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Thermal sub-grid boundary layer modelling around bubbles at moderate Reynolds and Prandtl numbers

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Abstract

This work focuses on thermal sub-grid modelling around bubbles at turbulent Reynolds numbers (up to 400) and moderate Prandtl numbers (up to 5). The increasing availability of computational resources allowed us to perform direct numerical simulations of bubbles' dynamics in swarms at turbulent Reynolds numbers for RANS Euler-Euler modelling purposes. The very local thermal effects are not captured as precisely close to the interface due to phase change at $Pr > 1$. Thermal sub-grid boundary layer modelling has been considered to enhance temperature prediction in the bubbles' interface region. First, the current Front-Tracking framework `TriocFD` used at CEA will be presented. The literature in terms of boundary layer modelling for concentration will be briefly described. Then, the sub-grid temperature modelling approach on a steady single rising bubble in an axisymmetric configuration has been performed *a priori*. Some analytical solutions in a $2D$ local spherical coordinate system have been derived. These radial solutions show free parameters that are fitted according to the temperature values in the bubble's neighbouring resolved field. The temperature gradient prediction performance will determine the choice of the analytical model over more complex approaches and its range of validity. In a second step, the micro-macro regions coupling of a one-dimensional analytical solution to the Stefan problem has been investigated. The analytical solution has been used locally to correct both diffusion, interfacial temperature gradient and liquid temperature extension over time (as part of a Ghost-fluid method). Some hints to perform more complex modelling will be finally given.

Introduction

Previous studies, on bubbles' swarms and channels, have proved that second-order dynamical quantities were converged enough to perform proper modelling for averaged simulations at a reasonable cost. However, in presence of phase change, the temperature field is converging at a lower rate and thus requires a finer spatial resolution.

Well-established numerical methods such as Front-Tracking are taking advantage of the One-fluid formulation to solve a unique set of equations (momentum and mass) while calculating volumetric averaged physical parameters in mixed cells. The literature has reached another consensus on temperature resolution. To ensure energy conservation, it needs to be solved separately for each fluid domain and matched at the interface using the saturation temperature condition.

A major strength of the One-fluid formulation is that the common high-order operators can still be used across the interface when the velocity is continuous. In presence of phase change, the normal temperature gradient jump at the interface is directly related to the normal velocity jump. The construction of continuous ghost fields is thus inevitable in order to keep using both convective and diffusive schemes in the interfacial region.

To mitigate the error in the interfacial quantities, some authors used adaptative mesh refinement tech-

niques (AMR), a second mesh for solving the temperature or quadratic temperature extensions... Increasing the mesh refinement makes the time-step smaller whereas a limited rate of convergence is expected for quadratic temperature extensions. These methods thus do not seem sufficient to perform parametric studies of bubble's swarms and generate enough data for modelling purposes (Data mining, Tensor Basis Neural Network extension to two-phase flows...).

As a consequence, the focus has been brought to the use of a simplified substitute radial model in the interfacial region. Starting from steady-state simulations, some authors (Bothe 2013; Weiner 2020) used a self-similar solution of a steady advection-diffusion equation in the context of thin concentration films around a single bubble. Other publications (Aboulhasanzadeh 2012; Weiner 2022) are attaching to the Front-Tracking markers the energy contained in a thin radial control volume. However, the methods lack two-way coupling because the Eulerian field is not modifying the sub-grid model. Both approaches are interesting but there is still a need to unify and generalise them for larger boundary layer thicknesses and time-dependent solutions. The ultimate purpose of the present work is to study and model realistic boiling situations observed in nuclear and solar power plants.

From a simple approach to boundary layer modelling

In our numerical approach, a normal temperature gradient is computed for pure interface neighbouring cells at a distance $\frac{d_i}{2}$ from the interface (2^{nd} order). The temperature gradient was then historically corrected using a one-dimensional pure radial diffusion sub-grid model (decreasing exponential solution). The normal temperature gradient, stored at the pure cells' centres (distance d_i) is then diffused by an iterative neighbouring averaging procedure. A continuous Eulerian normal temperature gradient field is then obtained.

In the second phase, the ghost-field is obtained in both the mixed cell and the other's phase region using the latter temperature gradient field. This extended temperature field is thus embedding the saturation temperature condition.

Thermal (or concentration) boundary layer modelling has been investigated (Aboulhasanzadeh 2012; Bothe 2013; Weiner 2020, 2022) and seems promising to enhance the latter extrapolation procedure. They managed to obtain robust results at very high Prandtl (Schmidt $\in [100; 10,000]$) numbers *i.e.* in presence of very thin layers. Major hypotheses have been made to use 2D self-similar quasi-static solutions by neglecting the local curvature effects.

Discussion and expectations

To start gradually to take into account the local curvature effect as well as both tangent and normal advection terms, which have proved to be dominant depending on the bubble curvilinear coordinate at moderate Prandtl numbers, a simplified 2D "spherical" solution has been derived in the interface vicinity (**Fig. 1**). The governing

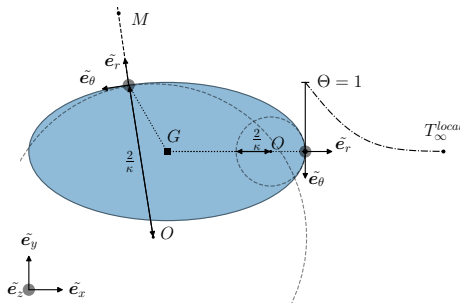


Figure 1: Local spherical coordinate system equation as well as the analytical solution are showed in **Eq. (1)** and **Eq. (2)**

$$\frac{\partial^2 \Theta}{\partial r^2} + \left(\kappa - \frac{u_r}{\alpha_l} \right) \frac{\partial \Theta}{\partial r} - \left(\frac{\kappa u_\theta}{2\alpha_l} \right) \frac{\partial \Theta}{\partial \theta} = 0 \quad (1a)$$

$$\Theta = \frac{(T - T_\infty^{local})}{(T_{sat} - T_\infty^{local})}; \quad \Theta(0, 0) = 1; \quad \Theta(\delta_\theta, 0) = 0 \quad (1b)$$

$$\frac{2}{r} = \kappa + o(1) \quad u_r = \text{const}_1; \quad u_\theta = \text{const}_2 \quad (1c)$$

A general solution depending on several free parameters is deduced. δ corresponds to the boundary layer thickness whereas δ_1 and δ_2 are damping factors com-

ing from solving a 2^{nd} order ODE and are linked by the mean curvature κ .

$$\Theta(r) = \left(1 - e^{\delta(1/\delta_2 + 1/\delta_1)} \right)^{-1} \left(e^{r/\delta_2} - e^{\delta(1/\delta_2 + 1/\delta_1)} e^{-r/\delta_1} \right) \quad (2)$$

$$\delta_2 = \frac{\alpha_l \delta_1}{\alpha_l + \delta_1 (u_r - \kappa \alpha_l)}; \quad 1/\delta_2 - 1/\delta_1 = u_r/\alpha_l - \kappa$$

This solution will be examined on a steady simulation *a priori*. As in sub-grid modelling, the refined extended temperature field will be filtered to mimic an equivalent under-resolved simulation in the boundary layer region.

Simultaneously, the so-called one-dimensional Stefan problem allowed us to understand more deeply the coupling between the micro and macro-regions while emphasizing the need for a local model to better predict the temperature distribution in the interface region (see **Fig. 2**). The associated figure is showing where the temperature field, as well as the temperature gradient evaluation, are corrected using the analytical solution once the growth rate γ has been found using the nearest pure cell temperature value. A significant improvement has been observed in the case of non-linear profiles compared to the previous ghost-linear extension method and additional work concerning energy conservation will be undertaken on this 1D mock-up.

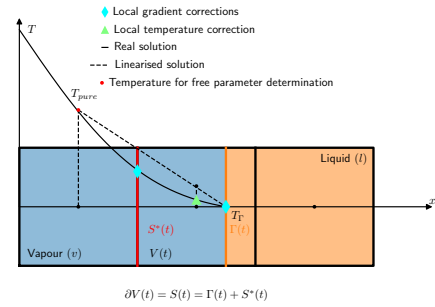


Figure 2: Micro-Macro region coupling illustrated on the Stefan problem

Conclusion

In the proposed approach, a local analytical solution taking into account the transverse advection and curvature effects has been derived in a local spherical coordinate system. The profile has been fitted in the interface region using a filtered temperature field. We observed that the fitting step may be tedious (*e.g.* Newton-Raphson). From this assessment, solving an ODE in the radial direction while modelling the transverse term $\frac{\partial \Theta}{\partial \theta}(r)$ as in **Eq. (3)** using the resolved field as a boundary condition will be also worth considering. In that case, higher order terms (velocity and curvature) could be taken into account to enhance the temperature gradient prediction.

$$u_r(r) \frac{\partial \Theta}{\partial r}(r) + \frac{u_\theta(r)}{r} \frac{\partial \Theta}{\partial \theta}(r) = \alpha_l \left(\frac{2}{r} \frac{\partial \Theta}{\partial r}(r) + \frac{\partial^2 \Theta}{\partial r^2}(r) \right) \quad (3)$$

The coupling of the analytical solution in the Stefan problem has been enlightening and the micro-macro coupling has proved to work in this pure diffusion case. The

gain in knowledge will allow a more straightforward 3D implementation. The local temperature and growing convergence rate have been observed but a more precise energy conservation understanding should be necessary at the instants where the interface is crossing a cell.

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