Modeling Partially Absorbing Biosensors

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Abstract

Designing and constructing a lab-on-a-chip device poses a variety of questions. Transport of all required substances, detection of the analyte and its deposition on a sensor have to be incorporated. Different strategies have been developed to achieve good coverages of the sensor, like employing electric or magnetic gradients. On the basis of a ramp like structure [1],(Figure1), the binding of the analyte to a sensor surface is being simulated. As the number of binding sites on the surface is limited, the binding probability of particles to the surface change over time. This way it is possible to measure the amount of analyte bound to the sensor and calculate capture rates as functions of time.

Everything is calculated using various interfaces of COMSOL Multiphysics®. Only half of the geometry is modeled, as it has a plane of symmetry (see Figure 1). For the computation of the fluid flow, additional auxiliary domains are added in front and at the outlet of the structure. The Laminar Flow interface is then used to generate the fluid profile corresponding to the inlet velocity and the geometry. Given that 3D simulations require high resolution meshes, the convection-diffusion-reaction equation is simulated on a 2D plain, which is the cross section of the structure along the plain of symmetry. As the fluid profile is computed in 3D, most of the 3D features are reproduced. The analyte distribution is generated by the Transport of Diluted Species interface. Here the sensor surface receives a flux boundary condition which is then coupled to either a boundary ODE or the Surface Reactions interface. The laminar flow is computed using a stationary linear solver, uncoupled to any other interface. The rest is calculated using a standard time-dependent solver.

The results so far are on the one hand as expected but some on the other hand still need improvement. The overall occupation of binding sites (Figure 2) behaves as expected and shows a decay of free binding sites as time goes by. But these results are dependent on the used mesh parameters. This is most likely due to the transition between a totally reflecting surface and the partially absorbing one (Figure 3). Prior to the absorbing surface the concentration goes above average, which leads to an increase in binding events. This error progresses all over the sensor area and may be the origin of the mesh dependence.

As soon as the mesh dependence is eliminated, the simulation can be compared to experiments, in order to determine the appropriate rate constants. Then the model could be used to optimize the structure or it could be extended to emulate more complex behavior, for example multiple species binding to each other, surface transport and things alike.
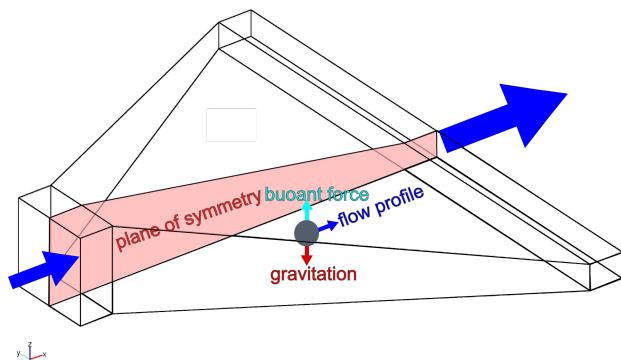
Figures used in the abstract

Figure 1: Ramp structure with all contributing effects on the particle

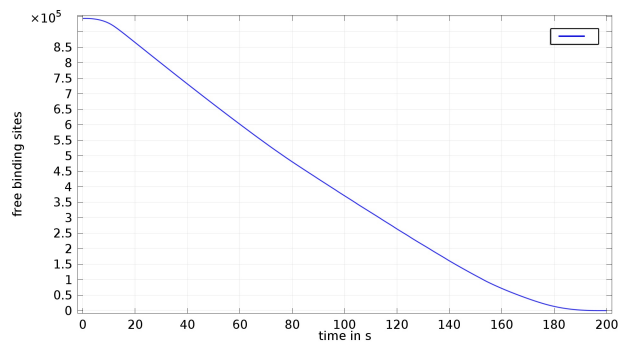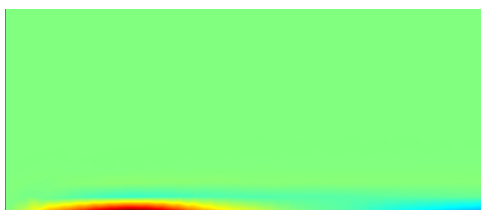**Figure 2**: Timedependent decrease of free binding sites

Figure 3: Transition between totally (left) and partially (right) reflecting boundaries