2013 nanoHUB-U Course on
"Principles of Electronic Nanobiosensors"

Beating the diffusion limit

Muhammad A. Alam
Network of Computational Nanotechnology
Discovery Park, Purdue University.

In this HW problem set, we will discuss approaches to beat the diffusion limit. There are four problems (two Octaview codes are also provided). The basic concepts we discussed in the class are simple, but we must solve a few specific problems to make sure the concepts are fully understood. See HW1 for additional information regarding the two software packages to be used: Octaview and BiosensorLab. We will discuss the solutions at the end of the week.

Problem 2.1: *Beating the diffusion limit.*

Let us use the following example to illustrate the efficiency of biobarcode sensors in being able to detect analytes at ultra-low concentrations within a very short period of time. Assume the analyte density of 1 pM, diffusion coefficient of the analyte molecule is D=10^{-5} cm^2/Sec and its radius is a0=10 nm. The density of magnetic particles introduced in the solution is ρ_{MP}=1 mM.

(a) Calculate the number of biomolecules that have escaped capture after t=1 nanosecond, 10 nanoseconds, and 100 nanoseconds.
(b) How long should we wait before 99% of the target particles are captured?
(c) None of the times calculated above change if the analyte density is reduced to 1 fM. Can you explain why?

(Hint: Be careful about units when calculating τ.)

Problem 2.2: *Beating the diffusion limit by super-hydrophobic surfaces.*

(a) Show that, the contact angle θ^* of a droplet can be designed by the following formula: $\cos\theta^* = \phi\cos\theta_E - (1-\phi)$, where, ϕ is the fractional area covered by the pattern (see lecture slides), and θ_E is the contact angle of the water droplet on a flat surface.
(b) What is the value of θ_E for Teflon and SU-8 (google it)? Which one of them is more hydrophilic?
(c) Using the relationship in part (a), plot θ^* as a function of the design parameter ϕ for Teflon and SU-8. Would it be possible to design a super-hydrophobic surface from the hydrophilic material you identified in part (b)? A superhydrophobic surface is characterized by a contact angle exceeding 145 degrees.

(Note: Octaview code is provided).

Problem 2.2: ***Beating the diffusion limit by flow.***

Consider a disk sensor embedded in fluidic channel with w=4 μm, h=1 μm. The analyte concentration is ρ_0 = 1fM and its diffusion coefficient is D=150 μm^2/s.

(a) Write the expressions for Pe and total flux I.
(b) Plot the total flux I as a function of the sensor radius a. Calculate for both volumetric flow $Q =$ 0.1 and 10 $\mu L/min$.
(c) From the lecture slides, you should expect $ln(I) \sim (5/3)ln(a) + c$, where c is a parameter that depends on variables other than the radius, a. Confirm this approximate relationship from the plot in part (b).

(Note:. Octaview code is provided).

Problem 2.4: ***Diffusion in confined geometries.***

Consider two concentric cylinders of radius a and b, respectively. The cylinder (with radius a) is a perfect sink. The particles are being injected at a radius x_0 from the center.

(a) Use the 'charge control model' to show that

$$\tau = \frac{b^2}{2D} ln\left(x_0/a\right) + \frac{1}{4D}\left(a^2 - x_0^2\right)$$

(b) Calculate the MFPT based on the diffusion equivalent capacitance approach.

$$\frac{\tau}{A} \approx \frac{1}{2\pi D} ln\left(x_0/a\right)$$

(c) Show that when $b \gg a$, the results in part (a) reduces to that of part (b), suggesting that the diffusion equivalent capacitance provides excellent approximation to the exact result.

This completes the problem set for HW2