

Influence of Lift Forces on Particle Capture on a Functionalized Surface - Supporting Information

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S1: Lagrangian Simulation

A set of particles is initialized with a homogeneous concentration at $x < 0$. At each time step dt , particles are convected along x over a distance $v_x(z)dt = \frac{6Q}{W_c H^3} \left(\frac{H}{2} + z\right) \left(\frac{H}{2} - z\right) dt$, *i.e.* as in a Poiseuille velocity profile. Then, each particle moves along z over a distance $v_{\tilde{z}_{\text{Lift}}}(z)dt$ due to lift forces, and of a distance $\sqrt{6Ddt}$ in a random $3D$ direction due to Brownian motion. The value of the diffusion coefficient D is computed using Einstein law.¹ If, due to random walk, a particle is found outside the channel, it is set in a mirror position with respect to the wall separating it from the channel. A particle disappears from the simulation when it reaches a preset position $x = x_{\text{end}}$. The corresponding exit time and exit height are recorded.

At the end of the simulation, for each height interval $[z; z + \Delta z]$, the number of particles per unit of time that exited this portion of height can be computed. This quantity theoretically equals to $c(x_{\text{end}}; z)v_x(z)\Delta z$. The local concentration is then obtained by dividing the former quantity by $v_x(z)\Delta z$.

Table S1: ξ as a function of the Lifto-Diffusive Number \mathcal{N}_{LD} .

\mathcal{N}_{LD}	ξ
0,01	9,99E-01
0,1	9,92E-01
1	9,19E-01
3	7,76E-01
5	6,53E-01
7	5,48E-01
10	4,20E-01
15	2,67E-01
20	1,67E-01
25	1,04E-01
30	6,39E-02
35	3,89E-02
40	2,36E-02
45	1,42E-02
50	8,46E-03
60	2,97E-03
70	1,03E-03
80	3,51E-04
90	1,19E-04
100	3,98E-05
150	1,57E-07
200	5,77E-10

S2: *Lidi* - Software User Manual

In this section, we present a detailed example of use of the free of access software *Lidi*, available at <http://lidi.ens-rennes.fr/download>. This software can automatically compute, without requiring a powerful computer, the equilibrium concentration profile, the Lifto-Diffusive number \mathcal{N}_{LD} , the correction factor ξ and the critical flow rate Q_c . It also includes

the simulation code used in this article to compute the transient profiles of Figure 7.

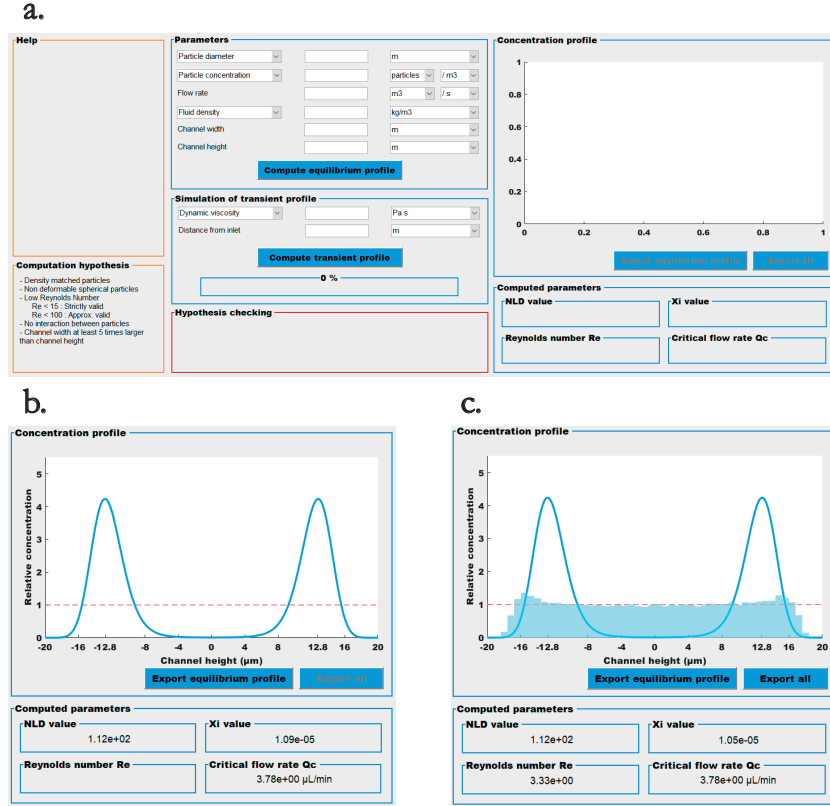


Figure S1: Screenshots from the free-of-access software *Lidi*. (a) Complete software view. (b) Result panels after equilibrium profile computation. (c) Result panels after transient profile computation.

Panels Description

The software is composed of 7 panels (see Supplementary Figure 1). From left to right :

- The **Help** panel displays information on any element the mouse pointer is on.
- The **Computation hypothesis** panel reminds the physical hypothesis under which the software gives accurate results.
- The **Parameters** panel has to be fill in for the calculation to be performed. Then, the user can click on the Compute equilibrium profile button to launch the computation,

giving equilibrium concentration profile together with \mathcal{N}_{LD} , ξ and Q_c values. Detail of the inputs are described in the Input Description section.

- The **Simulation of transient profile panel**. These additional parameters are required only for running the transient concentration profile simulation. Details of the inputs are described in the Input Description section. A progress bar indicates the progress of the simulation once launched.
- The **Hypothesis checking panel** shows warning messages after computation if some parameters seem not physical or in contradiction with the validity hypothesis described in the Computation hypothesis panel. When a warning message is displayed, the results given by the software could be inaccurate or completely wrong.
- The **Concentration profile panel** displays the concentration profile, both at equilibrium (as a blue line) and transient (as a dark blue histogram). A red dashed line is also plotted, representing the initial flat profile. Two buttons allow exportation of the profile (either the equilibrium one or both). The input parameters are also recorded in the exportation folder.
- The **Computed parameters panel** shows the \mathcal{N}_{LD} , ξ and Q_c values after any computation. After transient simulation, it also shows the Reynolds number Re value.

Inputs Description

In the case of multiple choices for the input parameters, they are clearly indicated in the following text through the punctuation /. For both the input parameters and the units, the choice can be made in the software using a scrolling list. The accepted number formats are 0.2 or 0,2 or 2e-1 or 2E-1.

Inputs for Equilibrium Computation

- **Particle diameter/Particle radius**

Enter the particle size. In case of a polydispersed particle population, we recommend to run a different computation for each range of size, as the larger particles could be focused while the smaller could display a flat profile. Under the hypothesis that particles do not interact, their respective concentration profiles are independent.

- **Particle concentration/Relative concentration**

Two options are proposed:

- Particle concentration: Enter the exact injected particle concentration.
- Relative concentration: As long as the particles do not interact, the result does not depend on the particle concentration. As such it is possible to normalize the concentration profile by the initial bulk concentration. This option has the advantage to provide a generic result for all concentrations, given the other experimental parameters are constant. Consequently, no input is required with this option.

- **Flow rate**

Enter the injection flow rate.

- **Liquid density/Liquid relative density/Water density**

Three options are proposed:

- Liquid density: Enter the Liquid density
- Relative liquid density: Enter the liquid density relative to water density
- Water density: The software will consider that the surrounding liquid has the same density as water at room temperature ($\rho = 10^3 \text{ kg/m}^3$). No input needed.

- **Channel width and Channel height**

Enter the width and the height of the considered channel. The software supposes that the channel width is larger than the channel height (at least 5 time larger), so that the concentration profile is homogeneous along the width of the channel. If not, a warning message will invite the user to change these values.

Inputs for Transient Computation

- **Dynamic viscosity/Kinematic viscosity/Water viscosity**

Three options are available:

- Dynamic viscosity: Enter the value of the dynamic viscosity η .
- Kinematic viscosity: Enter the value of the kinematic viscosity $\nu = \eta/\rho$.
- Water viscosity: The software will consider that the surrounding liquid has the same dynamic viscosity as water at room temperature ($\eta = 10^{-3}$ Pa s). No input needed.

- **Distance from channel inlet**

The distance between the channel inlet (where particle concentration is flat) and the position where the transient concentration profile will be computed. The more this value is important, the more the computation will be long.

Detailed Example

The example detailed below corresponds to particles of 1 μm diameter flowing in water in a channel whose dimensions are 200 μm x 40 μm , with a flow rate of 40 $\mu\text{L}/\text{min}$. The transient concentration profile desired is taken 5 cm far from the channel inlet.

1 - Computation of the equilibrium profile

The input parameters are entered in the Parameters panel to perform the equilibrium profile.

- For the particle size, two options are valid:
 - choose *Particle diameter*, choose unit μm and enter 1.
 - or choose *Particle radius*, choose unit μm and enter 0.5.
- In this example, the *Relative concentration* option has been chosen. The real concentration profile for any experiment can be obtained by multiplying the relative concentration profile by the mean experimental injection concentration.
- For the flow rate, choose units μL and $/\text{min}$ and enter 40.
- For the liquid density, three options are valid:
 - choose *Liquid density* and choose the unit kg/m^3 and enter 1000
 - or choose *Liquid relative density* and enter 1.
 - or choose *Water density*.
- For the channel height and width, the largest dimension must be the width. If not, a warning message will pop in red after the computation in the hypothesis checking panel.
 - For the width, choose unit μm and enter 200.
 - For the height, choose unit μm and enter 40.

Then, click on the *Compute equilibrium profile* button. The concentration profile panel and the computed parameters panel refresh instantly to the state depicted on Supplementary Figure 1b. The *Export equilibrium profile* button is now activated. Click on it to export the concentration profile, the parameters and the computed parameters.

2 - Computation of the transient profile

To compute the transient profile, the Simulation of transient profile inputs need to be filled in:

- For the viscosity, three options are valid:
 - choose *Dynamic viscosity* and choose unit *Pa s* and enter 1e-3 or 0.001
 - or choose *Kinematic viscosity* and choose unit m^2/s and enter 1e-6
 - or choose *Water viscosity*
- For the distance from channel inlet, choose unit *cm* and enter 5.

Click on the Compute transient profile button. A progress bar begins to fill. This example is typically computed in a time between some seconds to one minute depending on the computer. The computed parameters panel then refreshes to the state depicted on Supplementary Figure 1c. The *Export all* button is now activated. Click on it to export the concentration profile, the transient profile, the parameters and the computed parameters.

References

- (1) Einstein, A. Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. *Annalen der physik* **1905**, 322, 549–560.