Coupling of boundary integral and finite element methods to model the deformation of a microcapsule in flow

J. Walter, A.-V. Salsac, D. Barthès-Biesel

Biomécanique et Bioingénierie (CNRS UMR 6600),
Université de Technologie de Compiègne, 60205 COMPIÈGNE

Résumé :

On propose une nouvelle méthode pour étudier l'interaction fluide-structure entre une microcapsule et un écoulement externe. Une méthode par éléments finis (pour la membrane) est couplée avec une méthode d'intégrales de frontière (pour les écoulements interne et externe) afin de modéliser la capsule en grande déformation. On montre que la méthode est numériquement stable, efficace et fournit des résultat en très bon accord avec des travaux précédents.

Abstract :

We introduce a novel method to study the fluid-structure interaction between a microcapsule and an external flow. A finite element method (for the membrane) is coupled with a boundary integral method (for the internal and external flows) to model the large deformation of the capsule. The method is found to be numerically stable, efficient and in very good agreement with previous studies.

Mots clefs : capsule, boundary integral method, finite element method, Stokes flow, 2D elastic membrane model

1 Introduction

Synthetic capsules are liquid drops or gels protected by a thin elastic membrane. Such artificial microcapsules have a very wide range of applications in cosmetic, food and pharmaceutical industries. They are used to protect fragile, volatile or active substances and to control the release rate as desired. Other instances are found in biomedical engineering, where microcapsules are used as vectors for targeted drug delivery or artificial blood manufacturing. In most applications, what is at stake is the characterization of the complex behavior of a deformable capsule in an external liquid flow. Numerical models of the fluid structure interactions are necessary to predict the capsule deformation in microflow conditions.
In many respects, the fluid structure interaction of microcapsules suspended in an external flow is unconventional. (*i*) The capsules are closed surfaces suspended in a fluid. They are therefore not subjected to any boundary condition on the displacement apart from spatial periodicity. (*ii*) At the small scale of the capsule, the inertial forces of the internal and external flows are negligible compared to the viscous forces. The fluid flows can therefore be modeled using the Stokes equations (balance between viscous and pressure forces). (*iii*) The inertial force of the capsule wall can be equally neglected. Consequently the problem does not contain any dynamics and can be seen as a succession of equilibrium states. The drawback is that the stability of the equilibrium is not necessarily satisfied. (*iv*) The capsules are subjected to not only large displacements but also large deformations, which must be taken into account in the numerical model used to simulate the membrane mechanics.
This problem has been studied for the past three decades and different strategies have been considered to derive numerical solutions. Many studies have used a fluid solver based on the boundary integral method to solve for the Stokes flow equations. The velocity field at any position within the fluid domain is given by surface integrals calculated on the geometric boundaries. This method therefore has the advantage of reducing the geometric dimension of the problem by one, which largely decreases the total number of nodes.
The model the most used for the capsule wall is that of a 2D hyperelastic membrane : the wall is considered to be infinitely thin and to have a negligible bending stiffness. Two approaches may be considered to model the capsule membrane mechanics : the equations of the force equilibrium on the capsule wall may either be written locally at each point (strong form) or globally integrated over the capsule surface (weak form). Most capsule studies have used the strong form of the equations. Capsules in simple shear flows have been considered by Pozrikidis (1995), Ramanujan & Pozrikidis (1998) [1, 2] and more recently by Li & Sarkar (2008) [3], who computed the membrane load as a piecewise constant function. Lac *et al.* (2004) and Lac & Barthès-Biesel (2005) [4, 5] used instead bi-cubic B-splines as interpolation functions in order to compute the loads with high accuracy. An alternative option is to write the balance equations in their weak form and to use a Finite Element

(FE) method. The local equilibrium equations are converted into their variational equivalent. Only two groups [6, 7, 8] have implemented a FE method, that was each time coupled with an immersed boundary method to compute the motion of a capsule in shear flows. However their FE method is based on the use of linear interpolation functions and lacks generality in the implementation.
Previous studies have shown that, for certain ranges of the governing parameters, the capsule wall undergoes compression and tends to buckle. Thus, bending effects must be taken into account in order to properly model the wall mechanics. However no satisfying model for the bending stiffness of a capsule has been implemented yet. The FE method has the advantage of offering a framework suitable for the modelling of thin shells.
In this paper we propose a novel coupling technique between a finite element method to simulate the large deformation of the capsule wall and a boundary integral formulation of the Stokes flow equations. It is validated on a membrane model for which the bending stiffness is neglected. We show that the method is numerically stable and, as a test case, we study the deformation of a capsule in a simple shear flow and compare the results with previous studies.

2 Problem statement

We consider an initially-spherical capsule (radius a) consisting of a liquid droplet enclosed by an infinitely thin membrane characterized by a surface shear modulus G_s. The capsule is suspended in a viscous liquid undergoing an unbounded shear flow. The velocity of the unperturbed flow is denoted $\underline{v}^\infty$ and the shear rate $\dot{\gamma}$. Both fluids are assumed to be Newtonian and to have the same viscosity μ and density ρ. Dimensional analysis then shows that an important non-dimensional parameter is the capillary number

$$Ca = \frac{\mu \dot{\gamma} a}{G_s}\,, \tag{1}$$

which compares the viscous stresses exerted by the fluids to the elastic stiffness of the membrane.

2.1 Internal and external flows

The Reynolds number $Re = \rho a^2 \dot{\gamma}/\mu$ is small compared to unity, so that both the internal and external flows follow the Stokes equations. The velocity of the points of the capsule can then be related to the viscous stresses on the membrane through an integral equation over the deformed surface S :

$$\forall \underline{x}_0 \in S, \quad \underline{v}(\underline{x}_0) = \underline{v}^\infty(\underline{x}_0) + \frac{1}{8\pi\mu} \int_S \underline{\underline{J}}(\underline{x}_0, \underline{x}) \cdot [\underline{\sigma}](\underline{x})\, dS_{\underline{x}}\,, \tag{2}$$

where $[\underline{\sigma}] = (\underline{\underline{\sigma}}^{int} - \underline{\underline{\sigma}}^{ext}) \cdot \underline{n}$ is the viscous stress jump across the interface ($\underline{n}$ is the unit normal vector pointing outwards, $\underline{\underline{\sigma}}$ is the stress tensor in the fluids) and

$$\underline{\underline{J}}(\underline{x}_0, \underline{x}) = \frac{1}{r}\underline{\underline{\mathbb{1}}} + \frac{1}{r^3}\underline{r} \otimes \underline{r} \tag{3}$$

is Green's single layer kernel, with $\underline{r} = \underline{x}_0 - \underline{x}$ and $r = \|\underline{r}\|$.

2.2 Membrane mechanics

Following Skalak *et al.* [9], we treat the membrane as a purely bidimensional sheet of hyperelastic material. In particular, we neglect strain variations across the thickness and therefore the bending stiffness of the material. We introduce the displacement $\underline{U}(\underline{X}, t) = \underline{x}(\underline{X}, t) - \underline{X}$, where $\underline{X}$ and $\underline{x}$ are the positions of a given material point in the reference and deformed state. It is related to the velocity of the membrane through the kinematic condition :

$$\frac{\partial}{\partial t}\underline{U}(\underline{X}, t) = \underline{v}(\underline{x}, t)\,. \tag{4}$$

Dimensional analysis shows that the inertia of the membrane can be neglected compared to the viscous stress exerted by the flow. The motion of the membrane therefore follows the local equilibrium equation :

$$\underline{\nabla_s} \cdot \underline{\underline{T}} - \underline{q} = \underline{0}\,, \tag{5}$$

where $\underline{\underline{T}}$ are the bidimensional Cauchy tensions in the membrane, $\underline{\nabla_s}\cdot$ is the surface divergence operator on the deformed configuration and the load on the membrane $\underline{q}$ is equal to the viscous stress jump $[\underline{\sigma}]$.
We now have to turn (5) into a variational problem, with the load $\underline{q}$ as the unknown. Note that most finite element procedures look instead for the displacement field, treating the forces as known. That is not possible

when dealing with a capsule, as the lack of kinematic boundary conditions means that there is no unique displacement solution.
Let $\mathcal{V}$ be the Sobolev space H^1, and $\underline{\hat{u}} \in \mathcal{V}$ a virtual displacement field. The variational problem corresponding to (5) is thus :

$$\begin{aligned} &\text{Find } \underline{q} \in \mathcal{V} \text{ such that } \forall \underline{\hat{u}} \in \mathcal{V}, \\ &\int_S \underline{\hat{u}} \cdot \underline{q}\, dS = \int_S \underline{\underline{\hat{\varepsilon}}}(\underline{\hat{u}}) : \underline{\underline{T}}(\underline{U})\, dS \,, \end{aligned} \tag{6}$$

where $\underline{\underline{\hat{\varepsilon}}}(\underline{\hat{u}}) = \frac{1}{2}\left(\underline{\underline{\nabla_s \hat{u}}} + \underline{\underline{\nabla_s \hat{u}^T}}\right)$.
To close the problem, we need the (non-linear) relation between the displacement $\underline{U}$ and the tensions $\underline{\underline{T}}$. This is done trough the choice of a 2D strain energy function characterising the mechanics of the material. The strain energy w_s can be written as a function of the invariants

$$I_1 = \lambda_1^2 + \lambda_2^2 - 2\,, \quad I_2 = \lambda_1^2 \lambda_2^2 - 1\,, \tag{7}$$

where λ_1, λ_2 are the principal stretch ratios. Several laws have been proposed to model the behaviour of hyper-elastic membranes [10]. In this paper, we consider the neo-Hookean law (NH)

$$w_s^{NH} = \frac{G_s}{2}\left(I_1 - 1 + \frac{1}{I_2 + 1}\right), \tag{8}$$

and Skalak *et al.*'s law (Sk) [9]

$$w_s^{Sk} = \frac{G_s}{4}\left(I_1^2 + 2I_1 - 2I_2 + CI_2^2\right), \quad C > -1/2\,. \tag{9}$$

3 Numerical method

For a given deformed state of the capsule, we first solve the solid problem (6). $\mathcal{V}$ is discretized as a finite element space using an unstructured mesh, with quadratic (P_2) curved triangular elements.
The discretized problem leads to the following matrix system :

$$[M]\{q^N\} = \{R\}\,, \tag{10}$$

where $\{q^N\}$ corresponds to the degrees of freedom of the discretized load, $[M]$ has the structure of a mass matrix and $\{R\}$ corresponds to the right-hand side of (6) and depends non-linearly on $\underline{U}$. The tensions $\underline{\underline{T}}$ are computed directly using the strain energy function. Solving the solid problem consists in assembling $\{R\}$ and $[M]$ on the deformed state. Surface integration is performed using Hammer points on the elements. Eq. (10) is then solved using the sparse solver Pardiso [11, 12].
Once the load $\underline{q}$ is known, the velocity field is obtained explicitly from the boundary integral equation (2), which is discretized on the *same mesh* as for the solid problem, once again using Hammer points for the integration. Finally, the new position is obtained by convecting the nodes after integrating (4) numerically with a second-order Runge-Kutta method.
Tests performed using different mesh sizes and time steps show that the coupling between the boundary integral and the inverse finite element methods is numerically stable and converges in time and space. The numerical stability is conditional due to the explicit nature of the time integration scheme. That limits the time step as a function of Ca and the mesh size [13, 4].

4 Validation : capsule in a simple shear flow

We study the behavior of an initially-spherical capsule in a simple shear flow with the new coupling method. In order to validate the method and the non-classical inverse use of finite elements, the results are compared with three previous studies :

- the work of Lac *et al.* [4], who used the same method for the fluid problem (boundary elements), but a local approach for the solid problem, which is based on a discretization of the interface by bi-cubic B-splines ;
- the work of Li & Sarkar [3], who used the immersed boundary method for the flow and a local approach with a piecewise-constant load for the solid problem ;
- the work of Doddi & Bagchi [7], who also used the immersed boundary method for the fluid but finite elements to model the membrane, albeit with a method somewhat different from ours.

For the external fluid flow, we consider the undisturbed velocity field given by

$$\underline{v}^{\infty}(\underline{x}) = \dot{\gamma} x_2\, \underline{e}_1\,. \tag{11}$$

The capsule behavior is simulated using the NH law and the Sk law ($C = 1$). The P_2 triangular elements have 2562 nodes and the time step is $\dot{\gamma}\Delta t = 5 \times 10^{-3}$.
The capsule elongates under the influence of the shear flow as the capillary number is increased. Depending on the value of the capillary number Ca, three regimes are found, as first described by Lac *et al.* [4]. For $Ca < Ca_L$, folding occurs in the plane orthogonal to the main extension direction (hereafter called *the equator*). It is due to the presence of compression tensions in the membrane (fig. 1*a*). The folds disappear for larger values of the capillary number (fig. 1*b*). Indeed, as the capsule becomes more elongated by the shear flow, the value of the isotropic part of the tensions (related to the area dilation modulus) increases, which leads to positive tensions at the equator. For $Ca > Ca_H$, the elongated capsule behaves like a slender body submitted to a torque (due to the flow vorticity) and buckling occurs at the tips (fig. 1*c*). The critical values Ca_L and Ca_H separating those regimes are defined as the values between which the capsule takes a steady ellipsoidal shape, free of negative tensions.

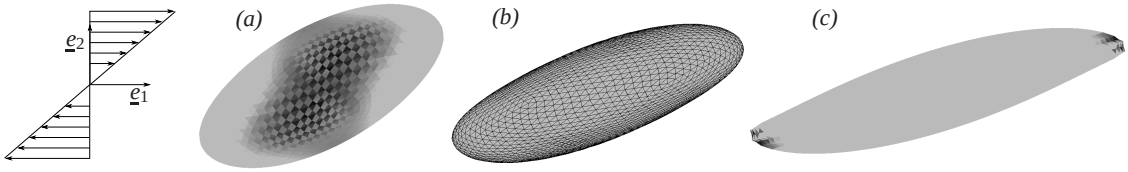

FIG. 1 – Deformed shape of a capsule, following the NH law, for different values of Ca : $Ca = 0.3$ (*a*), 0.6 (*b*), 1.2 (*c*). Light-grey zones are undergoing traction, while darker zones show areas where compression occurs. The mesh used for the computation is shown on figure *(b)*.

The critical values found with our coupling method are

$$Ca_L = 0.45\,, \quad Ca_H = 0.63\,, \tag{12}$$

for the NH law and

$$Ca_L = 0.4\,, \quad Ca_H = 2.4\,, \tag{13}$$

for the Sk law ($C = 1$). Note that we find exactly the same values for the critical capillary numbers as Lac *et al.* [4]. Doddi & Bagchi [7] also found negative tensions for low Ca, but did not quantify the limiting capillary number Ca_L. They did not consider large values of Ca and did therefore not comment on the existence of Ca_H. The three regimes were observed by Li & Sarkar [3]. They were, however, unable to characterize Ca_L and Ca_H, as they found negative tensions for all values of Ca, a phenomenon they ascribe to the lack of precision of their numerical method. Hence, our work is the only one beside [4] that determines Ca_L and Ca_H.
Another parameter to consider for the validation of the method is the Taylor parameter D_{ij}. It is an adequate parameter to characterize the deformation of capsules, since they typically assume an ellipsoidal shape at equilibrium. It is defined as

$$D_{ij} = \frac{|L_i - L_j|}{L_i + L_j} \quad (i, j = 1, 2, 3)\,, \tag{14}$$

where the L_i are the lengths of the principal axes of the ellipsoid. In particular, D_{12}^{∞} represents the Taylor parameter in the shear plane at steady state.
We compare values of D_{12}^{∞} with the previous studies for the NH law (fig. 2) and the Sk law (fig. 3). We find a good agreement for all values of the capillary number. In particular, our results are always well within 1% of those of Lac *et al.* [4] for both the NH and Sk laws. A 5% difference is, however, found with Li & Sarkar [3] for both laws. It is probably related to the crude description of the load used by these authors. The results of Doddi & Bagchi [7] are close to our results at low values of the capillary number but seem to diverge as Ca increases. This is somewhat surprising, as they also use finite elements to model the membrane.

5 Discussion and conclusion

We have developed a new numerical method to simulate the mechanical behavior of a capsule in an unbounded Stokes flow. This method couples a boundary integral method to model the internal and external flows with a non-classical inverse finite element model of the capsule membrane. Coupling those two techniques had never been attempted before and we have shown here that this coupling is feasible and numerically stable.
We have compared the results of our method with three previous studies and have found a good agreement. It may be noted, in particular, that our results are remarkably close to those of Lac *et al.* [4] (within 1%). Both studies find the same critical capillary numbers Ca_L and Ca_H, although two different methods are used to model the behavior of the membrane. This seems to indicate that the values of the critical capillary numbers have a physical relevance and are not a consequence of the numerical method used.

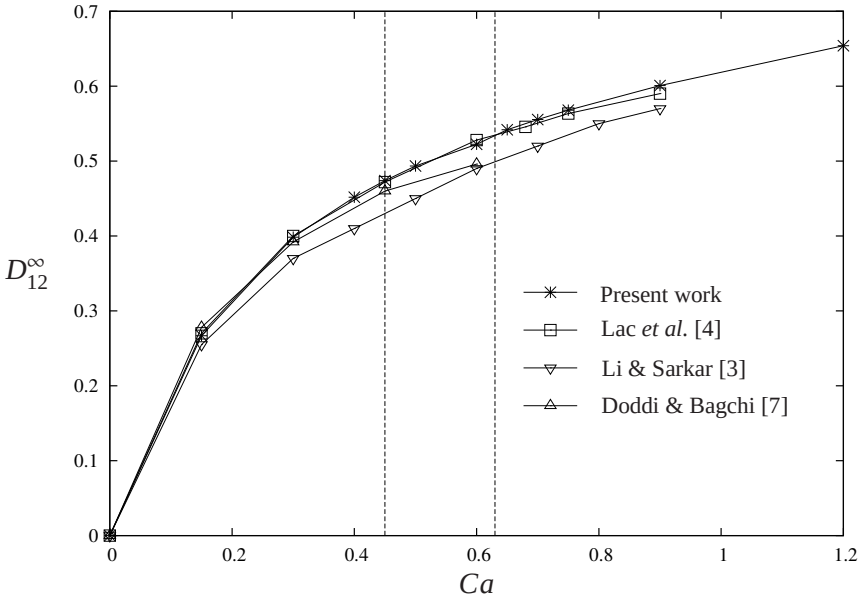

FIG. 2 – Values of D_{12}^{∞} as a function of Ca for a capsule following the NH law. The computation uses P_2 elements, 2562 nodes, $\dot{\gamma}\Delta t = 5 \times 10^{-3}$. Results are compared with [4, 3, 7]. Vertical lines indicate the critical capillary numbers Ca_L and Ca_H.

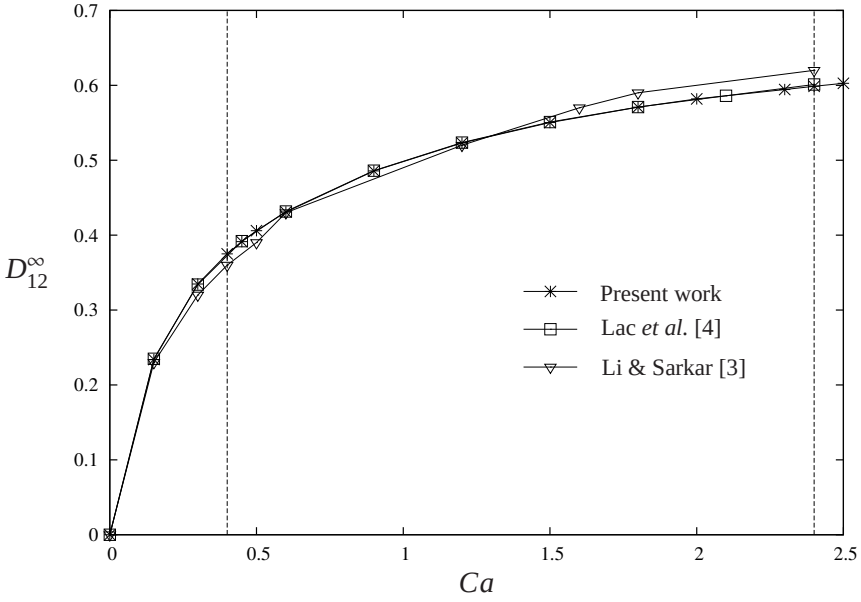

FIG. 3 – Values of D_{12}^{∞} as a function of Ca for a capsule following the Sk ($C = 1$) law. The computation uses P_2 elements, 2562 nodes, $\dot{\gamma}\Delta t = 5 \times 10^{-3}$. Results are compared with [4, 3] ; this case was not studied in [7]. Vertical lines indicate the critical capillary numbers Ca_L and Ca_H.

A major difference between our results and those of Lac *et al.* is the behavior of the numerical method when negative tensions appear. Whereas the technique used by Lac *et al.* fails when negative tensions appear ($Ca < Ca_L$ or $Ca > Ca_H$), our numerical method remains stable and a steady equilibrium state is achieved. This is probably due to the larger numerical stiffness of the finite elements as compared to the bi-cubic B-spline functions used by Lac *et al.* Neither Doddi & Bagchi [7] nor Li & Sarkar [3], who also used lower order discretization than Lac *et al.*, reported stability problems at low Ca, which would confirm the hypothesis. The stiffness introduced by the numerical method contributes to the stability of the problem because it enriches the membrane model with some bending rigidity. But being a byproduct of the numerical method, this small bending rigidity cannot be controlled. Consequently the folds that are observed for $Ca < Ca_L$ (fig. 1*a*) depend

on the mesh, with a wave length equal to the element size. Since we have not modelled a proper shell with bending stiffness, the folds are not physical, even though the occurrence of buckling and its location are.
The existence of folds for certain values of the capillary number shows the limit of a membrane model when simulating a capsule and the necessity to introduce some bending rigidity. In the range $[Ca_L, Ca_H]$, a membrane model is sufficient to obtain the mechanics of the deforming capsule, since no negative tensions are present at steady state. But beyond these limiting values, the capsule wall needs to be treated as a thin shell with a physical bending stiffness in order to properly model the buckling process. The framework of finite elements seems quite appropriate to implement such a shell model.

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