Modeling Drug Release From Materials Based on Electrospun Nanofibers

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Abstract

Electrospun nanofibers are prospective medicament carriers suitable for local administration of drugs in a controlled manner (1). Non-woven nanofibrous mats have shown potential for use in transdermal delivery systems and as implants releasing bioactive molecules including proteins, anti-cancer drugs or antioxidants. In this case, active substance is loaded into a nanofiber and release is carried out to the surrounding fluid. The release profile can be controlled by change of the fiber structure (solid fibers, core - shell fibers) (2), material porosity and spatial orientation of the fibers. This work contains our attempts to estimate impact of aforementioned structural parameters on drug release from the materials currently applied as a protective mats for neurosurgery.

We constructed a 3D finite element model for the representative nanofibrous cubic element using COMSOL Multiphysics®. Simulations were conducted in a geometry with regular and irregular fiber arrangement. Example of a cubic geometry of randomly oriented fibers is presented in Figure 1. Drug release from fibers was modeled by desorption - adsorption equation what is motivated by the fact that not entire drug is released from the nanofiber but part of it can be trapped inside the fiber. In our model the main transport process in the fluid surrounding fibers is diffusion which is also affected by the size of diffusing molecules and presence of fibers. The presence of fibers reduces overall diffusion coefficient, thus we introduced diffusion coefficient depending on porosity of the material, as purposed by Clague et al. (3).

Our results show that for the same material porosity drug release from the matrix of regularly oriented fibers is slower than from randomly oriented, isotropic nanofibrous material. Also by decreasing distance between the fibers drug transport rate is reduced. It means that if one intends to inhibit drug release in a given direction, highly oriented fibers constituting the outer barrier of a mat can help to reduce selectively its diffusive transport. Numerical results are verified with experimental data, and both show a good agreement of the release profiles. Through parameterized numerical studies one can find optimal geometry and structure of the nanofibers, avoiding tedious experimental tests.

Reference

1. Srouji, S. et al. Protein-2 Embedded Within Electrospun Scaffolds for Regeneration of Bone Defect: In Vitro and In Vivo Evaluation. 17, (2011).

2. Sirc, J. et al. Controlled gentamicin release from multi-layered electrospun nanofibrous structures of various thicknesses. International journal of nanomedicine 7, 5315–25 (2012).

3. Clague, D. S. & Phillips, R. J. Hindered diffusion of spherical macromolecules through dilute fibrous media. Physics of Fluids 8, 1720 (1996).

Figures used in the abstract

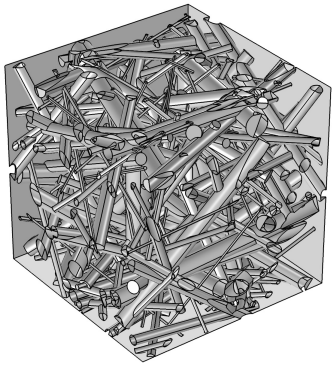

Figure 1: Nanofiber mesh with random fiber diameter and orientation.

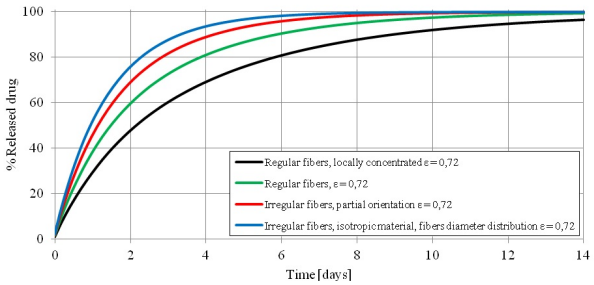

Figure 2: Drug release profile. Dependence on different material porosity and fiber arrangement.