ELECTRONIC SUPPLEMENTARY INFORMATION

Simple add-on devices to enhance efficacy of conventional surface immunoassays implemented on standard labware

Iago Pereiro, Anna Fomitcheva Kartchenko, Robert D Lovchik, Govind V Kaigala

IBM Research – Europe, Säumerstrasse 4, Rüschlikon, CH-8803, Switzerland.

E-mail: gov@zurich.ibm.com

Contents

SI.1 Shear rate under slide-based device	2
SI.2 Finite element simulations on the influence of flow conditions on kinetics of arrays of spots	3
Methodology	3
Results	4
SI.3 Vision of device designs for multiplexing	5
SI.4 Technical drawings of devices	6

SI.1 Shear rate under slide-based device

We used a 2D radial model COMSOL Multiphysics 4.4 to simulate shear rate conditions on the surface under the slide-based device (for the well-based device see Figure 5c in the manuscript). As seen, the shear rate is very uniform across the entire area below the tapered geometry until its edge. For an injected flowrate of 50 μ L/min, she created shear rate on the surface varies in a small range of 300-310 s⁻¹. The only exception to this is the small region below the central injection aperture, where shear rate increases symmetrically from a central point of null shear rate. At this point the lateral component of the flow velocity is zero.



Figure S1. FEM-simulation of shear rate conditions at the surface below the slide-based device. A profile of shear rate as a function of radius is provided between the inlet aperture and the surrounding groove.

SI.2 Finite element simulations on the influence of flow conditions on kinetics of arrays of spots

Methodology

We used COMSOL Multiphysics 4.4 to simulate the transport of species in a symmetrical quadrant of an array of spots. The volume of liquid analyzed had an inner radius of 0.15 mm and outer of 2 mm, and contained on its bottom surface 9 spots separated by 0.5 mm and of diameter 0.2mm, corresponding to a full array of 6x6 spots (Figure S1a).

The transport of the analyte was simulated with the Transport of Diluted Species module, making use of the convection-diffusion equation and assuming a constant diffusion coefficient and an incompressible fluid. For a concentration of analyte *c*:

$$\frac{\partial c}{\partial t} - \mathbf{D}\nabla^2 c + \vec{u}\nabla c = R \tag{1}$$

The magnitude of the convective flow in the volume of liquid \vec{u} was set as $\sigma.z$, where σ is the shear rate and z the orthogonal direction to the surface containing the array. We simulated both constant shear rate conditions, as created with the presented devices, and the equivalent conditions with a flat device without a tapered geometry. In this latter case $\sigma.z$ was multiplied by a factor $3Q/\pi H^2$ to account for the decaying shear rate. The shear rate σ was set at 300 s⁻¹, approximately corresponding to an injection flow-rate Q of 50 µL/min.

On the spots, we set a boundary condition with a flux of analyte *R* defined by first order Langmuir kinetics, where *b* is the density of bound analytes:

$$-F = k_{on} c (b_m - b) - k_{off} * b$$
⁽²⁾

The association rate constant k_{on} was fixed at 500 m³/mol.s and the dissociation rate constant k_{off} as 1×10^{-3} s⁻¹. The surface density of analytes b_m was set as 3×108 mol/m². The initial concentration in the volume was 0, and fixed at 6.7 mol/m³ in the inlet for the injected flow. Symmetrical boundary conditions were set on lateral and top surfaces.

The mesh of the volume was set with a free triangular mesh on the bottom surface that was swept in the direction *z*, and a boundary layer with 18 levels of increasing height was set at this surface, the initial elements of height 0.5 μ m. The total amount of elements in the mesh was 9.3x10⁶.

Results

As shown in Figure S1, the tapered geometry ensures a lower and more constant depletion layer over the spots of the array as compared with a device lacking this feature. In the latter, the depletion layer increases from spots 1 to 3 due to a decreasing shear. Additionally, much of the depletion of analyte from inner spots is transferred to the outer spots, increasing the size of the depletion layers downstream. For the tapered device this phenomenon is more attenuated, as the high shear inbetween spots minimizes the development of this layer. The sizes of the depletion layers, calculated as the height to reach 90% of the concentration of the injected reagent, were 2.5, 4.5 and 5.5 μ m for the tapered geometry and 3.5, 6.5 and 13.5 μ m for the flat geometry.



Figure S2. FEM-derived depletion layer over spots at 3 different distances from device inlet. (a) Section of the analyzed liquid volume over the spots, showing the concentration of analyte over each spot after 60 s of flow injection and flows from two different device geometries; (b) concentration profile of the resulting depletion layers for the three spots and two geometries.

SI.3 Filling of working area under tapered geometry



Figure SI 3. Injection of red colorant at 50 μ L.min⁻¹ from central aperture starting from a dry state. The liquid fills from the center towards the edges, filling first the areas where the ceiling is heigher.

SI.4 Technical drawings of devices



Figure SI 4. Technical drawing of the well-based device monolith with dimensions in mm.



Figure SI 5. Technical drawing of the slide-based device monolith with dimensions in mm.