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Transport model for drug release from delivery vectors accounting for chemical and microstructure properties

Arturas Ziemys

The Methodist Hospital Research Institute, USA

Abstract

Drug delivery vectors capture drug molecules by confining them inside matrix and then releasing them with a designed kinetics by diffusion. Drug diffusion is strongly affected by drug interaction with the media of drug vectors, and accurate prediction of drug release kinetics is not possible by common methods. In order to meet the need for the accurate release kinetics prediction, we have developed a novel physics-based deterministic method for drug diffusion in composite media that accounts for porosity of the microstructure as well as the interactions within microstructure which depend on drug and material properties of porous matrix.

A multiscale computational method was recently developed, incorporating solid-fluid interface effects into continuum models, and validated against experimental results. We have generalized our method to a robust approach to predict drug diffusion through nanopores, polymer matrix and composite cellular media containing cells and extracellular matrix. We showed that geometrical and material properties of solid phase, like polymer fibers, affect drug release along with drug physico-chemical molecule properties and size. Our drug diffusion transport method showed robustness and generality since it incorporates molecular level properties into the continuum model; it is computationally efficient, flexible and able to adequately include material properties of drug, as well as of the matrix of drug vector. This computational method offers a powerful tool in predicting drug release kinetics from drug delivery vectors, and can be used to optimize drug vector structure and chemistry, as well as drug penetration through biological media.

Biograpgy

Arturas Ziemys has PhD in biomedical sciences and molecular biophysics, focusing his research is on drug transport models. He is a co-author of 25 peer-reviewed papers and holds professional awards. Milos Kojic is a mechanical engineer by training with over 30 years of experience in development of computational methods and software for solid and fluid mechanics. He is the founder and PI of a Finite Element program used in research and industry. Miljan Milosevic has PhD in mechanical engineering developing multiscale transport models