A discrete multi-physics model to simulate the mechanical properties of breakable capsules.

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ABSTRACT

A capsule consists of a thin membrane (or shell) enclosing an active (often in liquid form) substance. In many applications, the purpose of the capsule is to ensure a controlled release of the liquid inside. In this context, capsules are widely used in a variety of fields including cosmetics, food, textiles, pharmacy, agriculture and, more recently, for self-healing materials such as self-repairing concrete or asphalt. Mechanical characterization is essential to design the capsules for a timely release of the active substance. However, currently they are designed by trial and error; computer simulations, therefore, have the potential to significantly accelerate their design by providing a method for calculating in the behaviour of the capsules beforehand. Conventional modelling techniques like the Finite Element Method can be used to calculate the stresses in the membrane, but are less effective when the simulation also includes the fracture of the membrane and the consequent release of the fluid inside.

In this paper, a discrete multi-physics (DMP) approach is used to investigate the mechanical response (including breakage and liquid release) of core-shell capsules under compression. The model is based on a particle framework that combines Smoothed Particle Hydrodynamics for modelling the fluid, with the Mass and Spring Model for modelling the elastic membrane. The meshless nature of DMP allows including in the model the fracture of the capsule's shell and the interactions between the active liquid and the solid shell.

The simulations accounts for a parallel plate compression test of a single core-shell capsule. The inputs of the model are the size of the capsule, the thickness of the shell, the internal structure, Young's modulus of the shell material and the fluid properties like density and viscosity. Outputs of the model are the fracture type, maximum force needed for the fracture and the displacement-strain curve. Data are validated by reproducing equivalent experimental test in the laboratory. By means of this methodology, it is possible to optimise the size, thickness of the shell, internal structure and type of material, in order that the capsule breaks and releases the internal liquid at the right time. The authors expect that the use of this model will easy the design of the capsules in the future.

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