Understanding the Role of Nanomaterials in DNA Biosensors Through Finite Element Analysis

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Abstract

Tremendous progress is being made in the integration of nanoparticles into micro-analytical systems for biosensing. These materials are shown to enhance the analyte capture capability of biosensing platforms by offering higher surface area to volume ratio and more efficient interaction with biomolecules of the same size [1]. Furthermore, in the context of clinical diagnostics, low detection limit has to come hand-in-hand with short sample-to-answer time for the platform to be acceptable.

We have implemented a computational model that considers the sensor's geometry, size, analyte concentration and type to predict the number of nucleic acid molecules captured by functionalized electrodes in clinically relevant durations. The model, originally developed by Erickson et. al. [2], is based on the finite element method using COMSOL Multiphysics®, in which analyte transport in the bulk phase is modeled as 3D diffusion, and analyte transport on the sensor (solid phase) is modeled as 2D surface diffusion. The adsorption to the sensor surface and hybridization on the functionalized part of the sensor are modeled as 2nd-order reactions. The models are being used to understand the role of nanomaterials in biosensing. This enables the collective optimization of the sensor's sensitivity and speed by changing the geometry and size of the nanoparticles.

The development of this model required the determination of several model parameters that are not well characterized. The number of parameters was reduced from the model by Ericson et. al. [2] by nondimensionalization. After this sensitivity analyses have been performed to determine the important parameters and these parameters are being determined through inverse modelling for fitting to experimental results under controlled conditions. The details of the model development and the findings from the models will be presented.

Reference

1. Bin, X., Sargent, E. H., and Kelley, S. O., Nanostructuring of sensors determines the efficiency of biomolecular capture. Analytical chemistry, 82(14), 5928–31 (2010).

2. Erickson, D., Li, D., and Krull, U. J., Modeling of DNA hybridization kinetics for spatially resolved biochips. Analytical Biochemistry, 317(2), 186–200 (2003).