A Model of Gas Bubble Growth by Comsol Multiphysics

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Abstract: We use Comsol Multiphysics to model a gas bubble expansion in a viscous liquid initially at rest, a very common system for lightweight foamed materials from metal production and polymer processing. The aim of the present work is to develop a first computational model for the growth of gas bubbles under simpler conditions, modeling both the gas and liquid flow and to verify its validity by comparing the numerical results with existing analytical solutions. The two dimensional isothermal model developed in Comsol Multiphysics considers a gas bubble growing due to a pressure difference with a surrounding Newtonian liquid. Surface tension effects on the gas-liquid interface are considered. The model equations are solved on a fixed grid, built both in the gas than in the liquid region. In order to capture the front between the two fluids we exploit the capability of the level set method.
The numerical results of the computational model compare well with analytical solutions from theory and obtained for a few simple cases. This first computational work is a basis for considering successive more realistic foam expansions.

Keywords: Bubble growth, multiphase flow, level set.

1. Introduction

Gas bubble growing in a surrounding liquid matrix is an important and complex phenomenon in many technological fields. An interesting case is encountered in cellular metals and metal foams production, when nucleated gas bubbles expand and move in a confined liquid metal before to cool and solidify. 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 [1]. The process depends on simultaneous mass, momentum and energy transfer between three phases: solid, liquid and gas. Furthermore, other physical phenomena should be taken in account in the system, like complex interface processes, bubble motion, coexistence, coalescence and collapse of bubbles. 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. Then, these mechanisms can be modelled and studied by applying computational techniques, although the computational work is very challenging: the phenomenon are not independent among them and many times are simultaneous. Multiphase flow modelling is also required because of the presence of more phases: the solid metal matrix containing the foaming agent not yet fully melted, the gaseous phase made up of bubbles and the liquid phase composed of a melted metal matrix. Mass and heat transfer should be also taken into account in the modelling work to give the most accurate results. 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 very strategic and this is dependent on the ability of controlling the gas bubble growth.

It is understood that the improving of foaming quality and cost-effectiveness may be also realized by means of simplified computational models. Attention will be demanded by the presence of a dynamic interface between the gas bubbles continuously originating and the surrounding liquid. To accurately compute the evolution of interfaces, many computational methods are been designed in the past. Lagrangian methods use a numerical grid which follows the fluid and tracks the interface, while by Eulerian methods the interface is captured on a stationary grid. 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 [2] 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.

As a first effort to understand metal foaming mechanisms, we consider the growth of a gas bubble embedded in a viscous liquid. We take into account 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, a commercial simulation tool based on finite elements method which includes the level set method in its Chemical Engineering Module [3].

2. Theory and model description

In this section we describe the two dimensional model and the assumptions which are been done to reasonably simplify the problem. This is due also for managing the computational job in a common laptop machine.

2.1 Theory

Let us to consider a gas bubble growing due only to a pressure difference with a surrounding limited amount of liquid matrix. The problem is assumed two dimensional, no heat transfer and mass diffusion are taken into account. The system is thus isothermal and there are not gradients of species concentration. The gas in the bubble follows the ideal gas law while the liquid is considered to be an incompressible Newtonian fluid. Furthermore, the gas and the liquid are assumed to be immiscible.

Figure 1 shows a schematic of a circular gas bubble with initial radius and pressure respectively equal to R_0 and $p_{G,0}$. The expansion takes place in a liquid matrix Ω modeled as a circular region of radius R_Ω. For symmetrical considerations it is possible to reduce the modeled region, both for the gas bubble and the liquid (see section 2.2). The gas liquid interface is a free surface with uniform surface tension coefficient σ, with κ representing the local curvature and **n** the unit normal to the interface.

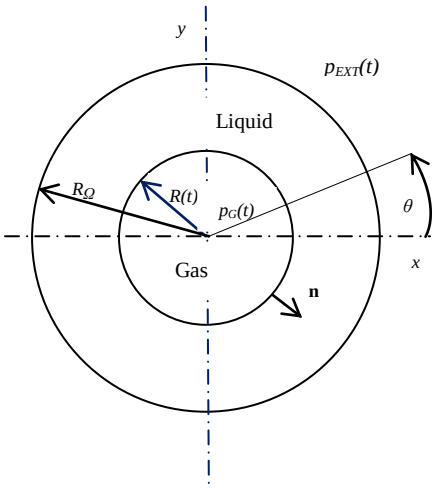

Figure 1. Schematic of a gas bubble growth in a liquid region with the considered symmetry: at the beginning $R(t)=R_0$, $p_G(t)=p_{G,0}$ and $p_{EXT}(t)=p_{EXT,0}$.

At any time t, T is the constant absolute temperature of the system and $R(t)$ and $p_G(t)$ are the bubble radius and gas pressure, respectively.

At the beginning ($t=0$), with the liquid at rest and by calling with $p_{EXT,0}$ the initial ambient pressure imposed on the boundary of Ω, the Laplace's equation states that stress balance at the surface of a circular bubble of radius R_0 is:

$$p_{G,0} - p_{EXT,0} = \sigma\kappa \qquad (1)$$

where:

$$\kappa = 1/R_0 \qquad (2)$$

for a circular bubble. Substituting Eq.2 into Eq.1, it is written as:

$$R_0 = \frac{\sigma}{p_{G,0} - p_{EXT,0}} \qquad (3)$$

which gives the radius of the bubble at $t=0$ when the liquid is still at rest. Consequently, given σ, the bubble will expand or contract and the liquid will flow if the pressure difference $p_{G,0} - p_{EXT,0}$ changes its value. For a gas bubble expansion, a common case could be represented by a sudden lowering of the ambient pressure. Under this condition, a new equilibrium state

will be reached by the bubble and, with the liquid at rest again, the bubble radius at equilibrium is:

$$R_{eq} = \frac{\sigma}{p_G - p_{EXT}} \qquad (4)$$

Here p_G and p_{EXT} are the new equilibrium values of the pressure, for the gas and the ambient respectively. On the other hand, the ideal gas equation followed by the specie inside the bubble is:

$$pV = n\Re T \qquad (5)$$

where V represents the volume (area for a two dimensional problem) of the bubble, $\Re$ is the universal gas constant and n is the number of moles. We assume that during bubble expansion the behavior of the gas is polytropic, thus for an isothermal process it follows:

$$p_{G,0}A_0 = p_G A \qquad (6)$$

being A_0 and A the equilibrium bubble areas for the pressure $p_{G,0}$ and p_G, respectively.

2.2 Governing equations

To simulate numerically the isothermal growth of a gas bubble embedded in a viscous liquid and the fluid flows that originate, we use the classical equations of fluid dynamics coupled to the level set method available in Comsol Multiphysics. As we said before, the method is very well suited to describe the motion of the interface during the gas expansion. We assume the liquid to be an incompressible Newtonian fluid and take into account the compressibility of the gas in the bubble. For gas flows with low Mach numbers (approximately $Ma < 0.3$), a weakly- compressible model can be used. In this model, the gas density $\rho_G(t)$ is given by the ideal gas law (5), 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 (Two Phase Flow, Level Set Application Mode, [3]):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (7)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

$$-(\frac{2\eta}{3} - \kappa_{DV})(\nabla \cdot \mathbf{u})\mathbf{I}] + \mathbf{F} + \rho \mathbf{g} + \mathbf{F}_{ST} \qquad (8)$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot [\varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|}] \qquad (9)$$

In the momentum transport equation, the scalar magnitudes ρ, η and κ_{DV} are the fluid density, dynamic viscosity and bulk viscosity, respectively. Among the other terms, $\mathbf{u}$ is the fluid velocity, $\mathbf{I}$ is the identity tensor, $\rho\mathbf{g}$ is the gravity force and $\mathbf{F}$ takes into accounts other body forces. The term $\mathbf{F}_{ST}$ accounts for the surface tension force acting at the interface between the two fluids (see [3] for more details on $\mathbf{F}_{ST}$ modeling).

The advection of the level set function ϕ in the computational region is given by Eq. 9. 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 $0.5 < \phi \le 1$ for the other (gas in the model). 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. 9.

To solve the governing equations we have select a Cartesian system of coordinates (*x*,*y*) and applied the symmetry conditions shown in Figure 1. The computational domain Ω has been reduced again, giving a circular surface with azimuthal angle $0 \le \theta \le \frac{\pi}{4}$. In the domain the external boundary of Ω has been set as an outflow with a Dirichlet condition $p_{EXT}(t) = 0$ on the pressure and vanishing viscous stresses.

At $t = 0$, starting with gas and liquid phases at equilibrium, we impose a pressure value greater than σ/R_0 on the gas bubble. Forces $\rho\mathbf{g}$ and $\mathbf{F}$ are set to zero, then we drive the interface motion by analytically computing the density

variation $\rho_G(t)$. Using cylindrical coordinates (r,θ), the incompressible liquid motion is radially oriented and the velocity field u is only a function of (r,t). The interface velocity may be obtained by the velocity field at $r=R$, this leads to:

$$u(r,t) = \frac{dR(t)}{dt}\frac{R(t)}{r}, \quad r \geq R \qquad (10)$$

In the absence of tension surface effects and considering the stress at $r=R$, the bubble radius may be calculated by solving an ordinary differential equation, as explained in [4]. Successively, for $p_{EXT} = 0$ the density variation is computed as:

$$\rho_G(t) = \frac{\rho_{G,0}}{(1+\frac{p_{G,0}\,t}{\eta_L})} \qquad (11)$$

Instead, for $\sigma \neq 0$ we solve the respective ordinary differential equation and calculate $R(t)$, numerically, by the solution:

$$[C - AR(t)]^C \exp^{AR(t)} = [C - AR_0]^C \exp^{A(R_0 - At)} \qquad (12)$$

where $C = \frac{p_{G,0}R_0^{\,2}}{2\eta_L}$ and $A = \frac{\sigma}{2\eta_L}$.

Finally, the radius $R(t)$ from Eq.12 is substituted into Eq.6, modeling a density change for an isothermal process with surface tension phenomenon at interface.

3. Simulations

Our main interest is to simulate a gas bubble expansion in a liquid metal during foam processing, in order to capture the interface and analyze fluid flows similar to those we could have within moulds. However, multiphase phenomenon in metal foam production give strong property gradients at fluid interfaces, which cause computations to be carried out with some difficulties. Considering these complexities, we start to study simpler problems, as first examples of future more realistic simulations. Consequently, we have set the values of fluid properties shown in Table 1. Other parameters used in the model are given in Table 2. In this way we model flows with moderate density and viscosity differences, as well as surface tension. The density of the liquid is taken to be 10 kg/m^3, while the initial gas density $\rho_{G,0}$, computed by Eq. 5, is 0.02613 kg/m^3 which gives a density ratio of approximately $4\text{x}10^2$. In the same way the viscosity ratio is near 10^2. The surface tension coefficient is zero in the first simulated case and equal to 0.01 N/m for other computations.

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

Magnitude	Symbol	Value
Universal gas constant	$\Re$	8.314 J/(mol·K)
Gas molar mass	M	2 g/mol
Gas density	ρ_G	Eq.5, Eq.6, Eq.11
Liquid density	ρ_L	10 kg/m^3
Gas viscosity	η_G	10^{-3} Pa·s
Liquid viscosity	η_L	10^{-1} Pa·s
Gas bulk viscosity	κ_{DV}	0 Pa·s
Surface tension coefficient	σ	0 N/m
		10^{-2} N/m
Initial bubble radius	R_0	10^{-2} m
Initial bubble pressure	$p_{G,0}$	0.2 Pa
		1.2 Pa; 2.2 Pa
Ambient pressure	p_{EXT}	0 Pa
Constant temperature	T	933 K

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

Magnitude	Symbol	Value
Max element size of the mesh	-	10^{-4} m
Time stepping	-	set by the solver
Relative tolerance	-	10^{-3} s
Absolute tolerance	-	10^{-4} s
Interface thickness	ε	10^{-4} m
Reinitialization	γ	$0.01 \div 0.02$ m/s

To solve the model equations, the global computational domain Ω has been meshed by 10^4 triangle elements approximately, corresponding to more than $8 \cdot 10^4$ degrees of freedom, number which could be still managed by a common laptop. Finally, calculations have been carried out with the direct solver PARDISO, Comsol Multiphysics version 3.5a. Although the partial differential equations of the model are non linear and time dependent, the convergence obtained during computations was good, giving a step-size near to 10^{-3} s with a solution time of 1.8 hours approximately, for a laptop with 2.8 GHz Intel Core2 Duo processor and 4 GB RAM.

The simulations started by initializing the level set function, using a pseudo-time equal to 10^{-2} s, such that ϕ varies smoothly from zero to one across the interface. Then, the transient mode was selected and computations were carried out in order to get bubble growth, interface motion and fluid flow, for three different conditions:

a) $\sigma = 0$ N/m, p = 0.2 Pa
b) $\sigma = 10^{-2}$ N/m, p = 1.2 Pa
c) $\sigma = 10^{-2}$ N/m, p = 2.2 Pa

4. Results and discussion

Figure 2 shows the bubble growth in the liquid region when tension surface is present and the initial gas pressure is equal to 1.2 Pa. The volume gas fraction is plotted 1.4 s after the growth starts, when the bubble has already reached its maximum expansion. We observe that the final bubble radius is equal to 0.012 m, in agreement with the analytical value given by Eq.4. For the same conditions, Figure 3 gives the pressure field both for the gas and liquid, which agrees with the values of pressure for a liquid again at rest ($p_L = p_{EXT}$) and with a static pressure jump equal to $\frac{\sigma}{R_{eq}} = \frac{0.01}{0.012} \cong 0.83\,\text{Pa}$

Figure 4 presents the change of areas, over time, obtained by integrating the level set function ϕ in the computational region. As shown in the figure, the gas area is growing only until to a certain time value ($t \approx 1\text{s}$), stating that for $t = 1.4\text{s}$ the bubble is in equilibrium with the liquid. Due to the expansion, the fluids acquire a

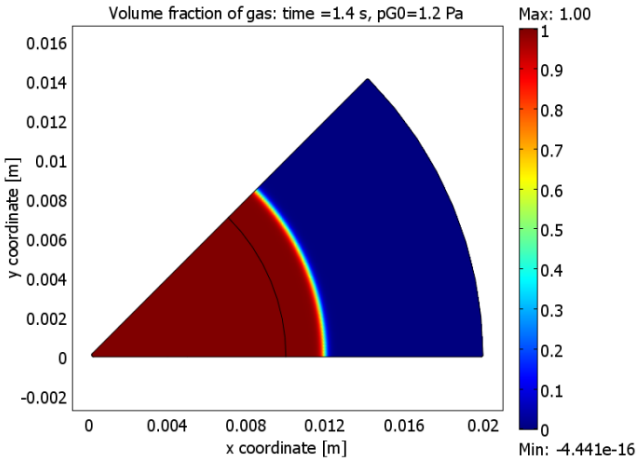

Figure 2. Growth of a gas bubble in a liquid corresponding to the simulated case b) of section 3.

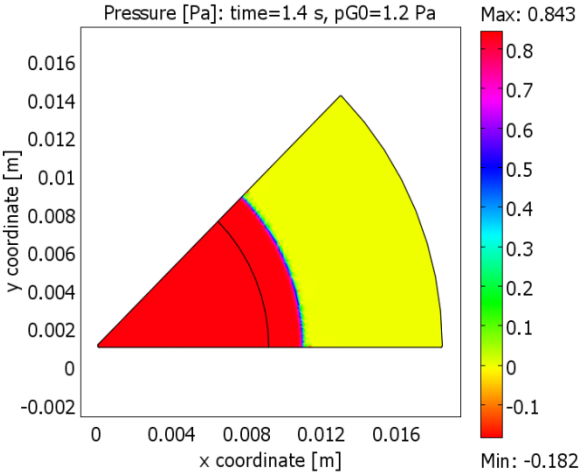

Figure 3. Pressure field in the gas and liquid corresponding to the simulated case b) of section 3.

significant motion, with the characteristic radial pattern depicted in Figure 5. In the figure we have plotted the pressure field superimposed on the contour of fluid velocity at $t = 0.2\,s$, for a gas bubble with an initial pressure equal to 2.2 Pa. As expected, the magnitude of the gas velocity increases with decreasing distance from the gas-liquid interface, where it reaches its maximal value, which is equal to 0.02 m/s approximately. Continuity between gas and liquid velocity can be well noted, indicating a correct coupling of the model at interface. At $t = 0.2\,s$ the bubble is still expanding, far from

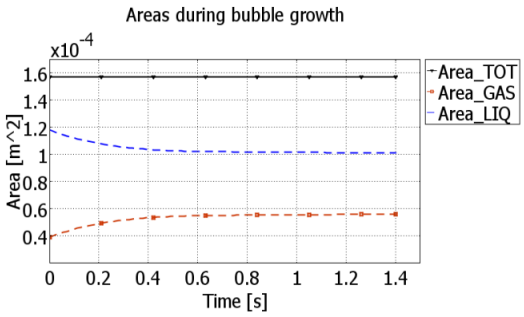

Figure 4. Values of total (black line), gas (brown dashed line) and liquid (blue dashed line) area, corresponding to the case b) of section 3.

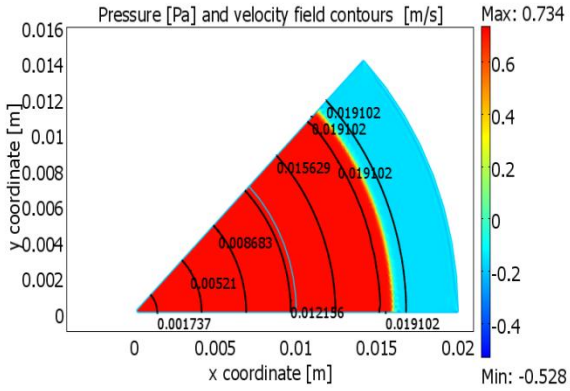

Figure 5. Pressure and velocity field during the growth of a gas bubble in a liquid, corresponding to the case c) of section 3: t = 0.2 s after growth starts.

the static equilibrium. In fact, the radius for this latter condition is given by $R_{eq} = \frac{p_{G,0} R_0^{\,2}}{\sigma} = 0.022\ \mathrm{m}$, which is obtained introducing Eq.4 into Eq.6. In correspondence of that radius the pressure would be equal to $\frac{\sigma}{R_{eq}} = \frac{0.01}{0.022} \cong 0.45\,\mathrm{Pa}$. This value is lower than the maximum pressure present at that moment within the bubble, close to 0.73 Pa, as we may observe in the same Figure 5.

5. Conclusions

A model by Comsol Multiphysics has been presented for the simulation of gas bubble growth with flow in the liquid and inside the gas region. No mass and energy transfers has been considered, bubble growth is due to only a pressure difference. Flows in both the fluids are calculated using a weakly-compressible model coupled to a level set transport equation which captures the front between the two phases. Gas density has been modeled starting from the gas ideal equation, also in presence of surface tension effects. The resulting model performs well, giving results which agree with analytical solutions. Although the model takes into account moderate density and viscosity difference values for the fluids, simplifying in this way the numerical computations, it represents a good basis for future and more realistic simulations of foam expansions.

6. References

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