Multiphysics Modeling of a Gas Bubble Expansion

B. Chinè[*1,2] and M. Monno[1,3]
[1]Laboratorio MUSP, Macchine Utensili e Sistemi di Produzione, Piacenza, Italy;
[2]Instituto Tecnològico de Costa Rica, Escuela de Ciencia e Ingenieria de Materiales, Cartago, Costa Rica; [3]Politecnico di Milano, Dipartimento di Meccanica, Milano, Italy.
*Corresponding author: Laboratorio MUSP, Località Le Mose, SS 10, 29100 Piacenza, Italy;
bruno.chine@musp.it

Abstract: In this work we use Comsol Multiphysics 4.2 to model a gas bubble expansion in a viscous liquid initially at rest. The aim of the present work is to improve a computational model developed early under simpler conditions [1], by considering now the expansion of a spherical bubble and more realistic physical properties. Surface tension effects on the gas-liquid interface are set for an aluminum-hydrogen system and a step function is considered for modeling the pressure on the boundary. Due to the axial symmetry, the model equations are solved on a two-dimensional mesh with adaptive mesh refinement in time. In order to capture the interface between the two fluids, the capabilities of the level set method are exploited. The numerical findings verify that the computational model is effective. The simulations, carried out for different cases, predict well bubble expansion, interface movement and fluid flow.

Keywords: Bubble expansion, multiphase flow, level set.

1. Introduction

Bubble expansion phenomena plays an important role during metal foam processing. To produce a metal foam, a liquid metal (e.g. Al) can be foamed directly by injecting gas (H_2) or gas releasing blowing agents (solid particles), or by producing supersaturated metal-gas solutions [2]. There is then a simultaneous mass, momentum and energy transfer between three phases, solid, liquid and gas. Experimental works carried out by observation techniques cannot be sometimes applied owing to the specific properties of liquid metals: they are hot, opaque and very reactive with oxygen. These mechanisms could then be modelled and studied by applying computational techniques, although the computational work is very challenging. On the other hand these phenomenon have major effects on the quality of metal foams. To give an example, during mould filling the desired metal foam density is dependent on the ability of controlling the gas bubble expansion.

To accurately compute the evolution of interfaces in bubble dynamics, one interesting alternative Eulerian numerical formulation is provided by the level set method, which embeds the interface as the zero level set of a function. The method was first introduced by Osher and Sethian in 1988 [3] and has encountered extensive applications in multiphase flow modelling. Level set techniques have the additional advantage that they can easily provide accurate values for the normal direction and the curvature of a physical interface.

Our multiphysics modelling work takes into account the expansion of a gas bubble embedded in a viscous liquid. The model considers the interface movement which is due to a pressure difference between the two phases. To model and solve the governing equations of the problem, we will use Comsol Multiphysics 4.2, in particular the level set interface available in the CFD module [4].

2. Model description and equations

In this section we formulate the model and the assumptions done to reasonably simplify the problem.

2.1 Model

At time $t = 0$, we consider a spherical gas bubble of initial radius R_0, density $\rho_{G,0}$ and initial pressure $p_{G,0}$ in static equilibrium with a surrounding liquid matrix of initial pressure $p_{EXT,0}$. The gas in the bubble is considered to be compressible and following the ideal gas law, while the liquid is an incompressible Newtonian fluid. Gas and the liquid are immiscible, and

there is spherical symmetry in the system. Further on, no heat transfer (T is the constant absolute temperature of the system) and mass diffusion are taken into account, although it is possible to extend this formulation to no-isothermal problems and analyze also concentration gradients. The state of the stress is then given by the classical Young-Laplace equation, relating the pressure discontinuity across the interface to the surface tension σ and curvature $\kappa = 2/R$ of the interface, that is

$$p_{G,0} = 2\sigma / R_0 + p_{EXT,0} \qquad (1)$$

In conjunction with these assumptions, we consider that $p_{EXT,0}$ decreases its value, which is the onset of bubble growth: thus, at any time t, $R(t)$ and $p_G(t)$ will be the new bubble radius and new gas pressure, respectively. Due to the spherical symmetry, the expansion causes the incompressible liquid to move radially oriented, where the velocity field u is only a function of the spherical radial coordinate r and time t.

Following the work of Gniloskurenko et *al.* [5], who studied a cavity growth in a liquid metal around a gas releasing particle, the interface velocity may be obtained by the velocity field at $r=R$, this leads to:

$$u(r,t) = \frac{dR(t)}{dt}\frac{R^2(t)}{r^2}, \quad r \geq R \qquad (2)$$

With tension surface effects and considering the stress at $r=R$, the bubble radius may be calculated by solving an ordinary differential equation, as shown in [5]. Successively, we use the Gniloskurenko et *al*. 's results, modeling the gas density $\rho_G(t)$ as:

$$\rho_G(t) = \frac{\rho_{G,0}}{\left\{1 + \frac{1}{4\eta_L}\left[p_{G,0} - (p_{EXT,0} + \frac{2\sigma}{R_0})\right] t\right\}^3} \qquad (3)$$

where η_L is the dynamic viscosity of the liquid.

2.2 Governing equations

To model the expansion in Comsol Multiphysics, we select instead a Cartesian system of cylindrical coordinates (r_{AX}, φ, z) and apply an axial symmetry condition around the z axis of the gas-liquid system, as depicted in Figure 1. With this assumption, the expansion takes place in a 2D liquid region Ω represented by a surface of radius R_Ω. The gas liquid interface is a free surface with uniform local curvature κ while **n** is the unit normal to the interface. The expansion of the gas bubble embedded in a viscous liquid is numerically simulated by using the classical equations of fluid dynamics coupled to the level set method available in Comsol Multiphysics 4.2. The method is very well suited to describe the movement of the interface during the gas expansion. The compressibility of the gas in the bubble is computed with a weakly- compressible model, valid for gas flows with low Mach numbers (approximately $Ma < 0.3$). In this model, the gas density $\rho_G(t)$ is given by the ideal gas law $pV = n\Re T$, after introducing the molar mass M and mass m ($n = m/M$). Then, for both the fluids, the coupled partial differential equations of the model are the following (Laminar Flow, Two Phase, Level Set Interface, [4]):

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = 0 \qquad (4)$$

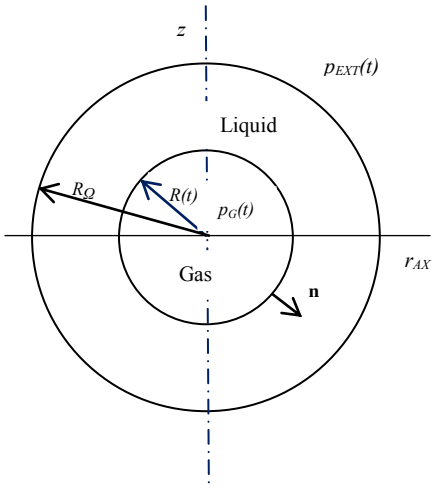

Figure 1. A gas bubble expanding in a 2D liquid region because of the axial symmetry around the z axis: at the beginning $R(t)=R_0$, $p_G(t)=p_{G,0}$ and $p_{EXT}(t)=p_{EXT,0}$.

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho(\mathbf{u}\bullet\nabla)\mathbf{u}=\nabla\bullet[-p\mathbf{I}+\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})$$
$$-\frac{2\eta}{3}(\nabla\bullet\mathbf{u})\mathbf{I}]+\mathbf{F}+\rho\mathbf{g}+\mathbf{F}_{ST} \quad (5)$$
$$\frac{\partial\phi}{\partial t}+\mathbf{u}\bullet\nabla\phi=\gamma\nabla\bullet[\varepsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}] \quad (6)$$

The momentum transport equation (Eq. 5) relates the fluid velocity **u** to gravity force $\rho\mathbf{g}$, other body forces **F**, and the surface tension force $\mathbf{F}_{ST}$ acting at the interface between the two fluids (see [4] for more details on $\mathbf{F}_{ST}$ modeling). In the same equation **I** the identity tensor. The advection of the level set function ϕ in the computational region is given by Eq. 6. To compute this field, a signed distance function at $t=0$ is used to build the function ϕ which corresponds to the interface at the level set $\phi=0.5$. In the same step the values of ϕ inside the two phases are setting as $0\le\phi<0.5$ for one fluid (in our model is the liquid) and $0.5<\phi\le1$ for the other (gas in the model). In Eq. 6 the parameter γ represents the reinitialization parameter and controls the re-initialization performed at some later point in the calculation beyond $t=0$, need to preserve the values of distance close to the interface. Finally ε is the interface thickness parameter which adds extra numerical diffusion in order to stabilize the computations of Eq. 6.

Boundary conditions are applied by considering the axial symmetry and also the symmetry around the r_{AX} axis. In this way, we reduce the computational domain of Figure 1 to a circular region with $0\le r_{AX}\le R_{\Omega}$ and $0\le z\le R_{\Omega}$. Finally, the external boundary of the Ω domain is outflow with Dirichlet condition $p_{EXT}(t)=0$ and vanishing viscous stresses.

Multiphase phenomena in metal foam production give strong property gradients at fluid interfaces, which cause calculations to be carried out with some difficulties, due to instabilities in numerical computations. Moreover, depending on the pressure difference between gas and liquid phase and the value of η_L, the expansion could be very fast. In fact, by means of equation (3) a gas bubble with $R_0=10^{-4}$ m would obtain an average interface velocity of ~ 0.25 m/s for a pressure difference of 10 Pa and $\eta_L=10^{-3}$ Pa·s. Consequently, a step function is introduced in the model for setting the condition $p_{EXT}(t)=0$ on the boundary and, in order to obtain convergence and compute a more accurate numerical solution, the mesh is refined in the proximity of gas-liquid interface.

3. Numerical settings

To simulate a hydrogen bubble of radius 0.01 m expanding in aluminum liquid, we use the values of fluid properties given in Table 1, while other parameters of the model are shown in Table 2. In all the computations, the value of the surface tension is set for a real aluminum-hydrogen system and gravity forces are not considered. The initial hydrogen density $\rho_{G,0}$, computed by the ideal gas law, is 0.02623 kg/m^3 and the constant hydrogen dynamic viscosity is 10^{-3} Pa·s.

When the initial pressure difference is large, we choose a higher value for the dynamic viscosity of the aluminum liquid, setting this to 10^{-1} Pa·s. This is needed in order to reduce the velocity of the process and get convergence in the simulations. In the same way, the density of the liquid is taken lower, equal to 10 kg/m^3, to reduce the strong density gradient across the interface. Instead, when the initial pressure difference between gas bubble and liquid is small (equal to 0.1 Pa), the values of aluminum viscosity and density are the real ones, close to 2.4x10 kg/m^3 and 4.5x10^{-3} Pa·s for a temperature of 933 K. Then, the maximum density ratio ρ_L/ρ_G used in the simulations is 9.1x10^4 approximately, while the minimum one is near to 3.8x10^2.

Using the maximum element size of Table 2 and depending on the computations (sharper properties differences needing finer meshes) the global computational domain Ω has been covered by $8\text{x}10^4\div10^5$ triangle elements, corresponding to more than $5\text{x}10^5\div6.5\text{x}10^5$ degrees of freedom. The calculations have been carried out with the direct solver PARDISO, Comsol Multiphysics version 4.2. The convergence obtained during computations was good, giving a step-size near to $10^{-3}\div10^{-5}$ s, function of the parameters of Table 2 and the

Table 1: Fluid properties used in the simulations of a gas bubble expansion in liquid.

Magnitude	Symbol	Value
Case A, B and C		
Universal gas constant	$\Re$	8.314 J/(mol·K)
Gas molar mass	M	2 g/mol
Gas density	ρ_G	Ideal gas and Eq.3.
Gas viscosity	η_G	10^{-3} Pa·s
Surface tension coefficient	σ	0.95 N/m
Initial bubble radius	R_0	10^{-2} m
Ambient pressure	p_{EXT}	0 Pa
Constant temperature	T	933 K
Case A		
Liquid density	ρ_L	10 kg/m^3
Liquid viscosity	η_L	10^{-1} Pa·s
Initial bubble pressure	$p_{G,0}$	400 Pa
Case B		
Liquid density	ρ_L	10 kg/m^3
Liquid viscosity	η_L	$4.5\text{x}10^{-3}$ Pa·s
Initial bubble pressure	$p_{G,0}$	190.1 Pa
Case C		
Liquid density	ρ_L	$2.4\text{x}10^3$ kg/m^3
Liquid viscosity	η_L	$4.5\text{x}10^{-3}$ Pa·s
Initial bubble pressure	$p_{G,0}$	190.1 Pa

Table 2: Model parameters used in the simulations of a gas bubble expansion in liquid.

Magnitude	Symbol	Value
Case A, B and C		
Max element size of the mesh	-	$1\text{x}10^{-4}$ m
Time stepping	-	set by the solver
Relative tolerance	-	10^{-3}
Absolute tolerance	-	10^{-4}
Case A		
Interface thickness	ε	$9\text{x}10^{-5}$ m
Reinitialization	γ	5.25 m/s
Case B		
Interface thickness	ε	$8\text{x}10^{-5}$ m
Reinitialization	γ	0.06 m/s
Case C		
Interface thickness	ε	$8\text{x}10^{-5}$ m
Reinitialization	γ	0.06 m/s

velocity of the expansion process. The solution time is of $2\text{x}10^4 \div 3\text{x}10^4$ s, for a PC with Intel Xenon CPU X5660, 6 core, 2.80 GHz, 12 GB RAM, 64bit and Windows 7 Operative System.

The simulations started by initializing the level set function, such that ϕ varies smoothly from zero to one across the interface. Afterwards, the time dependent solver carried out the computations in order to simulate bubble expansion, interface movement and fluid flow.

4. Results and discussion

Figure 2 shows the bubble growth in the liquid region for the *case A*. The volume gas fraction is plotted 0.001 s after the expansion starts, when the bubble has reached a radius of 0.0141 m. For the same conditions, Figure 3 gives the velocity field both for the gas and liquid. We can observe that the maximum value of velocity magnitude is 4.6 m/s on the gas side of the interface. Defining the Reynolds number as $\text{Re} = \dfrac{U R_0}{\upsilon_L}$, where U is the average velocity of the interface and $\upsilon_L = \dfrac{\eta_L}{\rho_L}$ the kinematic viscosity of the liquid, we obtain for the *case A* $\upsilon_L = 0.01 \text{m}^2/\text{s}$ and $\text{Re} \cong 5.3$. This expansion is

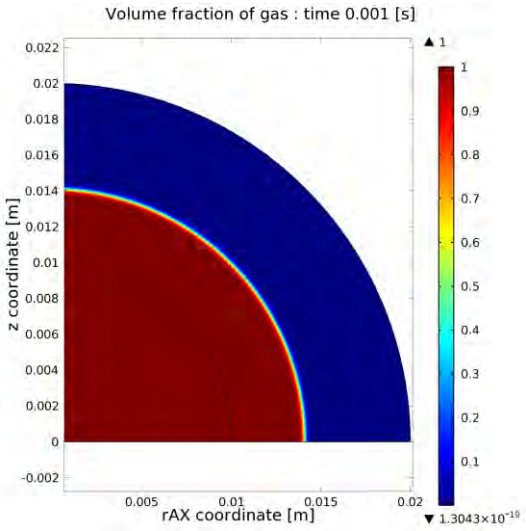

Figure 2. Expansion of a gas bubble in a liquid corresponding to the simulated *case A* (ρ_L=10 kg/m^3, η_L=10^{-1} Pa·s, $p_{G,0}$=400 Pa), after 0.001 s.

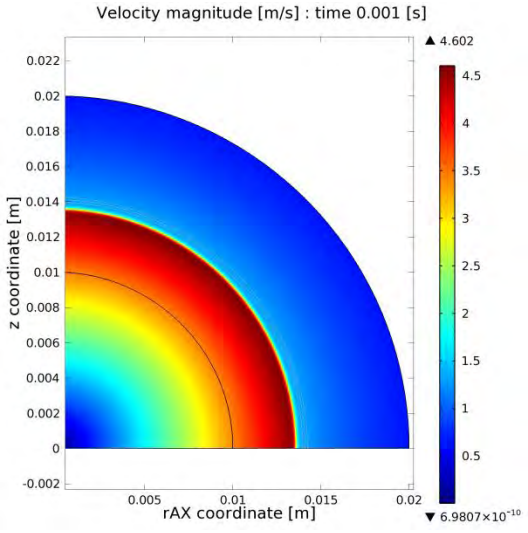

Figure 3. Velocity field in the gas and liquid region corresponding to the simulated *case A* (ρ_L=10 kg/m^3, η_L=10^{-1} Pa·s, $p_{G,0}$=400 Pa), after 0.001 s.

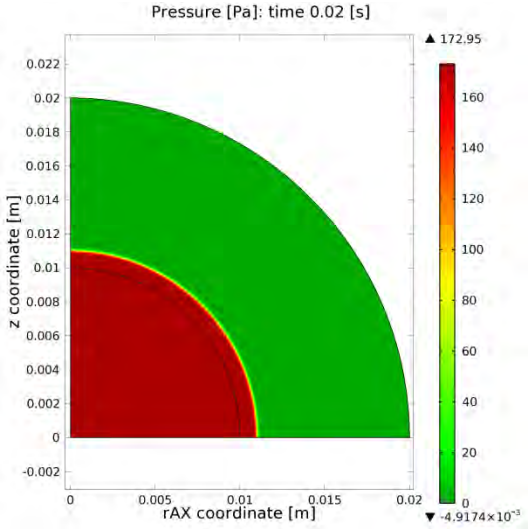

Figure 4. Pressure in the gas and liquid region corresponding to the simulated *case B* (ρ_L=10 kg/m^3, η_L=4.5x10^{-3} Pa·s, $p_{G,0}$=190.1 Pa), after 0.02 s.

quite fast, although the Reynolds number is limited by a larger value of υ_L.

In Figure 4 we have plotted the pressure for the *case B* at t=0.02 s, when the growing radius of the bubble is 0.0111 m. Note that for the spherical bubble, the gas pressure is uniform, but not constant, because the curvature of the gas-liquid interface decreases as the bubble expands. From the figure, we observe that the bubble has reduced the pressure of approximately 17 Pa from its initial value, while the pressure in the liquid demonstrates correctly the value p_{EXT} set on the boundary. The jump of dynamic pressure across the interface is about 173 Pa, lightly greater than the pressure discontinuity of $\frac{2\sigma}{R} = \frac{2(0.95)}{0.0111} \cong 171.2$ Pa, calculated under no flow conditions. The difference of a few Pa is just caused by the dynamic stress of the flow. For *case B*, the Re number is 1.22 and, as shown from the same Figure 4, the bubble experiences a movement which is slower if compared to the previous *case A*.

The most interesting simulation is, of course, *case C*, because it refers to the growth of a hydrogen bubble in liquid aluminum. Using the values of Table 1, the kinematic viscosity of the aluminum is $\upsilon_L \cong 1.9x10^{-6}$ m^2/s and the flow is characterized by $\mathrm{Re} \cong 293$. This time, the expansion is even faster and after only 0.006 s the bubble shows a radius of 0.01044 m, as indicated in Figure 5. As expected, due to the density difference between the gas and the liquid, the liquid moves away from the gas-liquid interface as the bubble grows and expands (see Figure 6). Furthermore, the magnitude of the liquid velocity decreases with increasing distance from the gas-liquid interface, as it can

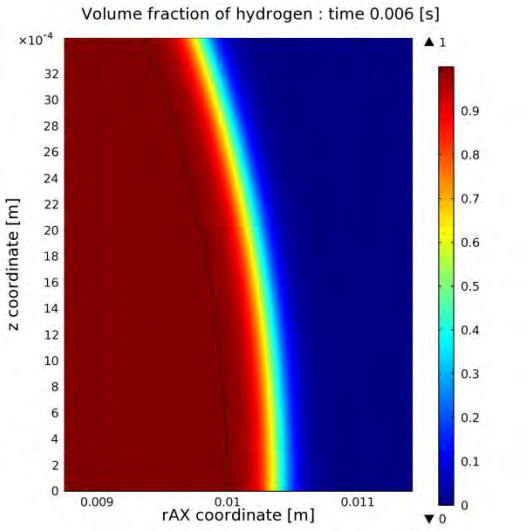

Figure 5. Expansion of a hydrogen bubble in liquid aluminum corresponding to the simulated *case C* (ρ_L=2.4x10 kg/m^3, η_L=4.5x10^{-3} Pa·s, $p_{G,0}$=190.1 Pa), after 0.006 s.

be observed in the same Figure 6.

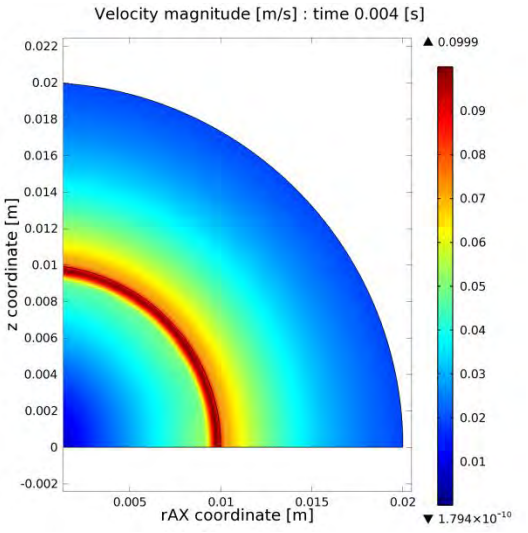

Figure 6. Velocity field of a hydrogen bubble expanding in liquid aluminum, corresponding to the simulated *case C* (ρ_L=2.4x10 kg/m^3, η_L=4.5x10^{-3} Pa·s, $p_{G,0}$=190.1 Pa), after 0.004 s.

5. Conclusions

A model by Comsol Multiphysics has been presented for the simulation of a hydrogen bubble expansion in liquid aluminum. Bubble expansion was driven by a pressure difference between the two phases in presence of surface tension effects, computing the flow both in the liquid and gas region. To set the external pressure on the boundaries, a step function has been used, while mesh refinement was applied in order to calculate the strong gradients close to the interface.

The numerical findings verify that the computational model, based on a level set technique for capturing the phase interface, is effective. The simulations, carried out for different cases, predict well bubble expansion, interface movement and fluid flow. We think to to extend the model in order to compute foam expansions, taking into account other mechanisms, like mass diffusion and heat transfer. However, when employing a comprehensive model for foaming process, a multiple bubbles model should be also considered.

6. References

[1] B. Chinè and M. Monno, A model of gas bubble growth by Comsol Multiphysics, *Proceedings of 2010 European Comsol Conference*, Paris, (2010).

[2] J. Banhart, Manufacture, characterization and application of cellular metals and metal foams, *Progress in Materials Science*, **46**, 559-632 (2001).

[3] S. Osher and J.A. Sethian, Fronts propagating with curvature dependent speed: Algorithms based on Hamilton-Jacobi formulation, *Journal of Computational Physics*, **79**, 12-49 (1988).

[4] Comsol AB, Comsol Multiphysics-CFD Module, *User's Guide*, **Version 4.2,** 201-264 (2011).

[5] S.V. Gniloskurenko, A.I. Raichenko, T. Nakamura, A.V. Byakova and A.A. Raichenko, Theory of initial microcavity growth in a liquid metal around a gas-releasing particle. II. Bubble initiation conditions and growth kinetics, *Powder Metall. And Metal Ceramics,* **41**, N.1-2, 90-96 (2002).

7. Acknowledgements

Authors gratefully acknowledge the collaboration provided by Dr. Valerio Marra (Comsol AB, Brescia, Italy) for his technical suggestions concerning Comsol Multiphysics version 4.2.