Modeling the rupture of microcapsules in flow

Post doc Advisors:

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Context of the study:

A micro-capsule is a fluid droplet enclosed in a thin membrane with hyperelastic properties. When suspended in a confined carrying fluid, it experiences large deformation under the hydrodynamic constraints of the internal and external fluids. The objective of the project is to study the occurrence of rupture as the capsule deforms under flow and determine the capsule dynamics before and after rupture. One application of the project is oriented towards drug targeting and the triggering of rupture to release drugs contained within microcapsules.

Keywords: capsule suspension, membrane rupture, model reduction, fluid-structure interaction, drug targeting

Project partners:

- **Biomechanics and Bioengineering Laboratory**: "Biological Fluid Structure Interaction" team
  Anne-Virginie SALSAC (CR CNRS), Badr KAOUI (CR CNRS), Anne LE GOFF (MCF), Dominique BARTHES-BIESEL (Emeritus Professor)

The team has an expertise both in numerical simulation (development of state-of-the-art fluid-structure interaction codes dedicated to capsule dynamics) and in microfluidic experiments, which is unique at the international level in the field of modeling of capsule flows.

- **Roberval Laboratory**: "Computational mechanics" team
  Adnan IBRAHIMBEGOVIC (Professor), Pierre VILLON (Professor)

The team is specialized in the development of numerical tools to model complex multiphysics problem in mechanical engineering, correlate experiments and numerical simulation and optimize large-scale problems with a multi-scale approach, using various strategies of model reduction.

- **Laboratory of Applied Mathematics of Compiègne** (LMAC): "Stochastic Systems" team
  Salim BOUZEBDA (MCF), Nikolaos LIMNIOS (Professor)

The team is specialized in weak approximations of stochastic processes and semi-markovien processes. It works on the study of their stability and stationarity and on non-parametric estimation.

Post doc description:

The project is dedicated to model the rupture of microcapsules subjected to an external flow. The burst of a capsule under shear was first observed by Chang & Olbricht (1993), but no systematic study was performed ever since. There is only sparse experimental data and hardly any numerical model (one exception being Ghaemi et al. 2015) of this key phenomenon.

The **objectives** of the project are to tackle the following *scientific challenges*:

- Task 1: Build-up of a **3D numerical model** of a capsule flowing in a cylindrical tube and of its deformation **before and after rupture**. It will account for:
  - **Heterogeneous capsule states** (state heterogeneity of a capsule before and after rupture + variability of properties in a capsule population, which can be seen as "sub-systems")
  - **Multiphysics** problem: strong coupling between suspension flow - capsule wall deformation
  - **Multi-scale phenomena** (deformation @ capsule scale, rupture @ membrane scale)

The numerical model will be inspired by the existing Boundary Integral – Finite Element model of a capsule flowing in a tube (Hu *et al.* 2012). It will be enriched to account for the membrane bending rigidity (e.g. Dupont et al. (2016) shell model) and plasticity. It will be used to predict the location of rupture based on a rupture criterion. A possibility will then be to use an embedded discontinuity approach to represent mode I and mode II failure mechanisms (Nikolic *et al*. 2015).

- Task 2: Build-up of **reduced models** of the capsule motion before and after rupture

Reduced models of capsule deformation will be built from the capsule shapes predicted, before and after rupture, by the 3D simulations (task 1). The shapes will be interpolated using Principal Component Analysis and Diffuse Approximation to replace the geometry-based variables with the smallest set of variables needed to represent an admissible shape for a given precision (Raghavan *et al*. 2013).

- Task 3: Statistical study to predict **likelihood** and **moment of rupture** for a **capsule population**

In case of a 1-year extension of the project, a statistical analysis will be conducted. Given a sample of capsules with a variability in mechanical properties and size, the goal will be to determine the probability of capsule rupture within the sample and the moment of rupture. Method such as the change point problem (Bouzebda 2014) or semi-Markov model (Bouzebda & Limnios 2012) will be considered.

Integration in Labex Scientific Program:

The project, which does not have any other funding source and which **could unfortunately not be embedded within a DEFI team** owing to the absence of any project linked to Mechanical Engineering, will *encompass 2 scientific themes* of the MS2T Labex:

- "**Optimized design of TSoS**" (in particular "Multi-level and multiphysics optimization")
- "**Management of uncertainties**" ("Modeling of uncertainties", "Robustness in uncertainties")

It will be *rooted on* the results of the *PhD thesis of B. Sévénié* (2016), who provided the proof-of-concept that a reduced-order model was accurate to model the deformation of a capsule in a bifurcated channel.

Project planning:

The objective of the 1st year will be to build (*i*) a *3D numerical model* predicting capsule rupture and simulating its deformation before and after the event, as well as (*ii*) *a reduced model* of these 2 stages. If extended for a 2nd year, the objective will be to predict whether rupture is likely to occur for a given capsule sample with a probability distribution in properties and estimate the moment of rupture.

Candidate's profile: **Potential Candidate identified** (see attached documents)

The competences of the successful candidate will be multidisciplinary: Solid background in solid mechanics, Multiphysics modeling and numerical analysis, Notions of biomechanics and bioengineering. Knowledge in model reduction will be a plus.

Documents required to apply:

Send to Anne-Virginie Salsac (a.salsac@utc.fr):

- Curriculum vitae
- Motivation letter
- At least two references and/or recommendation letters
- A statement of research experience and interests

Location:

Laboratory Biomechanics and Bioengineering (BMBI), UMR CNRS-UTC 7338
Université de Technologie de Compiègne (UTC), CS 60319, 60203 Compiègne cedex – France

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