3D Numerical solution for quenching process using an adaptative multiphase flows

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Résumé :

Différentes étapes du procédé de trempe ont encore besoin d'être modélisées, en particulier les phénomènes liés à l'ébullition : l'ébullition nuclée, la génération et le détachement du film de vapeur lors de l'ébullition film. Une méthode LevelSet est utilisée pour décrire l'interface entre les phases. La surface de tension est modélisée en combinant le modèle " Continuum Surface Force" avec un gradient défini directement au nœud. En adoptant cette approche, les premières simulations d'ascension de bulle et de coalescence sont en accord avec ceux de la littérature. Les différentes étapes de génération et de détachement du film de vapeur seront modélisées lors du procédé de trempe en 3D.

Abstract :

Different stages of the thermal modelling of the quenching process need to be treated, from nucleate boiling to generation and growth of a vapour film. The interface between each phase flow will be determined using a level set method. Surface tension is evaluated using the " Continuum Surface Force", the main challenge in this approach is to compute the curvature of the fluid interface as a second derivative of the LevelSet function since a linear finite element method is used. In this paper, the normal and the curvature are calculated based on the recovered gradient at the nodal points. By using this whole numerical approach, the results concerning the bubble rising problem are in good agreement with those found in the literature. The proposed method demonstrates the capability of the model to simulate the generation and the detachment of film vapour from a heated source.

Mots clefs : **Surface tension ; LevelSet ; Two-phase flow**

1 Introduction

The quenching process is an efficient way to control mechanical and metallurgical characteristics of final metallic parts. Nevertheless, the heat transfer between the part and the quench fluid must be very well controlled to avoid defects like cracks, heterogeneous distribution of mechanical and metallurgical properties. The framework of this study is the improvement of the heat transfer knowledge between the solid part and the fluid thanks to an innovative numerical description of the fluid behavior at the interface and, especially, of the phase change (liquid, vapour) phenomenon of the cooling fluid. Modeling the multiphase flow during the quenching process is a challenging .
In the literature, different approach has been used to simulate boiling heat transfer that occur during the quenching process ; were propose in here a modified formulation to study the formation and the evolution of a bubble or a film vapour via a germination and a growth approach.

Numerical simulation of such a problem is a great challenge due to : the accuracy of the interface, the discontinuities between the fluids properties, the topological change in the bubble shape and the effect of surface tension. In fact, two techniques are available to capture the interface : front tracking (lagrangian, i.e. explicit mesh) and front capturing (eulerian, i.e. fixed mesh) methods. Each of these robust approaches have their own advantages and disadvantages [1], the most important advantage of

LevelSet methods is that the interfaces can easily merge and the coalescence between bubbles is well presented.

The numerical treatment of surface tension is the second challenge in the numerical simulation of multi phase flows. In literature, surface tension forces can be mathematically modeled as interfacial bondary conditions or as a continuum surface force (CSF) as presented by Brackbill [3]. In the current paper, the surface tension is calculated by the CSF in conjunction with the LevelSet function, to avoid spurious oscillations generated by the descretisation of regularised delta function, a smooth delta function has been implemented [4]. Since in this eulerian formulation, a piecewise linear basis functions is used, computation of the local curvature as a second derivative of the LevelSet function presents another difficulty [12], then the gradient in use was computed directly at the nodes of the mesh.

The outline of this paper is organized as follows : first, we introduce the governing equations in Section 2. The LevelSet approach and the mixing law are presented in section 3. Modelling of surface tension based on a new gradient is presented in section 4. Numerical results and comparisons of our numerical predictions with available experimental data on bubble rising and coalescence in liquids is presented in Section 5. The generation and the detachement of vapour is also treated in section 4.

2 Governing Equations

2.1 Growth velocity

Several experimental studies have been performed to compute the growth rate of bubbles, Barthès [2] shows that the characteristic length $R(t)$ varies as a function of the time t, the Jacob number Ja_l and the liquid thermal diffusivity a_l .

$$R(t) = C_0^* Ja_l \sqrt{a_l t} \qquad with \qquad Ja_l = \frac{\rho_l c_l \left(T_{l-\infty} - T_e\right)}{\rho_v L} \tag{1}$$

Here, $T_{l-\infty}$ denotes the far field liquid temperature and T_e the ebullition point. To compute the interface growth velocity, we use the same approach as Zabaras [15] then the Gibbs Thomson relation is adopted and the growth velocity is defined as follows :

$$\boldsymbol{v} = C_0 \left(T - T_e\right) n \tag{2}$$

Where C_0 is the growth constant function of the used fluid.

2.2 Conservation of energy

The heat transfer governed by the energy equation accounts for the Stephan condition by treating its contribution as an external force term as follows, (3) :

$$\begin{cases} \dfrac{d\boldsymbol{H}}{dt} - \boldsymbol{\nabla} \cdot (k \nabla T) \\ \boldsymbol{H} = \rho c_p \left(T - T_e\right) + \rho_v L H(\alpha) \end{cases} \tag{3}$$

Here, L is the latent heat of vaporisation per unit mass and $H(\alpha)$ is the smooth Heaviside function defined in section 3. By substituting $\boldsymbol{H}$ in the first equation of system (3) we obtain(4) :

$$\begin{cases} \rho c_p \dfrac{dT}{dt} - \boldsymbol{\nabla} \cdot (k \nabla T) = \left[\rho_v L + \left(T - T_e\right)\left(\rho_v c_p^v - \rho_l c_p^l\right)\right] \delta_\Gamma^e(\alpha) \dfrac{d\alpha}{dt} & \text{in}\Omega \\ T(\boldsymbol{x}, 0) = T_0 & \text{in}\Omega \\ \boldsymbol{\nabla} T(\boldsymbol{x}, t).n = 0 & \text{in}\partial\Omega \end{cases} \tag{4}$$

2.3 Momentum equation

In this section, we consider two fluids in a domain Ω which are separated by an interface Γ. $\Omega \subset \mathbb{R}^n$ is the spatial domain at time $t \in [0,T]$, where n is the number of space dimensions. We consider the following velocity-pressure formulation of the Navier-Stokes equations governing unsteady incompressible flows :

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u}) - \boldsymbol{\nabla} \cdot \boldsymbol{\tau} = \rho \mathbf{g} \text{ in } \Omega \times [0,T] \quad (5)$$

$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0 \text{ in } \Omega \times [0,T] \quad (6)$$

where ρ and $\mathbf{u}$ are the density and the velocity, $\mathbf{g}$ the density and $\boldsymbol{\tau}$ the stress tensor.

In bubble rising, surface tension plays an important role in defining final bubble's shape and bubble departure. To account for the surface tension effects at the interface between fluids, the surface stress boundary condition is added as follows :

$$\boldsymbol{\tau . n} = \sigma \boldsymbol{\kappa . n} \quad , \quad [\mathbf{u}] = 0 \quad (7)$$

where σ is a physical constant depending on the fluids, κ is the signed mean curvature of the surface and n is the unit mormal vector at the interface.

3 LevelSet approach

Coupez proposed an extended convected Level-Set function, similar to the one introduced in Coupez [16], to track the interface between fluids. The basic idea of this method is to use both the physical time and the convective time derivative in the classical Hamilton-Jaobi reinitialisation equation. An hyperbolic tangent of the LevelSet function presented in (figure 1) is used, where ϕ stands for the standard distance function.The level-set evolution equation is then given by

$$\begin{cases} \frac{\partial \alpha}{\partial t} + \boldsymbol{u}.\nabla \alpha + \lambda s \left[|\nabla \alpha| - \left(1 - \alpha^2\right) \right] = 0 \\ \alpha(t=0,x) = \alpha_0(x) \end{cases} \quad (8)$$

λ is a coupling constant depending on time discretization and spatial discretization, typically $\lambda \simeq h/\Delta t$ and $\boldsymbol{u}$ is the convection velocity, s is the signed function.
Once the level-set function is defined, it can be used to easily separate both phases and to define the density ρ and the viscosity μ on the whole domain. At the interface, the sharp discontinuity of fluid properties is smoothed over a transition thickness using the following expressions :

$$\rho = H(\alpha)\rho_1 + (1 - H(\alpha))\rho_2 \quad (9)$$

$$\mu = H(\alpha)\mu_1 + (1 - H(\alpha))\mu_2 \quad (10)$$

where H is a smoothed Heaviside function given by :

$$H(\alpha) = \begin{cases} 1 & \text{if } \alpha > \varepsilon \\ \frac{1}{2}\left(1 + \frac{\alpha}{\varepsilon}\right) & \text{if } |\alpha| \leq \varepsilon \\ 0 & \text{if } \alpha < -\varepsilon \end{cases} \quad (11)$$

Here ε is a small parameter lower than the truncation thickness.

4 Surface Tension

In many fluid flow problems, surface tension plays a significant role by inducing microscopic localized surface forces that exerts itself in both normal and tangential directions. The computation of the surface tension force by using the continuum surface force (CSF) depends on the location and the derivatives of the interface. Adopting the CSF, the interfacial force is taken into account as a right hand side source term added to the momentum equation by using the following expression :

$$\boldsymbol{F}^{CSF} = \sigma \kappa \boldsymbol{n} \qquad with \quad \kappa = -\nabla \cdot n \quad and \quad n = \nabla \alpha \quad (12)$$

The main challenge in this approach is to compute the curvature of the fluid interface as a second derivative of the Level set function since a linear finite element method is used. In this paper, the normal and the curvature are calculated based on a continuous gradient operator, known as the recovered gradient, based on the length distribution tensor and the projection of the gradient along the edges as follows :

$$\left(\tilde{\nabla} u_h\right)^{\mathrm{i}} = \arg\min_{\mathbf{G}} \left(\sum_{j\in\Gamma(i)} \left| (\mathbf{G} - \nabla \mathrm{u_h}) \cdot \boldsymbol{X}^{\mathrm{ij}} \right|^2 \right) = \arg\min_{\mathbf{G}} \left(\sum_{j\in\Gamma(i)} \left| \left(\mathbf{G} \cdot \mathbf{X}^{\mathrm{ij}} - \mathrm{U}^{\mathrm{ij}} \right) \right|^2 \right) \tag{13}$$

Consequently the gradient $\tilde{\nabla}^i$ is given by

$$\tilde{\nabla}^i = \left(X^i\right)^{-1} U^i \qquad where \qquad U^i = \sum_{j\in\Gamma(i)} \mathrm{U}^{\mathrm{ij}} \mathrm{X}^{\mathrm{ij}} \tag{14}$$

where $\boldsymbol{X}^{\mathrm{ij}}$ is the edge vector made of nodes i and j sharing at least one element and X^i denote the positive tensor at the node i, U^{ij} is the difference of the function u at the node j and at the node i. The

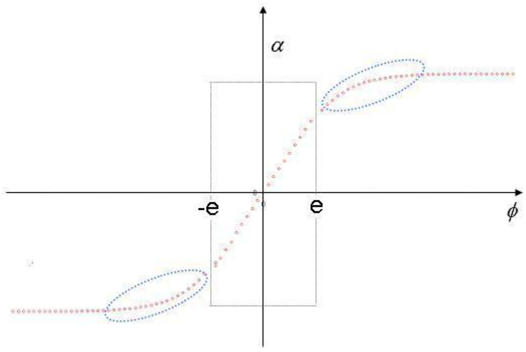

FIGURE 1 – The hyperbolic tangent $\alpha(\phi)$

advantage that offers the use of the recovered gradient is the superconvergent of the Laplace operator in triangular meshes as presented by Zhang [17]. Once the normal and the curvature are computed, (12) is multiplied by a smoothed Dirac delta function $\delta^e_\Gamma(\alpha)$,and then surface tension is modeled as a volume force [3].

$$\delta^e_\Gamma(\alpha) = \begin{cases} 0 & \text{if } |\alpha| > e \\ \frac{1}{2e}\left[1 - \left(\frac{\alpha}{e}\right)^2\right] & \text{if } |\alpha| < e \end{cases} \tag{15}$$

Additional force term (16) is once added to the Navier-Stokes equations and represents the surface tension as a continuous three dimensional effect across a given interface.

$$\int_\Omega \sigma \tilde{\nabla} \cdot \left(\tilde{\nabla}\alpha(\mathbf{x})\right) \tilde{\nabla}\alpha(\mathbf{x}) . \delta^e_\Gamma(\alpha(\mathbf{x})) d\mathbf{x} \tag{16}$$

5 Numerical Examples

The implemented surface tension coupled to an extended convected Level Set method is validated for incompressible two-phase flows. Firstly, bubble coalescence in 3D is presented, secondly the generation and the detachment of a vapour film during the quenching process are simulated. All the numerical implementations were carried out using the CimLib parallel finite element library [11].

5.1 Bubble coalescence

In this three dimensional example, the domain $\Omega = [0.01; 0.01; 0.02]$ with two bubbles initially located, respectively, at $(0.005; 0.005; 0.005)$ and $(0.005; 0.005; 0.00797)$, are considered. The bubbles have an initial diameter equal to $D = 2.6\ mm$. The aim of this multi-phase flow is to simulate bubble coalescence. The surface tension coefficient is $5.8 \times 10^{-4}\ N.m^{-1}$ and the gravity is $g = -8.65\ m.s^{-2}$. The physical parameter for the surrounding fluid are $\rho_1 = 880 kg.m^{-3}$ and $\mu_1 = 0.0125 N.s.m^2$, for the bubble $\rho_1 = 440 kg.m^{-3}$ and $\mu_1 = 0.00625 N.s.m^2$. As time progresses, the lower bubble is deformed and the upper bubble shape changes from a sphere to a cap shape (figure 2 at times $t = 0\ s$, $t = 0.015\ s$, $t = 0.045\ s$, $t = 0.06\ s$, $t = 0.075\ s$, and $t = 0.15\ s$). The average mesh size is $0.0003\ m$. It can be noted that at time equal to $0.15\ s$, the two bubbles merge together to become a single bubble with a cap shape. Our results are in good agreement with those found by [13].

FIGURE 2 – Isovalue zero of the level set function for bubble coalescence

5.2 Vapour generation-film boiling

The aim of this test is to bring out the generation of a vapour film around a solid object, close to the quenching problem. Using the immersed volume method [7] and a stabilized finite element method for solving conjugate heat transfer [8], a hot solid is immersed inside a filled-water tank as shown in (figure 3). Therefore, we use a heat source to warm the surrounding liquid. As the growth velocity is proportional to the temperature difference, the vapour will appear when the liquid temperature is higher than the boiling temperature. The duration and the stability of the film boiling mode increase linearly with the growth of the bath temperature [9]. This boiling mode is the most noted for a bath having a temperature above 60 $^{\circ}C$. Therefore the water is initially considered at a temperature of 90 $^{\circ}C$. This computation is performed in a three-dimensional hexahedral domain with a heat source having as illustrated in (figure 3). The heat source is made of Inconel-718 at a temperature of 700 $^{\circ}C$. The vapour interface is initially coincident with the solid's boundary. As shown in figure 3, a continuous vapour layer forms between the heated solid and the surrounding liquid. The vapour is removed on the upper portion of the solid, which is determined by Taylor instability. From this test we can deduce that, in the quenching process, the dipped metal provides a natural generator of vapour.

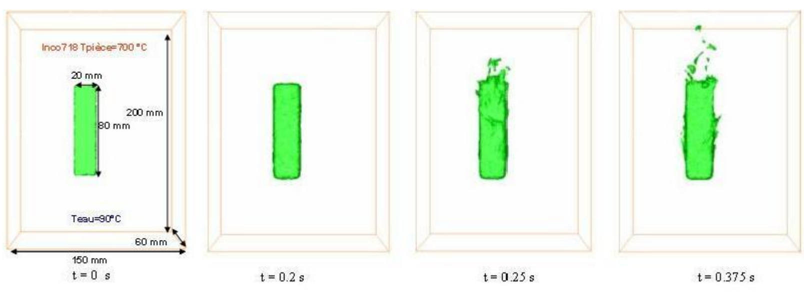

FIGURE 3 – Interface plot for a three-dimensional vapour film generation test

6 Conclusions

A novel numerical approach is presented for the simulation of phase change using the level set method to track the liquid-vapor interface and by solving one set of equations in both domains with different phase properties. To simulate multi phase flows where fluids are considered to be incompressible, the surface tension was computed by combining the continuum surface force (CSF) and a continuous gradient computed directly at the nodes of the mesh. The numerical three dimensional (3D) tests show that the proposed method is able to simulate the phase change during the quenching process. The used approach takes advantage of the level set method to capture the interface and to present the coalescence between bubbles. This method was also applied to simulate the generation of a film of vapour followed by its detachment.

Références

[1] Van Sint Annaland, M., Deen, N. G., Kuipers, J. A. M. 2005 Numerical simulation of gaz bubbles behaviour using a three-dimensional volume of fluid method. *Chemical Engineering Science.* **60** 2999-3011

[2] Barthès,M. 2005 Ebullition sur site isolé étude expérimentale de la dynamique de croissance d'une bulle et des transferts associés. *Ph.D. Thesis, Université De Provence.*

[3] Brackbill, J.U., Kothe, D.B., Zemach, C. 1992 A Continuum Method For Modeling Surface-Tension. *J. Of Computational Physics.* **100** 335-354

[4] Changl, Y.C., Hou, T.Y., Merriman, B.,Osher, S. 1996 A Level Set formulation of eulerian interface capturing methods for incompressible fluid flows. *J. Of Computational Physics.* **124** 449-464

[6] Coupez, T. 2010 Metric construction by length distribution tensor and edge based error for anisotropic adaptive meshing. *Journal Of Computational Physics.* **article in press**

[7] Hachem, E., Kloczko, T., Digonnet, H., Coupez, T. 2010 Stabilized finite element solution to handle complex heat and fluid flows in industrial furnace using the immersed volume method *International Journal for Numerical Methods in Fluids* in press, available online http ://dx.doi.org/10.1002/fld.2498

[8] Hachem, E., Kloczko, T., Digonnet, H., Coupez, T. 2010 Enriched finite element spaces for transient conduction heat transfer, Applied Mathematics & Computations *International Journal for Numerical Methods in Fluids* **217** 3929-3943

[9] Jérome,G. 2004 Etude Expérimentale des Aspects Thermiques lies Ã une OpÃ©ration de Trempe. *Ph.D. Thesis, Ecole Doctorale de Nantes.*

[10] Mcinnes, L.C., Balay, S., Gropp, W.D., Smith, B.F. 1995 Petsc User Manual. *Argonne National Laboratory(Technical Report - Revision 2.1.3)* Anl-95/11.

[11] Mesri, Y., Digonnet, H., Coupez, T. 2009 Advanced Parallel Computing In Material Forming With Cimlibl. *European Journal Of Computational Mechanics* **18** 669-694

[12] Nagrath, S., Kenneth, E.J., Richard, T., Lahey, Jr. 2005 Computation of incompressible bubble dynamics with a stabilized finite element level set method. *Computer Methods In Applied Mechanics and Engineering* . **194** 4565-4587

[13] Sousa, F.S., Mangiavacch, N., Nonato, L.G., Castelo, A., Tome, M.F., Ferreira, V.G., Cuminato, J.A., McKee, S. 2004 A front-tracking/ front-capturing method for the simulation of 3d multi-fluid flows with free surfaces. *Journal of Computational Physics.* **198** 469-499

[14] Smolianski, A. 2001 Numerical Modeling of two-fluid interfacial flows. *University of jyväskylä.*

[15] Tan, L., Zabaras 2006 Prost : A level set simulation of dendritic solidification with combined features of front-tracking and fixed-domain methods. *Journal of computed physics*

[16] Ville, L., Silva, L., Coupez, T. 2009 Convected Level Set Method For The Numerical Simulation Of Fluid Buckling. *International Journal For Numerical Methods In Fluids.*

[17] Zhang, Z., Victory, H.D., Jr., Dean, H. 1996 Prost : Mathematical Analysis of Zienkiewicz-Zhuś Derivative Patch Recovery Technique. *Numerical Methods Partial Differential Equations.*