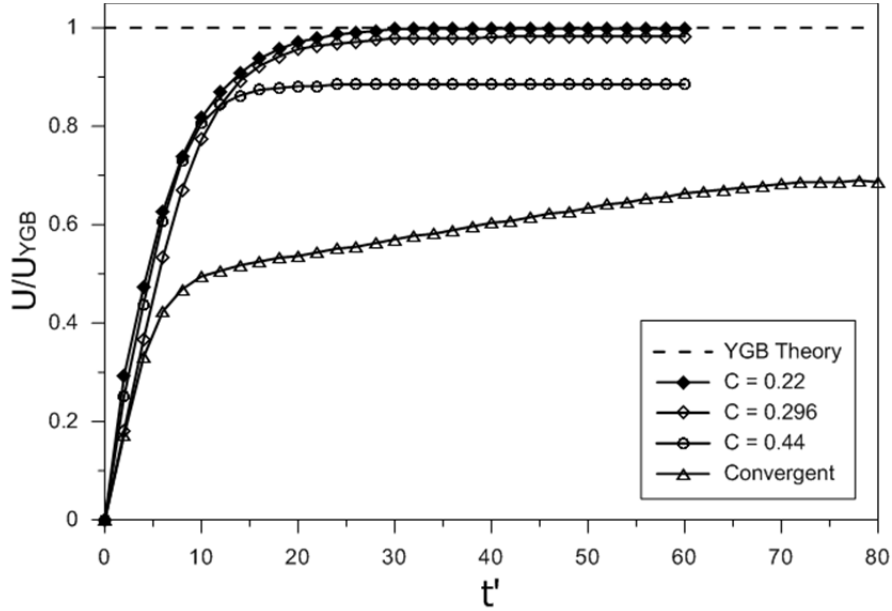


Fig. 5 Velocity history for various geometry and confinements C . The results are normalised using the YGB theoretical velocity. Notice the difference between the two cases $C = 0.296$ (still in good agreement with the YGB theory) and the case $C = 0.44$.

The last test considered was the simulation of a droplet migrating into a convergent channel, resorting to the same set-up adopted for the previous simulations. We used a convergent duct having “cold side” cross sectional area equal to the case of $C = 0.44$, with the cross-sectional area of the “hot side” being half of the cold one.

It is worth emphasising that in such case the droplet could not reach a steady state (its velocity increases monotonically until it suddenly decreases when the droplet is close to the hot wall). Such interesting behaviour, which would require further investigation, might be perhaps explained according to the presence of two different counteracting contributions: as the droplet migrates along the converging region, the degree of confinement increases, and on the basis of the previous findings, one should expect the velocity to decrease; however, since, the temperature field distribution is no longer linear, and the Marangoni stresses increase accordingly, one should expect the droplet to accelerate. Further studies are in progress along these lines to assess the role played in such dynamics by the relative importance of molecular and inertial transport terms in the governing equations.

Conclusions and Future Directions

In this work, we addressed the question of how a typical numerical framework for isothermal multi-phase flows can be adequately extended to make it suitable for the simulation of phenomena in which surface-tension gradients act as the main flow or pattern driver. In particular, starting from existing implementations in OpenFOAM of moving-boundary methods, some effort has been put into strengthening the used approach by incorporating in the algorithm the possibility to account for thermal effects of different nature. Special care has been devoted to numerical stability issues that are typical of such problems (in which the phenomena occurring in a limited neighbourhood of the interface separating the two liquids play a “crucial role”).

The framework has been successfully tested under restricted conditions, but future work shall be devoted to the application and testing of the resulting approach to more complex problems in which inertial terms in the momentum equation and convective-transport terms in the energy equation dominate over the corresponding molecular-transport terms.

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