

Sensor in a microfluidic channel. Estimation of the time needed to reach equilibrium.

The following simplified mathematical description is meant to be used for an estimation of the characteristics of molecular detection on sensors placed on the side of a microfluidic channel, given the geometrical dimensions, the flow rate, the diffusion constant and the concentration of target molecules.

In the hypothesis of “perfect collection” ($k_{\text{off}} \rightarrow 0$ and $k_{\text{on}} \rightarrow \infty$), the time τ_{eq} needed to reach the density Γ_{eq} (the equilibrium density of target molecules on the surface of the sensor) depends only on the DIFFUSION and CONVECTION phenomena which determine the number of molecules that reach the surface of the sensor per unit time (i.e. J_D , the collection rate). Finally, the time τ_{eq} to reach the equilibrium density on the sensor is determined by the total number of target molecules on the sensor at equilibrium ($\Gamma_{\text{eq}} * \text{Sensor-surface}$) divided by the rate of arrival of target molecules on the surface of the sensor (J_D).

Let's define the parameters of the system:

Q volumetric flow rate

H height of the channel

W_c width of the channel in the direction normal to the flow

W_s width of the sensor in the direction normal to the flow

L length of the sensor in the direction of the flow

C concentration of target molecules in the sample

D diffusion constant of the target molecules

δ extension of the depletion region

Expression of the collection rate J_D

If the flux of molecules is:

$$j_D = -D \nabla C = -D \left(\frac{C_{\text{depl}} - C}{\delta} \right) = D \frac{C}{\delta} \quad (1)$$

then the collection rate is

$$J_D = j_D * \text{section crossed by the flux} \quad (2)$$

The section crossed by the flow is the boundary of the depletion region normal to the direction of the flux.

Two cases are possible depending on whether convection wins over diffusion: (CASE 1: the depletion zone extends only in the region right above the sensor leaving most of the channel height unaffected)

$$J_D = D \frac{C}{\delta} L W_s \quad (3)$$

or diffusion wins over convection (CASE 2: the depletion zone extends towards the entire height of the channel and upstream):

$$J_D = D \frac{C}{\delta} H W_c \quad (4)$$

In order to determine which of the two cases is verified, it is useful to compare the time needed for a molecule to diffuse across the height of the channel ($\tau_{H,D} = H^2/D$) and the time spent to travel the same distance by convection ($\tau_{H,C} = H^2 W_c/Q$).

$\tau_{H_D} / \tau_{H_C} = Pe_H \ll 1$ Diffusion wins, CASE 2

$\tau_{H_D} / \tau_{H_C} = Pe_H \gg 1$ Convection wins, CASE 1

where $Pe_H = Q/DW_c$ (5)

which does not depend on the height of the channel.

Hypothesis of strong convection and expression of the depletion region

In order to promote the delivery of molecules by convection, Q must be sufficiently high. In this hypothesis $Pe_H \gg 1$ and (3) hold.

The depletion region extends above the sensor for a distance δ_s . At height δ_s from the surface the molecule takes the same time to diffuse down to the surface and to flow the length of the sensor.

The time employed to cover the length L of the sensor by convection is

$\tau_{s_C} = L/(\text{velocity at height } \delta_s)$

$(\text{velocity at height } \delta_s) = (6Q/H^2W_c) * \delta_s$

on the other side, the time to reach the sensor by diffusion across the depletion region is

$\tau_{s_D} = \delta_s^2/D$.

From the identity $\tau_{s_D} = \tau_{s_C}$ we obtain the following relation:

$$\frac{\delta_s}{L} = \sqrt[3]{\frac{1}{6 Pe_H \lambda^2}} \quad (6)$$

where $\lambda = L/H$.

The expression in (6) can be employed to calculate the extension of the depletion region and include it in equation (3) to obtain the collection rate.

Moreover, we can define

$$Pe_s = 6 Pe_H \lambda^2 \quad (7)$$

and observe that

for $Pe_s \gg 1 \rightarrow \delta_s \ll L$ (the extension in z of the depletion region is smaller than the length of the sensor along the flow direction. Case verified for large(r) sensors).

For $Pe_s \ll 1 \rightarrow \delta_s \gg L$ (the extension in z of the depletion region is larger than the length of the sensor along the flow direction. Case verified for small(er) sensors).