Modeling Partially Absorbing Biosensors

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Motivation

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 coverage of the sensor, like employing electric or magnetic gradients[1]. On the basis of a ramp like structure [2],(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.

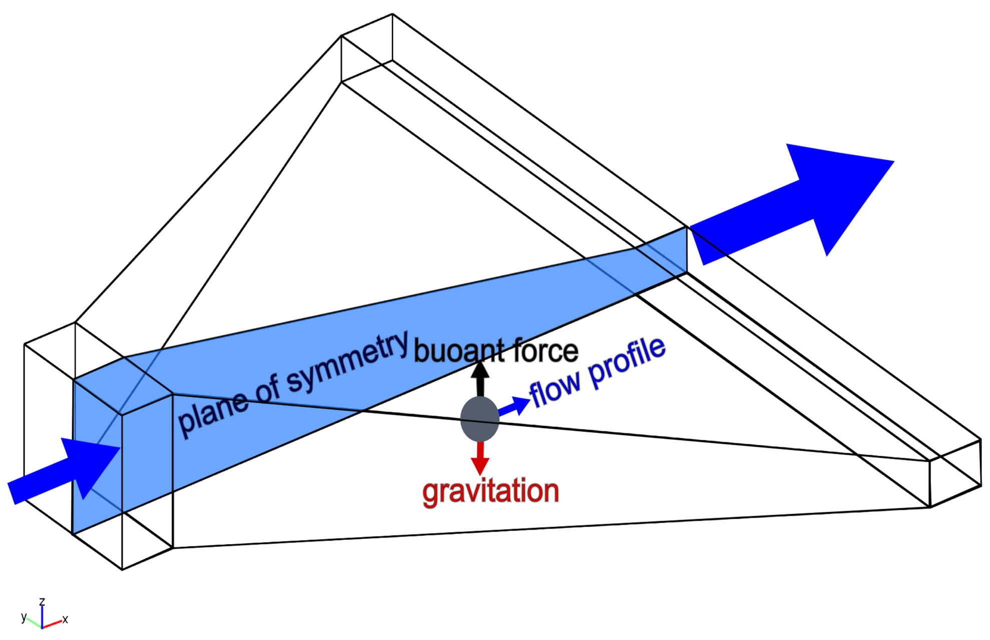

Figure 1. Model of the ramp structure with all contributing effects. Gravitation (red), buoyancy (black), and the flow profile (blue)

Governing equations

The equations needed to describe the ramp are the Navier-Stokes equation for incompressible fluids

$$\nabla p = \eta\,\Delta u + \rho\, f$$

with no-slip boundary conditions on all boundaries except the plane of symmetry, the inlet and the outlet, see Figure 1, were appropriate conditions are chosen.

The concentration profile is then calculated using an advection-diffusion equation

$$\frac{\partial c}{\partial t} + \nabla \cdot j = 0 \;\text{ with }\; j = D\,\nabla c - (u - g\mathbf{z})c$$

where the latter expression also accounts for gravitation and buoyancy. The inlet boundary is set to a constant concentration $c = c_0$, the outlet only allows convective transport. The sensor area is modeled with a Robin boundary condition [3]

$$D\frac{\partial c}{\partial \vec{n}}(\vec{x},t) = K\,c(\vec{x},t)\,\sigma(\vec{x},t)$$

Where K is a nonnegative reactivity constant and $\sigma(\vec{x},t)$ the ratio of unoccupied binding sites to the total of all binding sites.

References

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2. A. Weddemann, F. Wittbracht, A. Auge, A.Hütten, Positioning system for particles in microfluidic structures, *Microfluidics and Nanofluidics*, **7**, 849-655 (2009)
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Results

Due to stability reasons, the initial condition for the time-dependent simulation are set to the solution of stationary problem. This way the computation starts from an equilibrium state and depending on the reactivity constant K, the first time-steps do not resemble the real process (Figure 2a). Another issue to be solved is the dependence on K, here the simulations show similar behaviors on a wide range of reactivity values, which is not expected (Figure 2b). For any K the time until the sensor is totally covered is too short (in the order of seconds). At this stage it is only possible to make approximations about which areas of the sensor are occupied faster, thus being the most efficient. (Figure 3).

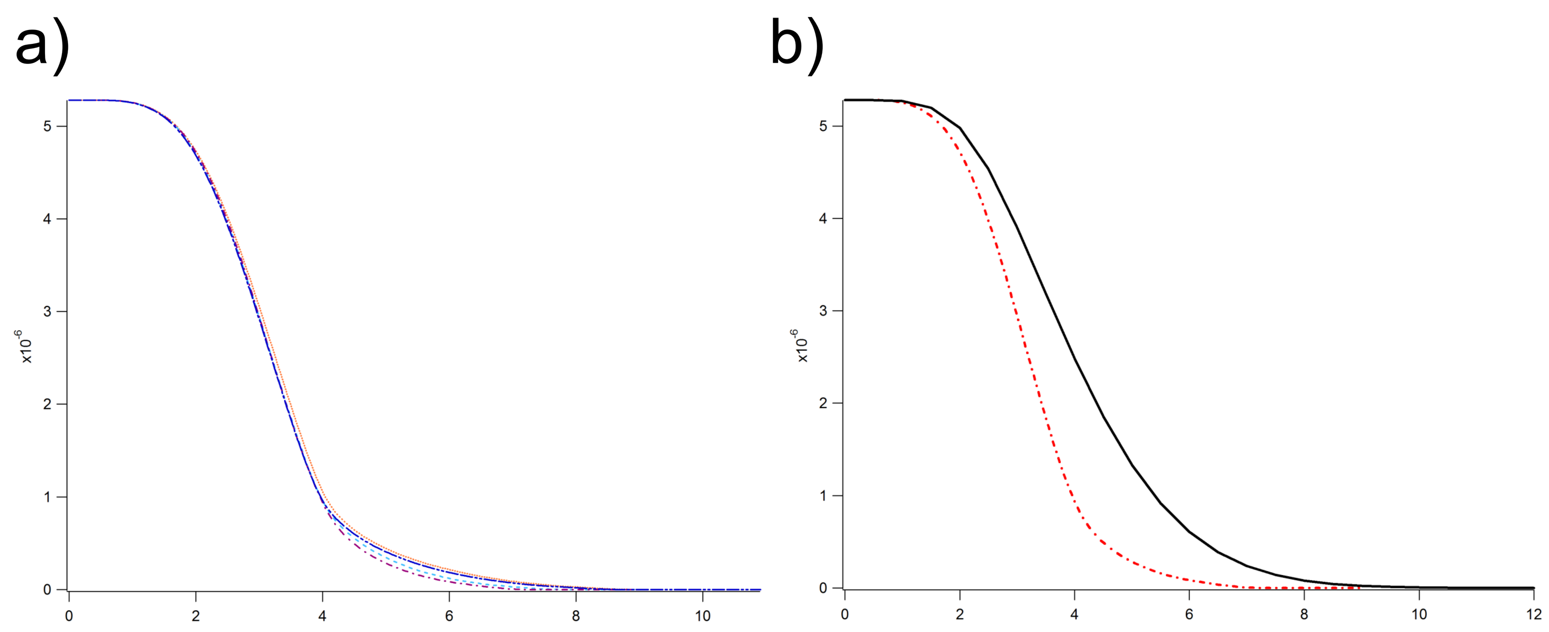

Figure 2. Evolution of free bindingsites for different reactivity parameters K. a) shows the evolution for a high reactivity of $K = 4 \cdot 10^{-5}\frac{m}{s}$ for different discretizations. b) shows the difference between high (red,dotted) and low (black) reactivities $K = 4 \cdot 10^{-7}\frac{m}{s}$

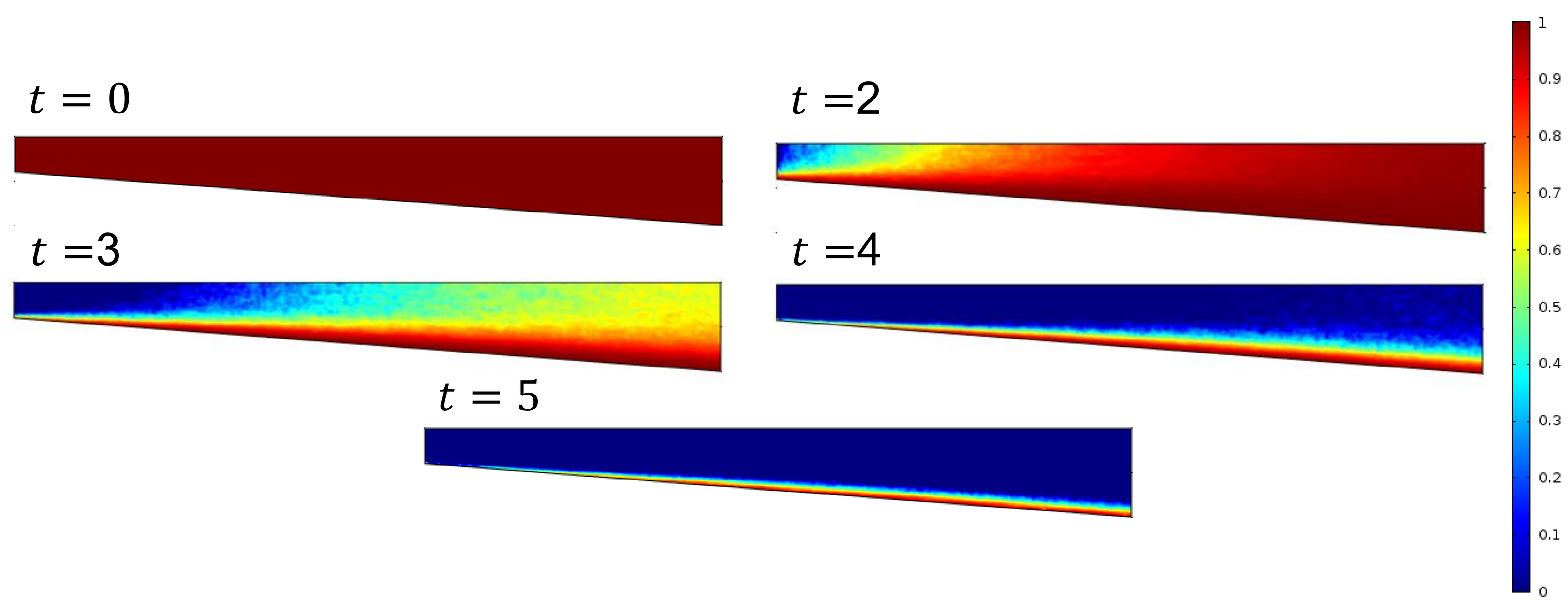

Figure 3. Ratio of free bindingsites to total bindingsites. Taken at $t = 0{,}2{,}3{,}4$ and $5s$

Conclusions

All in all the Robin boundary condition was implemented mostly successful with some alterations to improve stability. The independence of the reactivity is an obvious defect and needs further study. Experiments have to be carried out to testify the accuracy of the model. In case of a very small constant, other models would be more accurate and efficient.

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