Modeling of Transport Phenomena in Metal Foaming

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Abstract: Metal foams are interesting materials which include gas voids in the material structure with the real possibility to modify ad hoc their physical properties. During the foaming process of a metal, simultaneous mass, momentum and energy transport mechanisms arise. In this work we propose a model considering mass transfer phenomena coupled to the growth and motion of a gas bubble in the liquid metal. The diffusion of the gas in the liquid is studied by applying the Fick's law and convective transport. The equilibrium concentration at the gas-liquid interface is modeled by the Sievert's law with surface tension effects included. The numerical results of the simulation show that the computational model, using the phase field method for capturing the phase interface, can be effective. The computations simulate satisfactorily mass transfer, bubble expansion, interface movement and fluid flow. In this way other physical mechanisms of foaming could be included in a future more comprehensive model.

Keywords: metal foams, multi-phase flow, transport phenomena, gas diffusion.

1. Introduction

Metal foams [1,2] are interesting materials with many potential applications in engineering. Foamed metals or alloys include gas voids in the material structure with the real possibility to modify ad hoc their physical properties. Therefore, a wide range of possibilities arise in the automotive, aerospace, nautical, railway, building, civil engineering and medical industries. It is possible to manufacture foamed component via the powder metallurgical route, i.e. starting from a compacted mixture (precursor) of metal (or metal alloy) and blowing agent powders, such as Al and titanium hydride (TiH_2). Remelting the precursor leads to in situ gas evolution within the metal as the blowing agents release H_2 gas. With this process, closed molds can be filled with foam, and structural foam parts of complex shape can be manufactured. Shaped sandwich panels with two dense face sheets and a cellular core can also be made [1].

During the foaming process of a metal, simultaneous mass, momentum and energy transport mechanisms arise between different phases, the solid one (mold walls and the solidified metal), the liquid metal (Al) and the gas (H_2 gas bubbles and the surrounded air). Furthermore, other physical phenomena like complex interface processes, bubble motion, coexistence, coalescence and collapse of bubbles, have place. Experimental works carried out by observation techniques cannot be sometimes applied owing to the specific properties of liquid metals, since they are hot, opaque and very reactive with oxygen. Hence the computational techniques could represent a useful tool to investigate these mechanisms, although the computational work is very challenging, because the phenomena are not independent among them and are simultaneous. The ultimate aim of our underway researches is to simulate the expansion of a metal foam in a mold, by taking all these mechanisms into account. Following our previous efforts to simulate the foaming process of a metal [3], we develop a model, by COMSOL Multiphysics® version 4.3b, which considers mass transfer phenomena coupled to the growth and movement of a hydrogen gas bubble in liquid aluminium. The purpose is to model the expansion of H_2 gas in metal foam, resulting from the diffusion of the gas towards the bubble. In the previous work this expansion was modeled by means of a specific expansion rate [3].

The structure of the paper is the following. The description of the physical and mathematical model is given in Section 2, while Section 3 deals with the use of Comsol Multiphisics®. Finally the computational results are presented in Section 4 and the conclusions in Section 5.

2. Model description and equations

2.1 Physical model

We consider that under the precursor heating, the foaming agent starts to release H_2 gas in the melted aluminium. The gas dissolves in the aluminium and insoluble gas diffuse towards existing bubbles or nuclei, which causes them to inflate. The gas in the bubble is considered as an ideal gas and the equilibrium concentration at the gas-liquid interface is given by the Sievert's law . Because of surface tension effects, the thermodynamical equilibrium at the gas-liquid interface between the hydrogen partial pressure p_g in the gas bubble and the dissolved hydrogen in the liquid aluminium is expressed by the Gibbs-Thomson equation [4,5].

Fig. 1 shows an isolated circular H_2 gas bubble surrounded concentrically by a shell of liquid Al. In this 2D model gravity is absent and the system is considered isothermal. The melted metal is considered as an incompressible Newtonian liquid of constant viscosity. At the boundary of the system with external radius R_{ext} the pressure is fixed at atmospheric pressure p_{ATM}. We define r the radial coordinate, t the time, $R=R(t)$ the time-dependent bubble radius, p_g the pressure of hydrogen in the bubble, σ the interfacial surface tension, V the molar volume and C the molar concentration. Following the work of Atwood *et al.* [4] the hydrogen concentration at the interface between the gas bubble and the melt is:

$$C_H^* = S_H^L \exp\left(\frac{\sigma V}{R(t)\,\Re\, T}\right) \qquad (1)$$

where $\Re$ is the universal ideal gas constant, S_H^L the hydrogen solubility in liquid aluminium and T the absolute temperature. The hydrogen solubility is computed by the equation:

$$\log S_H^L = -\frac{2760}{T} + 2.796, \quad \text{ml/100g STP} \qquad (2)$$

given in ml of hydrogen dissolved in 100 g of aluminium under standard conditions of temperature and pressure.

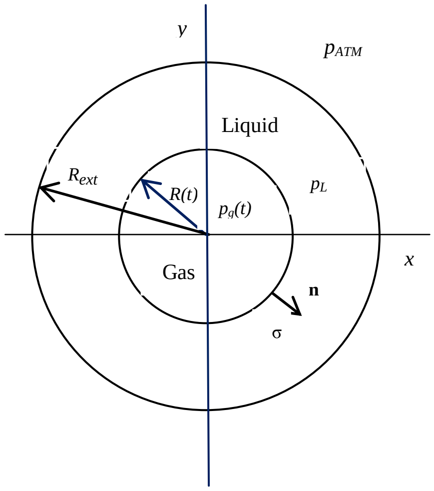

Figure 1. Schematic of a hydrogen gas bubble expanding in a 2D liquid aluminum.

In Eq. 1 the exponential term accounts for the effects of curvature according to the Gibbs-Thompson equation [4,5]. By assuming a supersaturated aluminium melt of initial hydrogen concentration $C_H > C_H^*$, hydrogen will diffuse towards the bubble and the change of the bubble radius will depend on the concentration gradient of C_H at the interface. Therefore, by applying a mass balance at the interface we may relate the change of $R(t)$ to the concentration gradient of hydrogen.

2.2 Mathematical model

Eq. 3 gives the expression used by Atwood *et al.* [4] to compute the change of $R(t)$:

$$\left(C_g - C_H^*\right)\frac{dR(t)}{dt} = D_H\left(\frac{\partial C_H}{\partial r}\right)_{r\,=\,R(t)} \qquad (3)$$

where C_g is the hydrogen concentration in the gas bubble, $\left(\frac{\partial C_H}{\partial r}\right)_{r\,=\,R(t)}$ denotes the concentration gradient at the interface and D_H is the diffusion coefficient of hydrogen in liquid aluminium. We consider only H_2 gas in the bubble and express C_g by the ideal gas equation:

$$C_g = \frac{p_g}{\Re\, T} \qquad (4)$$

where the H_2 pressure is:

$$p_g = p_L + \frac{\sigma}{R(t)} \qquad (5)$$

with p_L denoting the pressure in the liquid aluminum. Equations 1 to 5 complete the mathematical model of the mass transfer mechanism coupled to the growth and movement of a H_2 gas bubble in liquid Al. The transport of the diluted H_2 in aluminium is modeled by the Fick's law of diffusion and taking the convection of species into account. In the model we use the laminar equations of fluid dynamics and the phase field method in order to capture the interface gas-liquid. We assume the liquid to be an incompressible Newtonian fluid and represent the compressibility of the gas through a weakly-compressible model, valid for gas flows with low Mach numbers (approximately $Ma < 0.3$).

The continuity and momentum equations modeled in Comsol Multiphysics® are the following [6]:

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = 0 \qquad (6)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \bullet \nabla)\mathbf{u} = \nabla \bullet [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \\ - \frac{2\mu}{3}(\nabla \bullet \mathbf{u})\mathbf{I}] + \mathbf{F}_{\text{st}} + \mathbf{F}_{\text{ext}} + \mathbf{F} \qquad (7)$$

The evolution of the phase field function ϕ in the fixed computational region is given by the Cahn Hilliard equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \bullet \nabla \phi = \nabla \bullet \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi \qquad (8)$$

where ψ is called *help variable*, given by:

$$\psi = -\nabla \bullet \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right) \frac{\partial f_{\text{ext}}}{\partial \phi} \qquad (9)$$

In Eq. 8 the parameter ε is a measure of the interfacial thickness, γ is the mobility and λ represents the mixing energy density. λ and ε are related to the surface tension coefficient σ through the expression:

$$\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\varepsilon} \qquad (10)$$

In the momentum transport equation, the scalar magnitudes ρ and μ are the fluid density and the dynamic viscosity, respectively. On the other hand **u** is the fluid velocity, **I** is the identity tensor and the term $\mathbf{F}_{\text{st}}$ accounts for the surface tension force acting at the interface between the two fluids. $\mathbf{F}_{\text{st}}$ is implemented as a body force linked to the chemical potential G of the multiphase system through the equation:

$$\mathbf{F}_{\text{st}} = \left(G - \frac{\partial f}{\partial \phi}\right) \nabla \phi \qquad (11)$$

where $\frac{\partial f}{\partial \phi}$ is a defined source of free energy.

The force arising due to a specific source of free energy is represented by $\mathbf{F}_{\text{ext}}$ and is computed according to:

$$\mathbf{F}_{\text{ext}} = \left(\frac{\partial f}{\partial \phi}\right) \nabla \phi \qquad (12)$$

Finally **F** models other body forces of the system.

The transport mechanism of hydrogen to the bubble is modeled by the convection diffusion equation available in the Transport of Diluted Species User Interface of COMSOL Multiphysics® [7], given by Eq. 13:

$$\frac{\partial C_H}{\partial t} + \nabla \bullet \left(- D_H \nabla C_H\right) + \mathbf{u} \bullet \nabla C_H = R_H \qquad (13)$$

where R_H is a reaction rate expression for the same species. We assume that the initial concentration of hydrogen in aluminium is $C_{H,0} > C_H^*$ and fix the same value $C_{H,0}$ on the external boundary of the shell $\left(r = R_{ext}\right)$. In the model R_H is set equal to zero.

3. Solution with COMSOL Multiphysics

To simulate a hydrogen gas bubble of radius 0.01 m expanding in liquid Al, we use the values of fluid properties given in Table 1, while other parameters of the model are shown in Table 2. The hydrogen concentration in the liquid on the gas-liquid interface is given by Eq. 1, while the initial hydrogen concentration $C_{H,0}$ in the bulk liquid Al is set in the simulations. The same value of $C_{H,0}$ is assigned to the shell boundary. The diffusion coefficient D_H is also selected and set in the numerical experiments. Because the expansion of a metal foam obtained via the powder metallurgical route is of the order of a few minutes when the metal is completely melted, we use larger values for the hydrogen diffusion coefficient, which normally is very small (close to 10^{-7} m^2/s).

The model equations are numerically solved with Comsol Multiphysics® 4.3b, using the CFD Module [6] and the Chemical Reaction Engineering Module [7]. Eq.1 modeling the transport of hydrogen in aluminium is implemented only in the shell, conversely the other equations are also solved in the gas phase. The ordinary differential equation modeling the change of the bubble radius *R(t)*, as a function of the concentration gradient of C_H at the gas-liquid interface (Eq.3), is coupled to the former equations. To compute this equation we add the Global ODEs and DAEs User Interface in order to evaluate the time dependent radius and modify the density of H_2 gas in the bubble. The gas density variation causes the interface to move forward.

The computational domain is obtained by meshing the circular region with nearly $7\text{x}10^4$ triangle elements. To solve the resulting system of equations we have used the BDF time dependent solver and the MUMPS direct solver for the integration in space. The computational model was run in a PC with Intel Xenon CPU X5660, 6 core, 2.80 GHz, 48 GB RAM, 64bit and Windows 7 Operative System. The solution time is approximately of 13600 s for a simulated foaming process of 0.14 s.

4. Results and discussion

Fig. 2 shows the hydrogen concentration field in the shell at time *t*= 0.14 s, while the

Table 1: Fluid properties used in the simulations of H_2 gas bubble growth in liquid Al.

Magnitude	Symbol	Value
Gas density	ρ_G	Ideal gas
Liquid density	ρ_L	$2.4\text{x}10^3$ kg/m^3
Gas viscosity	μ_G	10^{-3} Pa·s
Liquid viscosity	μ_L	10^{-1} Pa·s
Surface tension coefficient	σ	0.9 N/m
Gas bubble radius	R_0	10^{-2} m
Liquid shell radius	R_{ext}	$5\text{x}10^{-2}$ m
Ambient pressure	p_{EXT}	101.325 KPa
Constant temperature	T	933 K
Universal ideal constant	$\Re$	8.314462 J/mol K
Molar concentration of H_2 in the bubble	C_g	given by Eq. 4
Hydrogen solubility in liquid aluminium	S_H^L	given by Eq. 2
Hydrogen concentration in the liquid on the gas-liquid interface	C_H^*	given by Eq. 1
Initial hydrogen concentration in the shell and on the boundary	$C_{H,0}$	set in the simulations
Diffusion coefficient of hydrogen in aluminium	D_H	set in the simulations

Table 2: Model parameters used in the diffuse interface model.

Magnitude	Symbol	Value
Max element size of the mesh	-	$6\text{x}10^{-4}$ m
Interface thickness	ε	$3\text{x}10^{-4}$ m
Mobility tuning parameter(*)	χ	1 m·s/kg

(*) This parameter determines the time scale of the Cahn-Hilliard diffusion and therefore governs the diffusion related time scale of the interface [6].

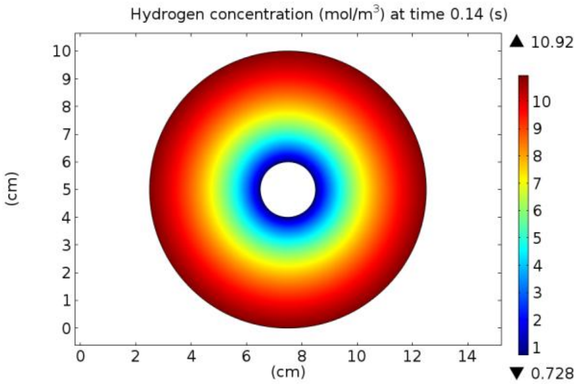

Figure 2. Values of hydrogen concentration in the shell of aluminium melt ($C_{H,0} = 15xC^*_H$, $D_H = 10^{-3}$ m^2/s).

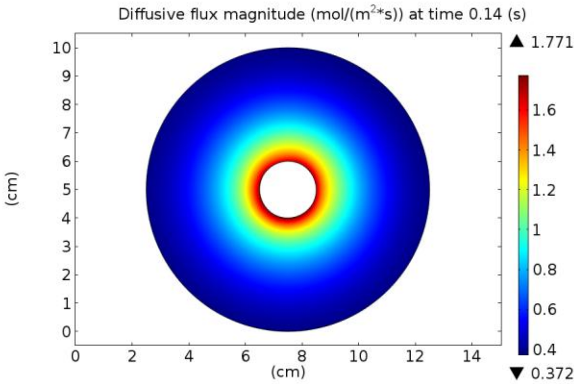

Figure 3. Values of the diffusive flux magnitude of hydrogen in the shell of aluminium melt ($C_{H,0} = 15x C^*_H$, $D_H = 10^{-3}$ m^2/s).

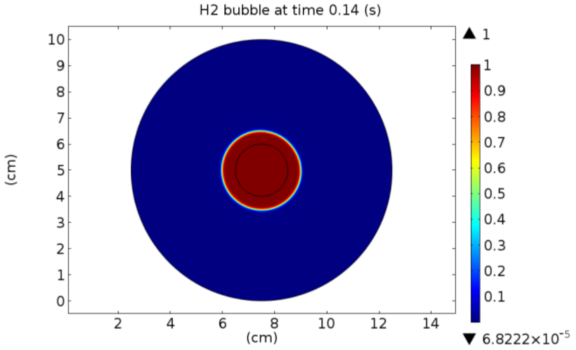

Figure 4. Position of the H_2 gas-liquid aluminium interface after t = 0.14 s ($C_{H,0} = 15xC^*_H$, $D_H = 10^{-3}$ m^2/s).

diffusive flux magnitude of hydrogen is given in Fig. 3. We observe the usual concentric pattern indicating the radial transport of the hydrogen from the peripheral region to the bubble. As the convection diffusion equation was solved only in the shell, the central region is void. For the same time, Fig. 4 gives the position of the gas liquid interface, from which it is possible to get the fast expansion of the bubble. This is confirmed by the plot of Fig. 5 which shows the change of the bubble time dependent radius, given by Eq. 3.

The significant motion acquired by the two fluids is depicted in Fig. 6. Here it is evident the characteristic radial pattern of the expansion flow, where the magnitude of the liquid velocity decreases with increasing distance from the gas–liquid interface. Finally, Fig. 7 gives the pressure field in the system.

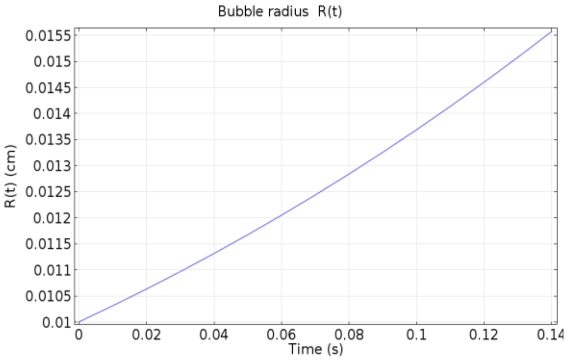

Figure 5. Plot of the gas bubble time dependent radius ($C_{H,0} = 15xC^*_H$, $D_H = 10^{-3}$ m^2/s).

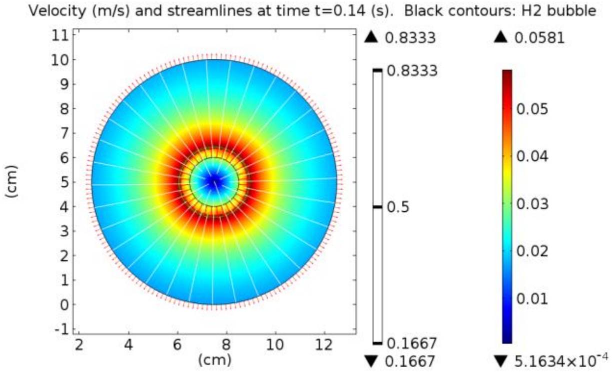

Figure 6. Plot of velocity field and streamlines in H_2 bubble and aluminium shell; position of the gas-liquid interface is given by the contours ($C_{H,0} = 15xC^*_H$, $D_H = 10^{-3}$ m^2/s).

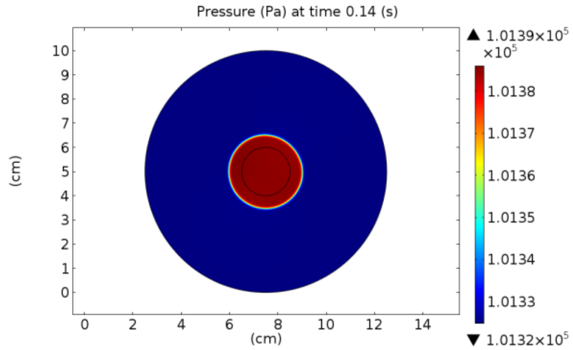

Figure 7. Plot of the pressure field in H_2 bubble and aluminium shell after t =0.14 s ($C_{H,0}$ = 15xC^*_H, $D_H = 10^{-3}$ m^2/s).

5. Conclusions

We have proposed a computational model considering mass transfer phenomena coupled to the growth and motion of gas bubbles in the liquid metal. The diffusion of the gas in the liquid has been simulated by applying the Fick's law and convective transport. The equilibrium concentration at the gas-liquid interface has been modelled by the Sievert's law with surface tension effects included. The numerical results of the simulation has shown that the computational model, using the phase field method for capturing the phase interface, can be effective. The computations simulate satisfactorily mass transfer, bubble expansion, interface movement and fluid flow. In this way other physical mechanisms of foaming could be included in a future more comprehensive model.

6. References

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