

SUPPLEMENTARY INFORMATION

Underpinning transport phenomena for the patterning of biomolecules

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Finite element numerical simulations of transport of species and surface reaction were performed with COMSOL Multiphysics v4.2 (COMSOL, Inc., Burlington, MA). The governing equation, the convection-diffusion equation, defines the concentration of a species as a function of time under the influence of an advective flow:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) + \nabla \cdot (\vec{u}c) = R$$

where c is the concentration of species, D the diffusion coefficient, \vec{u} the velocity field and R the 'sink' or 'sources' of the species (∇ represents gradient and $\nabla \cdot$ divergence). We modelled the system as a 2D cross section, where we assume that any wall effects on fluid velocity in the width direction is negligible (valid if $W \gg H$). Assuming a constant diffusion coefficient and an incompressible fluid the equation simplifies to:

$$\frac{\partial c}{\partial t} - D\nabla^2 c + \vec{u}\nabla c = R$$

where R represents the 'sink' due to the transfer of species from the solution to the surface. This transfer of species was modelled assuming first-order Langmuir kinetics, with R equivalent to the binding rate of

the analyte on the surface
$$R = \frac{\partial b}{\partial t},$$

$$-R = k_{on} c (b_m - c_s) - k_{off} * c_s$$

c_s is the analyte concentration near the substrate surface, b the concentration of bound analyte on the surface, b_m the surface concentration of binding sites, and k_{on} and k_{off} the association/dissociation constants (see Eqn. 1 in Section 3 of main manuscript). This was modelled as a general form boundary PDE

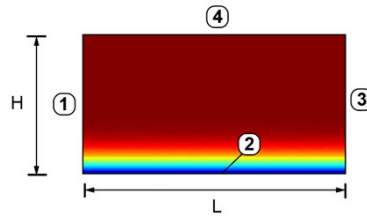
Three cases were analyzed: static diffusion (Section 3 of manuscript), laminar flows and laminar flows with recirculation (both in Section 6 of manuscript).

1. Static diffusion

FEM simulations of purely diffusive systems were performed in the absence of flow $\vec{u} = 0$,

$$\frac{\partial c}{\partial t} = D\nabla^2 c - R$$

The device geometry was defined according to:



with the following boundary conditions:

Surfaces 1, 2 and 3: $\vec{n} \cdot D\nabla c = 0$

Surface 4: $-R = k_{on} c (b_m - c_s) - k_{off} * c_s$

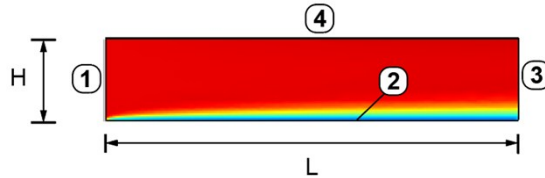
A global initial value of $c(t = 0) = c_0$ was imposed for all the cross section.

2. Laminar flow

Laminar flow was simulated with a parabolic flow profile in the horizontal direction:

$$\vec{u}(y) = v_{max} \left(1 - \left(\frac{y - H/2}{H/2} \right)^2 \right) \vec{e}_x$$

where \vec{e}_x is the unit vector in the direction of flow and v_{max} the maximum velocity of the profile in the center of the channel. The following boundary conditions were defined on each surface:



Surface 2: $c = c_0$

Surface 4: $-R = k_{on} c (b_m - c_s) - k_{off} * c_s$

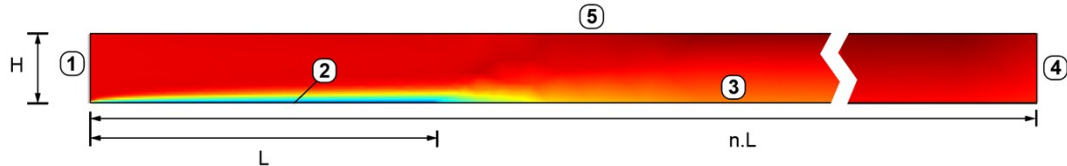
Surface 3: $\vec{n} \cdot D\nabla c = 0$

Surface 1: $\vec{n} \cdot (-D\nabla c + c\vec{u}) = 0$

And the global initial value was $c(x,y, t = 0) = c_0$

3. Laminar flow with recirculation

The recirculation of the laminar flow was simulated with the flow profile defined in 2, but the length of the model system was multiplied in the direction of flow to account for the volume of recirculated solution. $HxWxL$ represents the volume of reagent currently flowing over the substrate of interest and $HxWxLx(n-1)$ represents the volume of reagent recirculating before its next interaction with the substrate. The following boundary conditions were imposed:



$$c = \frac{\sigma}{H} \int_0^H c(x = n.L, y) dy$$

Surface 1:

Surface 2: $R = k_{on} c (b_m - c_s) - k_{off} * c_s$

Surface 4: $\vec{n} \cdot D\nabla c = 0$

Surface 3&5: $\vec{n} \cdot (-D\nabla c + c\vec{u}) = 0$

And global initial value of $c(x, y, t = 0) = c_0$

Surface 1 represents the continuity of surface 4 of a finite solution constantly recirculating in a loop. We assume a perfect mixing of the solution during recirculation. This is obtained by averaging the value of the concentration of species reaching surface 4 and imposing it as a constant uniform concentration at surface 1. Finally, to account for possible dilutions of the solution during recirculation, the concentration at surface 1 is multiplied by a factor σ representing the rate of dilution ($\sigma = 1$ when the dilution is null).