Diffuse Interface Models for Metal Foams

B. Chinè[*1,4], M. Monno[2,4], E. Repossi[3], M. Verani[3]
[1]Instituto Tecnològico de Costa Rica, Cartago, Costa Rica, [2]Politecnico di Milano, Dipartimento di Meccanica, Milano, Italy, [3]Politecnico di Milano, MOX-Dipartimento di Matematica, Milano, Italy, [4] Laboratorio MUSP, Macchine Utensili e Sistemi di Produzione, Piacenza, Italy
*Corresponding author: ITCR, School of Materials Science and Engineering, P.O. Box 159-7050, Cartago, Costa Rica, bchine@itcr.ac.cr; bruno.chine@musp.it

Abstract: Metal foams are cellular material of considerable interest because of their potential applications in many fields of the industry. To produce a metal foam, a well-established process is starting with a molten metal, then introducing blowing agents to create gas bubbles inside the metal. In this work we use COMSOL Multiphysics® and apply the diffuse interface methods of the phase field technique, in order to model the properties of metal foams and describe the movement of the gas-liquid interfaces. A metal foam represented by a number of bubbles moving in a laminar flow is modeled and simulated. Surface tension effects are considered and repulsive forces between neighboring bubbles are expressed through the disjoining pressure. The numerical results show that diffuse interface methods are effective to model this kind of complex phenomena and that fundamental mechanisms due to surface tension effects and disjoining pressure are well reproduced.

Keywords: metal foams, multi-phase flow, phase field, disjoining pressure.

1. Introduction

Metal foams are novel cellular materials with interesting potential applications in many fields of the industry. These materials can offer attractive combinations of low density, high stiffness to weight ratio, good energy absorption and vibration damping capacity. There are many technologies by which a foamed mechanical component can be produced [1]. A well-established process is starting with a molten metal, then introducing solid particles as blowing agents in order to create gas bubbles inside the metal, and finally filling a mold cavity. The successive solidification of the resulting system will give the characteristic cellular structure of the foamed component, represented by many voids in a metallic matrix. The foaming process of a metal is a complex operation which needs to be closely controlled in order to guarantee the wanted properties, by avoiding the formation of defects in the structure of the material. During the foaming process, solid particles and gas bubbles are transported in the liquid metal with important physical interactions arising between the different phases. Bubbles will interact between them, modifying their geometry and volume due to the pressure and surface tension effects. Also, it has been shown how solid particles get confined into bubble walls during foam expansion where they generate a repulsive force (o disjoining pressure) against further cell thinning [2]. Furthermore it is necessary to introduce a repulsive force in order to avoid no physical merging phenomena in the computation of foaming. Thus, the modeling of short-range molecular forces, and in particular of the repulsive forces between bubbles, might enable us to control the coalescence in the foaming process.

The laws of fluid mechanics govern the behavior of this physical system with the simultaneous presence of three phases, the liquid metal, the gas bubbles and the solid particles. On the other hand, a mayor understanding of the foaming process could be obtained if we are able to describe and then simulate the main phenomena occurring during the flowing of foam in a mold. In this work we use COMSOL Multiphysics® version 4.3b and apply the diffuse interface methods of the phase field technique available in the CFD module, in order to model the properties of metal foams and describe the movement of the gas-liquid interfaces. To analyze a practical case, a foam represented by a number of H_2 gas bubbles inside liquid aluminium is chosen as test and then simulated. We consider that the two-phase physical system is moving in a cavity under conditions of laminar flow. In the paper the description of the model and the resulting equations are given in Section 2. Section 3 deals with the use of Comsol Multiphisics® and the strategy need to obtain a numerical solution of the problem. Finally the computational results are presented in Section 4 and the conclusions in Section 5.

2. Model description and equations

The next sections give a description of the diffuse interface model, the equations governing the motion of a system of gas bubbles and liquid metal in a rectangular cavity and the assumptions for the modeling of the disjoining pressure.

2.1 Physical model

Let us to consider a number of gas bubbles (H_2) transported by liquid metal (Al) in a rectangular cavity, during the processing of metal foams from a molten metal. The problem is assumed two dimensional, no heat transfer and mass diffusion are taken into account. Gravity forces are not considered, that is the 2D cavity is set horizontally. The system is then 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.

Fig. 1 shows a schematic of a metal foam represented by H_2 circular gas bubbles in liquid Al. The bubbles have the same radius and pressure, respectively equal to R_0 and $p_{G,0}$. The gas-liquid interface is a free surface with uniform surface tension coefficient σ, κ represents the local curvature and **n** the unit normal to the interface. With the system at rest and by calling with p_L, the liquid pressure, the Laplace's equation states that the stress balance at the surface of a circular bubble of radius R_0 is equal to the capillary pressure:

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

with

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

When the fluids are in motion, the normal stresses boundary condition (1) at the interface is completed by also considering the projection of the viscous stress tensor in both the normal and the tangential direction. During the flow, a gas bubble could be pressed by other bubbles or against a solid wall, flattening the fluid films close to the interfaces. By assuming a homogeneous pressure in the bubble, Eq. 1 would give a larger pressure in the flattened liquid film ($\kappa = 1/\infty$) compared to the pressure in other areas where $\kappa = 1/R_0$. Hence, the liquid metal would be suctioned from the capillary films to the borders of the foam (Plateau borders) [2,3]. Then a film may collapse, causing the merging of the interfaces. The drainage of the intermediate thin films, induced by the capillary pressure, is slowed and eventually prevented when interactions between the film surfaces come into play. These effects are represented by a pressure, the disjoining pressure $\Pi(h)$, which results from the attractive and repulsive molecular forces in the thin film. In metal foaming process $\Pi(h)$ represents a stabilization effect suppressing the driving force for film thinning [2]. In our physical model, once the film *h* between the bubbles became sufficiently small, we take into account the disjoining pressure and rewrite Eq. 1 as:

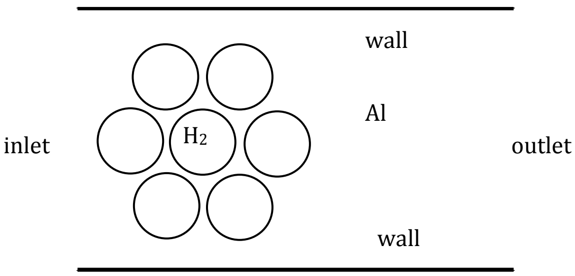

Figure 1. Schematic of a metal foam represented by hydrogen gas bubbles and liquid aluminium flowing in a rectangular cavity.

$$p_{G,0} - p_L = \sigma \kappa + \Pi(h) \qquad (3)$$

2.2 Governing equations

To model and simulate numerically the isothermal flow of gas bubbles embedded in a metal liquid moving in a cavity, we use the classical equations of fluid dynamics which are coupled to the phase field method for capturing the gas-liquid interfaces. We assume the liquid to be an incompressible Newtonian fluid and simplify the model by neglecting the compressibility of the gas bubbles. The flow is considered laminar because the Reynolds number is small. In metal foams processing, the effective viscosity of the melted fluid surrounding the gas bubble depends, other than on the temperature, on the presence of solid particles next to the bubble walls. More exactly, the viscosity of the surrounding fluid is almost one –two orders of magnitude higher than the aluminium viscosity. Gergely and Cline [4] used a liquid viscosity of 0.4 Pa·s for a liquid aluminium with solid particles, when simulating a metal foam obtained via the melted route. By considering the height of the cavity *H* as the characteristic length, the inlet velocity *U* of $5x10^{-2}$ m/s and the cinematic viscosity of the liquid $\upsilon_L = \frac{\mu_L}{\rho_L} = \frac{0.1\,\mathrm{Pa{\cdot}s}}{2.4x10^3\,\mathrm{kg\,m^{-3}}}$ equal approximately to $4.2x10^{-5}$ $\mathrm{m^2/s}$, it follows:

$$\mathrm{Re} = \frac{U_L\,H}{\upsilon_L} = 144 \tag{4}$$

with a simulated *H* equal to $12x10^{-2}$ m. Then for both the fluids, the coupled partial differential equations of the model are (Two Phase Flow, Phase Field Interface, [5]):

$$\frac{\partial\rho}{\partial t} + \nabla\bullet(\rho\mathbf{u}) = 0 \tag{5}$$

$$\rho\frac{\partial\mathbf{u}}{\partial t} + \rho(\mathbf{u}\bullet\nabla)\mathbf{u} = \nabla\bullet[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] \\ + \mathbf{F}_{\mathrm{st}} + \mathbf{F}_{\mathrm{ext}} + \mathbf{F} \tag{6}$$

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

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\bullet\nabla\phi = \nabla\bullet\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi \tag{7}$$

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

$$\psi = -\nabla\bullet\varepsilon^2\nabla\phi + (\phi^2-1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right)\frac{\partial f_{\mathrm{ext}}}{\partial\phi} \tag{8}$$

The phase field variable is $\phi = +1$ in one phase and is $\phi = -1$ in the other phase, with $\phi = 0$ describing the centre of the interface. Furthermore 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 next expression:

$$\sigma = \frac{2\sqrt{2}}{3}\frac{\lambda}{\varepsilon} \tag{9}$$

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

$$\mathbf{F}_{\mathrm{st}} = \left(G - \frac{\partial f}{\partial\phi}\right)\nabla\phi \tag{10}$$

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

On the other hand the force arising due to a specific source of free energy is represented by $\mathbf{F}_{\mathrm{ext}}$ and is computed according to:

$$\mathbf{F}_{\mathrm{ext}} = \left(\frac{\partial f}{\partial\phi}\right)\nabla\phi \tag{11}$$

Finally $\mathbf{F}$ models other body forces of the system.

2.3 Disjoining pressure

In our model the disjoining pressure is set by using Eq. 11. We follow the same method of Yue *et al.* [6] who simulated drop coalescences via diffuse-interface methods and explored the representation of short-range molecular forces in the diffuse-interface framework. Yue *et al.* obtained the counterpart of the disjoining pressure in this representation by considering a normal force balance in a thin liquid film sandwiched between semi-infinite domains of another fluid. They derived the next expression of *Π:*

$$\Pi(\phi) = -\frac{\lambda}{4\varepsilon^2}(\phi_0^2 - 1)^2 \tag{12}$$

where ϕ_0 is:

$$\phi_0 = -\tanh\left(\frac{h}{2\sqrt{2}\,\varepsilon}\right) \qquad (13)$$

Yue *et al.* set the value of $\phi = +1$ for two approaching drop phases and $\phi = -1$ for the bulk liquid. Hence, in a thin film the phase field variable will be equal to $\phi_0 \; > -1$, which represents the value of ϕ when the size of h is comparable to the size of ε. In the case of Eq. 12 the disjoining pressure is negative indicating attractive forces between the two interfaces. In the present model we consider a positive disjoining pressure, in order to model the repulsive forces between the gas bubbles of the metal foam. In Comsol Multiphysics® the disjoining pressure is introduced through Eq. 11 representing an external body force.

On the other hand, the phase field function is the same for all the gas regions, while Eq. 12 has to be applied only close to those interfaces which are getting closer. We can overcome the problem by assigning a marker c_i $(c_i = 1)$ to each bubble i and moving the marker like a species in the system, with the same velocity field of the corresponding bubble. The mechanism is modeled by the convection diffusion equation available in the Transport of Diluted Species User Interface of COMSOL Multiphysics® [7], given by Eq. 14:

$$\frac{\partial c_i}{\partial t} + \nabla \bullet \left(-D_i \nabla c_i\right) + \mathbf{u} \bullet \nabla c_i = R_i \qquad (14)$$

where D_i denotes the diffusion coefficient of the species c_i and R_i is a reaction rate expression for the same species. In the model R_i is set equal to zero and diffusion of the markers is avoided by assuming a very small value for D_i. Then, when the concentration of two markers is greater than a set value, the corresponding bubbles are considered to form a thin film and the disjoining pressure is activated by means of Eq. 12.

3. Solution with COMSOL Multiphysics

Real values of densities and viscosities for the gas and the liquid metal are used. To simulate a metal foam represented by hydrogen bubbles and liquid aluminium moving in a cavity, we use the fluid properties of Table 1. Table 2 gives the parameters of the diffuse interface model. The initial hydrogen density computed by the ideal gas law is approximately 0.026 kg/m^3 and the constant hydrogen dynamic viscosity is 10^{-3} Pa·s. The density of liquid aluminium is 2.4x10^3 kg/m^3 while its dynamic viscosity is set equal to 10^{-1} Pa·s. Surface tension effects are considered together with repulsive forces between neighboring bubble, due to the

Table 1: Properties of hydrogen gas bubbles and liquid aluminum used in the simulations.

Magnitude	Symbol	Value
Gas density	ρ_G	Ideal gas
Liquid density	ρ_L	2.4x10^3 kg/m^3
Gas dynamic viscosity	μ_G	10^{-3} Pa·s
Liquid dynamic viscosity	μ_L	10^{-1} Pa·s
Surface tension coefficient	σ	0.9 N/m
Radius of the gas bubbles	R_0	1.5x10^{-2} m
Number of gas bubbles	N	7
Height of the cavity	H	1.2x10^{-1} m
Length of the cavity	L	2.0x10^{-1} m
Inlet velocity of the metal foam	U	5x10^{-2} m/s
Ambient pressure	p_{EXT}	0 Pa
Constant temperature	T	933 K
Diffusion coefficient for species C_i	D_i	10^{-30} m^2/s

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

Magnitude	Symbol	Value
Max element size of the mesh	-	10^{-3} m
Interface thickness	ε	5x10^{-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 [5].

disjoning pressure. Without gravity forces surface tension and viscosity are in competition with each other, becoming important at small scales. We can estimate the relative strength of the two properties by using the Capillary number $Ca = \frac{\mu U}{\sigma}$. Considering the highest dynamic viscosity in the system, Ca is equal approximately to 5.6×10^{-3} denoting that interfacial tension are strong compared to viscous stresses.

The model equations are numerically solved with Comsol Multiphysics® 4.3b, using the CFD Module [5] and the Chemical Reaction Engineering Module [7]. The computational domain is obtained by meshing the rectangular cavity with nearly 4×10^4 triangle elements. The velocity of the foam is fixed on the inlet, slip conditions are applied on the walls and a null pressure with no viscous stress is set on the outlet of the cavity. The resulting system of equations is computed by using 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 13800 s for a metal foam with 7 bubbles and a simulated foaming process of 0.50 s.

4. Results and discussion

We begin our simulations considering a first case in which the disjoining pressure is not considered. Figs. 2 and 3 show the volume fraction of hydrogen after the foam flows in the cavity for t = 0.06 s and t = 0.012 s, respectively. Without repulsive forces the bubbles start to merge very quickly due to the capillary pressure. Fig. 4 represents the pressure field in the cavity, denoting higher values in the films, especially in proximity of the coalescing areas. A different situation is shown in Fig. 5 when the disjoining pressure $\Pi(h)$ balances the capillary pressure (see Eq. 3) in the films. In this case the drainage of the intermediate thin films, induced by the capillary pressure is slowed and prevented. At the same t = 0.012 s the H_2 gas bubbles are stable and convected by the fluid in the cavity without premature coalescing phenomena. Fig. 6 draws the body force due to the disjoining pressure at t =0.12 s which are responsible for establishing repulsive forces between the bubbles interfaces. Finally Fig. 7 gives the pressure field in the cavity at the same time. Comparing with Fig. 6, we observe that inside the metal foam the pressure values are now smaller emphasizing the stabilization

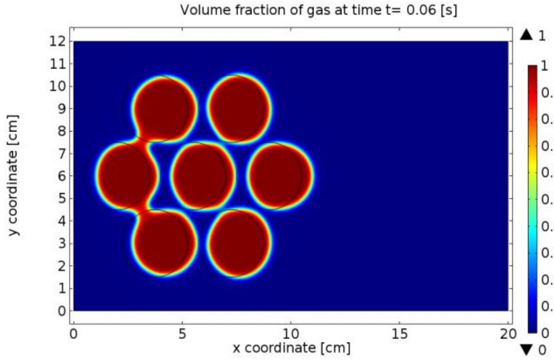

Figure 2. Volume fraction of H_2 in a metal foam flowing in a cavity after t =0.06 s with disjoining pressure equal to zero.

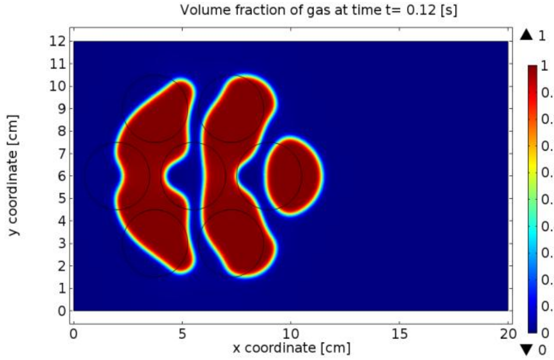

Figure 3. Volume fraction of H_2 in a metal foam flowing in a cavity after t =0.12 s with disjoining pressure equal to zero.

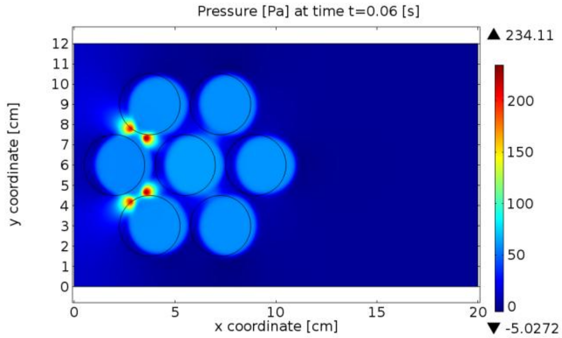

Figure 4. Pressure field in a metal foam flowing in a cavity after t =0.12 s with disjoining pressure equal to zero.

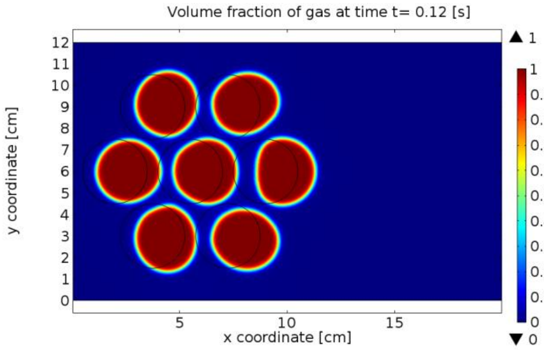

Figure 5. Volume fraction of H_2 a t =0.12 s when the disjoining pressure sets a repulsive stabilization effect between the bubbles interfaces.

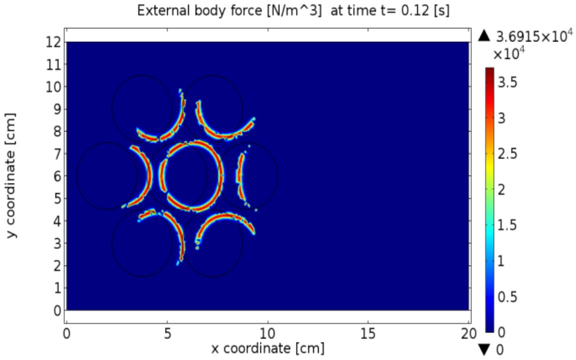

Figure 6. Body force due to the disjoining pressure at t =0.12 s giving repulsive forces between the bubbles interfaces.

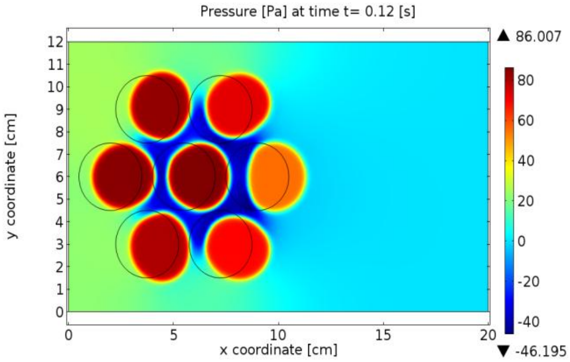

Figure 7. Pressure field in a metal foam flowing in a cavity after t =0.12 s when the disjoining pressure sets a repulsive stabilization effect between the bubbles interfaces.

effect of the disjoining pressure.

5. Conclusions

A metal foam represented by H_2 gas bubbles and liquid aluminium moving in a laminar flow has been modeled and simulated. Surface tension effects have been considered and repulsive forces between neighboring bubbles have been expressed through the disjoining pressure. The model uses a formulation of the disjoining pressure in the framework of the phase field method. The numerical results show that diffuse interface methods are effective to model this kind of complex phenomena and that fundamental mechanisms due to surface tension effects and disjoining pressure are well reproduced. The above results are encouraging for our under way researches [8] in the modeling of metal foaming processes.

6. References

[1] J. Banhart, Light-metal foams-History of innovation and technological challenges, *Advanced Engineering Materials*, **15**, 82-111. doi: 10.1002/adem.201200217 (2012).

[2] C. Körner, *Integral Foam Molding of Light Metals*, 124. Springer-Verlag, Berlin Heidelberg (2008).

[3] D. Weaire D. and S. Hutzler S., *The physics of foams*, Oxford University Press, Oxford (1999).

[4] V. Gergely and T.W. Clyne, Drainage in standing liquid metal foams: modeling and experimental observations, *Acta Materialia*, **52**, 3047-3058 (2004).

[5] Comsol AB, Comsol Multiphysics-CFD Module, *User's Guide*, **Version 4.3b,** (2013).

[6] P. Yue, J.J. Feng, C. Liu and J. Shen, Diffuse-interface simulations of drop coalescence and retraction in viscoelastic fluids, *Journal of Non-Newtonian Fluid Mechanics*, **129**, 163-176 (2005).

[7] Comsol AB, Comsol Multiphysics-Chemical Reaction Engineering Module, *User's Guide*, **Version 4.3b,** (2013).

[8] B. Chinè and M. Monno, Multiphysics modeling of a metal foam, *Proceedings of 2012 European Comsol Conference*, Milan, (2012).

7. Acknowledgements

One author (B. Chinè) gratefully acknowledges the financial aid provided by the Vicerrectoria de Docencia and Vicerrectoria de Investigaciòn y Extensiòn of the Instituto Tecnològico de Costa Rica.