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A DAMAGE MODEL TO ASSESS THE INITIATION OF RUPTURE OF LIQUID-CORE CAPSULES UNDER SIMPLE SHEAR FLOW

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Abstract

The present study aims at investigating the damage of capsules composed of a liquid core protected by a deformable solid envelope. When placed in suspension and subjected to an external flow, capsules are subjected to mechanical sollicitations which can lead to their rupture. A model of isotropic damage has been developed and implemented in a finite element model solving for the deformation of the capsule. It is integrated in a fluid-structure solver coupling the boundary integral method to the finite element method. We study the influence that various criteria of damage initiation have on the rupture kinetics for a capsule under simple shear flow.

1. Introduction

Capsules consisting of a liquid droplet enclosed by a thin elastic membrane are commonly encountered in nature in the form of cells, eggs and vesicles, and in numerous industrial processes. The protection and controlled release of active agents is of great importance for diverse applications in the food, cosmetic, bioengineering and medical engineering industry, among others. In medicine, encapsulation has opened the way to new treatment techniques like targeted drug/gene therapy [1]. New-generation bioartificial organs/cells are being developed, for instance, by encapsulating islets of Langerhans to treat diabetic patients [11] or hemoglobin to create artificial blood [7].

But when placed in suspension, capsules are subjected to intense solicitations from the surrounding flow, which may cause the mechanical degradation of the membrane. *In vivo* tests have shown that artificial blood cells could be easily damaged in circulation depending on the particle shape and deformability [7]: this example illustrates the importance to control rupture. Depending on the applications, capsule damage is to be prevented to preserve the inner substance, or, on the contrary, fostered and directed to allow a targeted release of the encapsulated substance. This necessitates to gain a good understanding of the capsule behavior under low-inertia flow conditions and of the parameters that control the initiation of rupture.

Early experimental studies, conducted on capsules in simple shear flows, showed the possibility of wrinkling formation at low shear rates [12] and of capsule burst at high shear [2]. The results by Chang and Olbricht indicated an initiation of rupture from one of the major axis tips of the ellipsoidal capsule shape. The crack then propagated in the plane containing the major axis that was perpendicular to the shear plane. Since then, the only studies that investigated the onset of rupture have been experimental [3, 5].

The objective of the study is to develop a damage model of a microcapsule subjected to a simple shear flow in order to assess the initiation of rupture of liquid-core capsules. Continuum Damage Mechanics (CDM), which is constructed on the basis of thermodynamics of irreversible processes, offers a theoretical framework to model structural damage. An overall presentation of CDM was recently published by Lemaître et Desmorat [6]. Contrary to crack propagation models, which represent the inherent geometrical discontinuity, the microdiscontinuities are not geometrically modeled in CDM. The local average damage state due to the microdiscontinuities is instead represented by a continuum variable: the damage variable. We propose to incorporate, for the first time, a CDM model into a fluid-structure interaction framework, in order to investigate the time-evolution of damage as the capsule deforms under flow.

2. Methods

We consider a spherical microcapsule of radius a enclosed in an elastic envelope of very small thickness with respect to its radius. The capsule is thus modeled as a two-dimensional incompressible membrane with surface shear elastic modulus G_s. It is placed at the center of an infinite shear flow of shear rate $\dot{\gamma}$, the unperturbed velocity field being $\underline{v}^{\infty}(\underline{x}) = \dot{\gamma} z \underline{e}_x$. The inner and outer fluids are the same incompressible Newtonian fluids of dynamic viscosity μ and density ρ. Gravitational and inertial effects being negligible due to the microscopic capsule size, the fluid-structure interaction problem is governed by only one non-dimensional parameter: the capillary number $Ca = \mu\dot{\gamma}a/G_s$.

2.1. Formulation of the problem

Internal and external flows

Inertial effects being neglected, the fluid problem is governed by the Stokes equations. At a given point $\underline{x}$ of the membrane S, the boundary integral formulation of the Stokes equations gives the relation between the velocity $\underline{v}$ and the stress $\underline{\underline{\sigma}}$ [9]:

$$\forall \underline{x} \in S, \quad \underline{v}(\underline{x}) = \underline{v}^{\infty}(\underline{x}) - \frac{1}{8\pi\mu} \int_S \underline{\underline{G}}(\underline{x}, \underline{y}) \cdot [\underline{\underline{\sigma}}] \cdot \underline{n}(\underline{y}) \, dS_{\underline{y}}, \tag{1}$$

where $\underline{\underline{G}}$ is the Oseen-Burgers tensor, $\underline{n}$ is the unit vector normal to S pointing to the external fluid and $[\underline{\underline{\sigma}}] \cdot \underline{n} = (\underline{\underline{\sigma}}_{ext} - \underline{\underline{\sigma}}_{int}) \cdot \underline{n}$ is the stress jump across the membrane.

Wall mechanics

The mechanical equilibrium of the membrane is written in terms of the tension $\underline{\underline{T}}$, corresponding to the resultant of the homogeneous stress $\underline{\underline{\sigma}}$ over the thickness. The principle of virtual work gives the relation between the tension $\underline{\underline{T}}$ and the external load $\underline{q}$:

$$\int_S \underline{\hat{u}} \cdot \underline{q} \, dS = \int_S \underline{\underline{T}} : \underline{\underline{\varepsilon}}(\underline{\hat{u}}) \, dS, \tag{2}$$

where $\underline{\hat{u}}$ is the virtual displacement and $\underline{\underline{\varepsilon}}(\underline{\hat{u}})$ is the symmetric part of $\underline{\underline{P_s}}.\underline{\nabla}\hat{u}$, $\underline{\underline{P_s}}$ and $\underline{\nabla}\hat{u}$ being the projector on S and the gradient of $\hat{u}$, respectively. Boundary conditions on the membrane are given in terms of external loading such that $\underline{q} = [\underline{\underline{\sigma}}] \cdot \underline{n}$.
In terms of kinematics, the no-slip condition holds and gives the relation between the velocity and the position of the corresponding point $\underline{x}_s$ of the membrane:

$$\underline{v} = \frac{d\underline{x}_s}{dt}. \tag{3}$$

In order to account for the progressive degradation of the membrane, we follow the standard framework of CDM [6]. The state variables of the model are the Green-Lagrange strain tensor $\underline{\underline{e_s}}$ and the damage variable d, chosen to be a scalar that ranges from 0 (sound material) to 1 (mesocrack initiation). The associated variables are the second Piola-Kirchhoff tension tensor $\underline{\underline{\pi_s}}$ and the specific elastic energy release rate Y, respectively. We consider isothermal and quasi-static transformations. Therefore, the specific free energy ϕ, defined on the initial configuration, is chosen to be:

$$\phi(\underline{\underline{e_s}}, d) = (1-d)\phi_{NH}(\underline{\underline{e_s}}), \tag{4}$$

where ϕ_{NH} is the specific free energy for a Neo-Hookean material:

$$\phi_{NH} = \frac{G_s}{2}(I_1 - 1 + \frac{1}{I_2 + 1}), \tag{5}$$

I_1 and I_2 being the invariants of $\underline{\underline{e_s}}$. The expression of the damage criterion f is chosen from the model developed by Marigo for quasi-brittle damage [8]:

$$f = Y - \kappa(d). \tag{6}$$

In this work, κ is chosen as a function of the two parameters Y_D and Y_C, respectively the damage threshold and the hardening modulus, in the form: $\kappa(d) = Y_D + Y_C d$. The damage evolution law, deriving from the normality law and consistency condition, writes:

$$\begin{cases} f < 0 \implies \dot{d} = 0 \\ f = 0 \implies d = \kappa^{-1}(Y) \end{cases} \tag{7}$$

where κ^{-1} designates the reciprocal of the bijection κ. For the purpose of the sensitivity analysis carried out in this work, we introduce the two non-dimensional parameters $\tilde{Y}_D = \frac{Y_D}{G_s}$ and $\tilde{Y}_C = \frac{Y_C}{G_s}$.

2.2. Numerical method

For a given deformed state of the membrane, the solid problem is solved with the Finite Element Method. At the material level, the evolution of the damage variable d (see equation (7)) is determined for each integration point using a return mapping algorithm [10]. On that basis, the external loading $\underline{q}$ is computed by solving the global problem (2).

For the fluid part, the velocity is computed explicitly at each node from equation (1), where $[\underline{\underline{\sigma}}] \cdot \underline{n} = \underline{q}$ results from equilibrium of the membrane. In order to handle the singularity of the tensor $\underline{\underline{G}}$ at the node $\underline{x}$ where the velocity has to be computed, polar coordinates centered on $\underline{x}$ are considered.

The same mesh is shared by the fluid and the solid problems. It contains 1280 quadratic triangular elements and 2562 nodes. It is constructed on the initially spherical shape (Figure 1a). We conduct a Lagrangian tracking of the nodes.

We follow the method proposed by Walter *et al.* [13] to couple the Finite Element Method with the Boundary Integral Method, and integrate equation (3) with a first-order explicit Euler scheme.

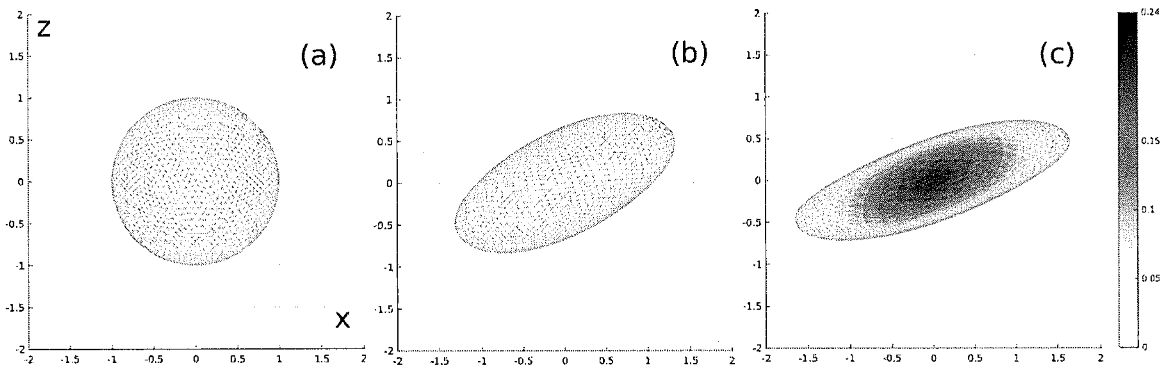

Figure 1: Typical 3D distribution of the damage state within the membrane of the capsule, which is represented with its mesh: (a) in the initial configuration, (b) at $Ca < Ca_C$ and (c) at $Ca_C < Ca < Ca_L$.

3. Results

The objective of this work is to assess the degradation process of the membrane leading to the initiation of rupture and to determine the influencing parameters. For a given set of the material parameters $\tilde{Y}_D$ and

$\tilde{Y}_C$, we are interested in determining the capillary numbers CaC and CaL, which respectively correspond to the onset of damage (critical value of Ca) and the rupture initiation (limit value of Ca). These capillary numbers depend on the material parameters $\tilde{Y}_D$ and $\tilde{Y}_C$. If $Ca < Ca_C$, the capsule is not damaged, and we recover the result presented in previous studies [4, 13]. The capsule elongates, having an ellipsoid-like shape whose major axis is contained in the shear plane. As the length of the major axis increases, the angle of the major axis to $\underline{e}_x$ reduces. The capsule finally reaches a steady shape and the membrane rotates around the vorticity axis $\underline{e}_y$ (Figure 1b). If $Ca_C < Ca < Ca_L$, while the length of the major axis increases and the angle of the major axis to $\underline{e}_x$ reduces, damage initiates from the two poles of the membrane crossing the vorticity axis $\underline{e}_y$. After damage initiation, two symmetric disjoint damaged areas, corresponding to areas where $d > 0$, develop around the two poles. As the capsule elongates, the two damaged areas spread, the maximum damage value increasing at the two poles till the membrane reaches the steady shape (Figure 1c). If $Ca > Ca_L$, the development of damage is similar to the previous case during the transitory regime, but the damage reaches the limit value $d = 1$ at the two poles. Therefore, the damage model indicates that the rupture initiates at the two poles located on the vorticity axis.
This work demonstrates that the chosen fluid-structure interaction strategy coupled with a damage model is capable of predicting the progressive degradation of the membrane till the onset of rupture.

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