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#### MODELLING OF DAMAGE AND STRAIN LOCALIZATION OF A CAPSULE IN FLOW<sup>†</sup>

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### **INTRODUCTION**

Capsules, which consist of a droplet surrounded by a thin elastic membrane, offer promising biomedical applications for the controlled release of active substances. However, one limitation comes from the lack of model of damage/rupture of capsules in flow. Recently, we developed a fluid-structure interaction (FSI) numerical model of a capsule in flow accounting for the diffuse damage mechanisms in the membrane [1]. The aim of the present work is to extend this model to take into account the subsequent phenomenon of strain localization, corresponding to the concentration of strain and damage in zones of very small thickness over the membrane. These localization zones are precursors of the onset of a crack. In order to take into account the effect of these very localized phenomena on the material response of the capsule wall, we follow a multi-scale approach based on the Embedded Finite Element method.

#### MODEL AND NUMERICAL METHOD

#### Macro-scale FSI problem

We consider an initially spherical liquid-core capsule surrounded by an elastic wall modeled as a twodimensional membrane S. The capsule is immersed in a simple shear flow. The internal and external flows are governed by the Stokes equations which are reformulated using a boundary integral method [1]. The membrane is in equilibrium at each instant. Therefore, the principle of virtual work gives a relation between the internal first Piola-Kirchhoff tension tensor P of the membrane and the external load vector q on the membrane:

for any virtual displacement 
$$\hat{\boldsymbol{w}}$$
,  $\int_{S_0} \nabla_s^0 \hat{\boldsymbol{w}} : \boldsymbol{P} \, \mathrm{d}S_0 = \int_S \hat{\boldsymbol{w}} \cdot \boldsymbol{q} \, \mathrm{d}S$ , (1)

where  $S_0$  is the reference configuration of S, and  $\nabla_s^0 \hat{w}$  is the surface gradient of  $\hat{w}$  over  $S_0$ . The motions of the fluids and the membrane are coupled by imposing the continuity of the velocities and stresses over S. The FSI problem is governed by the capillary number Ca (ratio of the fluid viscous forces to the membrane forces).

#### Micro-scale material problem

To take into account localized phenomena while computing the tensions P (eq. (1)), the deformation field is enriched locally. Following the strong discontinuity approach [2], the localization zones are represented at the micro-scale as lines  $\Gamma_0$  on which the membrane displacements are discontinuous. A discontinuity  $\Gamma_0$  affects the strains of the material points located in a neighbourhood  $S_{\mu} \subset S_0$  such that the micro-scale membrane displacement field in  $S_{\mu}$  is decomposed as  $u_{\mu} = u + M[[u]]$ , where u is the continuous membrane macroscale displacement associated with S, the vector [[u]] is the displacement jump on  $\Gamma_0$ , and the function M is

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discontinuous on  $\Gamma_0$ . The jump  $[\![u]\!]$  is determined from the equilibrium equation of a discontinuity:

$$t_{\Gamma} = P^+ \cdot N = P^- \cdot N, \qquad (2)$$

where  $t_{\Gamma}$  is the nominal traction vector acting on  $\Gamma_0$ ,  $P^+$  and  $P^-$  are the values of P on both sides of  $\Gamma_0$ , and N is the unit vector perpendicular to  $\Gamma_0$  on  $S_0$ . The local problem is closed using the constitutive laws of the bulk and discontinuity. For the material points of the bulk  $(S_0 \setminus \Gamma_0)$  it is the one associated with the model given in [1], which takes into account diffuse damage through the damage variable d, chosen as a scalar ranging from 0 (sound material) to the threshold  $d_c (\leq 1)$  corresponding to the introduction of a discontinuity  $\Gamma_0$  (see [1] for more details). The constitutive behaviour of the discontinuities is given by a brittle cohesive law relating the traction vector  $t_{\Gamma}$  to the displacement jump  $[\![u]\!]$ .

#### Numerical method

We perform a Lagrangian tracking of the membrane. At the beginning of a given time step, the current configuration of the membrane is known. We start by solving the solid problem using the finite element method. First, we solve the local equilibrium (eq. (2)) to determine the displacement jumps and compute the tensions. Then, we solve the global equilibrium (eq. (1)) to find the external load at the nodes. Next, we solve the fluid problem by computing the velocity of the fluids at the nodes using the boundary integral formulation. Finally, the velocity is explicitly integrated to update the position of the nodes for the next time step.

#### RESULTS

We have studied the damage and rupture mechanisms of a capsule as a function of the value of Ca for fixed values of the material parameters. Damage occurs when Ca is greater than a critical value  $Ca_c$ , and a larger threshold value  $Ca_h$  of Ca delimits two failure modes. For the first failure mode ( $Ca_c \leq Ca < Ca_h$ ), damage develops on the flanks of the capsule around the tip of the vorticity axis while the capsule elongates, and damage leads to the initiation of rupture when Ca is larger than a limit value  $Ca_\ell$ . If  $Ca < Ca_\ell$ , the capsule reaches a steady state of damage. For  $Ca_\ell \leq Ca < Ca_h$ , rupture initiates when  $d = d_c$  at the tips of the vorticity axis and the two cracks formed by the discontinuities then propagate perpendicularly to the direction of capsule elongates, and rupture initiates when  $d = d_c$  at the apices of the short axis of the capsule while the capsule elongates, and rupture initiates when  $d = d_c$  at the apices from which two cracks then propagate perpendicularly to the direction of capsule elongation (Figure 1a).



**Figure 1.** Damage of a capsule observed in the shear plane at an instant during cracks propagation in the cases (*a*)  $Ca_{\ell} \leq Ca < Ca_{h}$  and (*b*)  $Ca \geq Ca_{h}$ . The discontinuities are represented by the thick black lines.

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