COMSOL Multiphysics® Simulation of Functionalized 3D Biocompatible Porous Graphene Composites

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Abstract

Graphene is an allotrope of carbon having the structure of a plane sp2-hybridized atom with a band length of 1.42Å, and representing the basis of any carbonaceous material. This 2D material consisting on pure forms of carbon exhibits high crystalline and electronic quality. Thus, despite being alike an indefinitely large aromatic molecule, graphene has exceptional mechanical, electrical and thermal properties. Furthermore, being one-layer thick is almost transparent, thus interacting with light and with other materials in unprecedented ways within functionalized graphene embedded composites

G and GO related physics were introduced in COMSOL Multiphysics® through the bidirectional interface with MATLAB® via the LiveLink™ for MATLAB®. Material properties for G, porous G, and GO were new items added to the existing Material Library according to the state-of-art data from literature on the purpose of these specific simulations. For all the other related parts of the physical models the existing COMSOL Multiphysics® Material Library data were used.

The results of the COMSOL Multiphysics® simulations for functionalized 3D biocompatible porous graphene composites were validated using SoA literature data related to photodermal therapy (PTT), photodynamic therapy (PDT) and drug delivery through skin processes and parameters.

Figures used in the abstract

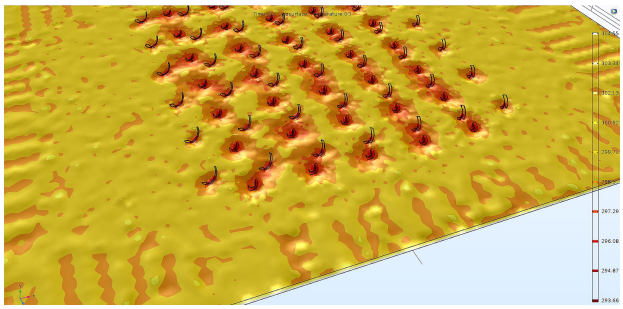

Figure 1: Isothermal response of G porous composite.