Simulating A Photothermal Elastic Capsule As A Drug Delivery Device

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Abstract

Our group developed an experimental millimetric capsule intended to release chemicals or drugs. The delivery mechanism of such device relies on the thermal expansion of carbon-elastomer composites which deform upon irradiation of light supplied by a Laser diode through an optical fiber. Experiments showed that the device can indeed deliver a marker liquid when the Laser was turned on; the whole process also revealed a mild deformation of the capsule geometry as well as the presence of millimetric bubbles appearing inside the capsule, which we suspect may play an additional role in the delivery mechanism. The experimental observations were further analyzed and explained conducting numerical simulations with COMSOL Multiphysics®. Although we split the whole problem into different study sets, we tried to include all the physics involved. Thus, we considered the absorption of light and consequent photothermal conversion into heat, this followed by the deformation of the elastic boundaries of the capsule that caused a thermal expansion releasing the diluted chemical species within an external fluid environment. In the simulations we replicated the cylindrical-shaped capsule using the 2D-axisymmetric geometry and several modules run in stationary or transient studies: the Heat Transfer Module, including a Lambert-Beer generation term assuming a diverging gaussian Laser beam profile, the Structural Mechanics Module, including an isotropic thermal expansion; we also included the CFD Module and Transport of Diluted Species interface (without diffusion) in order to simulate the release of a marker solution diluted in a liquid environment. Additionally, we ran simulations considering the isobaric expansion of an air bubble (with variable density due to the increment of temperature) to see if this kind of mechanism can also "squeeze" the liquid inside the capsule. Our simulations showed that the mechanism based on the elastic deformation of the capsule triggered by thermal stresses and the other one based on the isobaric expansion of trapped air bubbles can both promote the release of the capsule's content. Interestingly, the simulations also showed, however, that both mechanism have different time scales: the one based on elastic deformation occurs at short time scales and saturates very quickly, while the one based on bubble expansion can endure for longer time periods. In conclusion, our simulations demonstrated that these kind of delivery devices can be studied numerically using COMSOL® and we expect to continue studying these simulations using, for instance, other models of light absorption or elastic respond (nonlinear mechanical behavior) of the materials.
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