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Abstract

Modeling and Simulation of Magnetoliposome Formation by Encapsulation of Core-Shell, Magnetite-Chitosan Nanoparticles in Liposomes Enabled by a Low-Cost Microfluidic System †

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Abstract: Research in nanostructured materials has led to the development of different applications of relevance in the fields of medicine and biomedical engineering. In this regard, the field of drug delivery has probably benefited the most due to the possibility to engineer vehicles of high potency and increased activity and selectivity toward selected intracellular targets. Such vehicles can therefore potentially address one of the major cornerstones of modern pharmacology, which is increasing the bioavailibity of drugs of low permeability. Our research group has developed cell-penetration nanobioconjugates by interfacing several nanomaterials (e.g., chitosan, gelatin nanoparticles, graphene oxide, and magnetite) with translocaing peptides. The obtained nanobioconjugates have demonstrated facilitated cell internalization and endosomal escape abilities. To improve cell penetration even further, we encapsulated the magnetite-based nanobioconjugates into liposomes (to form magnetoliposomes) with very appealing results. Our plan is to expand the available nanoplatforms by combining the attributes of magnetite and polymeric nanoparticles through a core-shell system comprised of magnetite (core) and chitosan (shell). The encapsulation process has been successfully accomplished with the aid of passive micromixers with different channel geometries to favor intimate contact between the dispersed phase (nanoparticles) and the continuous phase (phospholipid solution). To model the encapsulation process, we implemented an Eulerian simulation in the software COMSOL Multiphysics® 6.0 (COMSOL Inc, Stockholm, Sweden) where mixing required the Navier-Stokes equations as governing equations of momentum transport, turbulence, eddie viscosity, and damping functions to approximate turbulence using the κ-ε turbulence model near the walls. The simulation was conducted for the different geometries (i.e., SARS, chambers, and serpentine) and for Reynolds numbers ranging from 0.2 to 10 Also, we tested a low Reynolds turbulent model using the κ-ε model given in the Euler-Euler module. The Euler-Euler approach showed that the encapsulation reaches higher encapsulation efficiency (EE%) values compared with the previously implemented mixture model. Our encapsulation results indicate that including the κ-ε turbulence model with low Reynolds turbulence model near the walls provide a higher agreement between in-silico and experimental approaches. Future work will be dedicated to evaluating

the performance of our previously tested magnetophoretic separators with the newly developed encapsulates, to assure sufficient purity for further biocompatibility testing.

Keywords: Microfluidics; MNP's; liposome; drug delivery systems; Euler-Euler approach

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