TITLE OF A FRACTAL GEOMETRY CONSIDERTION IN FLUID-ADSORPTION SIMULATION

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ABSTRACT

Fractal properties of the sensor surface affects the reaction kinetics for transport-limited bio-interactions at least limited range of scales. Fractal is considered how nature forms complex yet ordered geometry. However, bio-interaction model has been modeled in a simple Euclidian geometry for years although the sensor geometry and surface often features higher complexity. Also, current fractal modeling has not been extended to realistic 3D model yet. In this paper, protein interaction under the influence of flow is modeled and simulated with realistic 3D geometry and assumption of fractal sensor surface. A coupled fluid and reaction-transport model in the QCM disk-like fluid chamber was simulated for interaction between calmodulin and calcineurin as a model system. In classical analysis, the sensor surface is assumed to be uniform and homogeneous, and also overall binding kinetics is to be constant over time. The sensor surface can be irregular and have clusters due to surface defects, inhomogeneous deposition of capture proteins/DNA, nanoscale clustering of self-assembled monolayers. The surface irregularity can affect the binding kinetics of bio-molecular interactions. The differential equations were established

considering fractal geometry and kinetics, solved using the commercial PDF solver, COMSOL Multiphysics^{TM} . We used calmodulin and calcineurin as a model binding pairs to validate the mathematical model. The fractal surface assumption provided 20-30% improved results in predicting effects of flow rate and reaction kinetics on the binding. The results demonstrated that employing more realistic geometric features such as fractal surface to the mathematical modeling enables better prediction of the flow-driven bio-interactions. The results indicate that the intensity of sensor signal was dependent both on convection and on the contact time between the analyte and the immobilized probes. We demonstrate the advantages of the fractal reaction kinetics by comparing its results to the traditional kinetics. The results indicate that binding model with fractal kinetics is able to reproduce experimental data whereas the widely used traditional kinetics faces severe limitations. The model can be readily extended to a range of other binding reactions and potentially has a wide utility for various geometry of solid-state sensors.