SUPPORTING INFORMATION

Experimental and numerical study of band-broadening effects associated with analyte transfer in microfluidic devices for spatial two-dimensional liquid chromatography created by additive manufacturing

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A comparison between computational and experimental work was conducted for validation purposes of the computational setups. The examined device was the empty type X device (see Figure 1S, Table 1 and Figure 2).

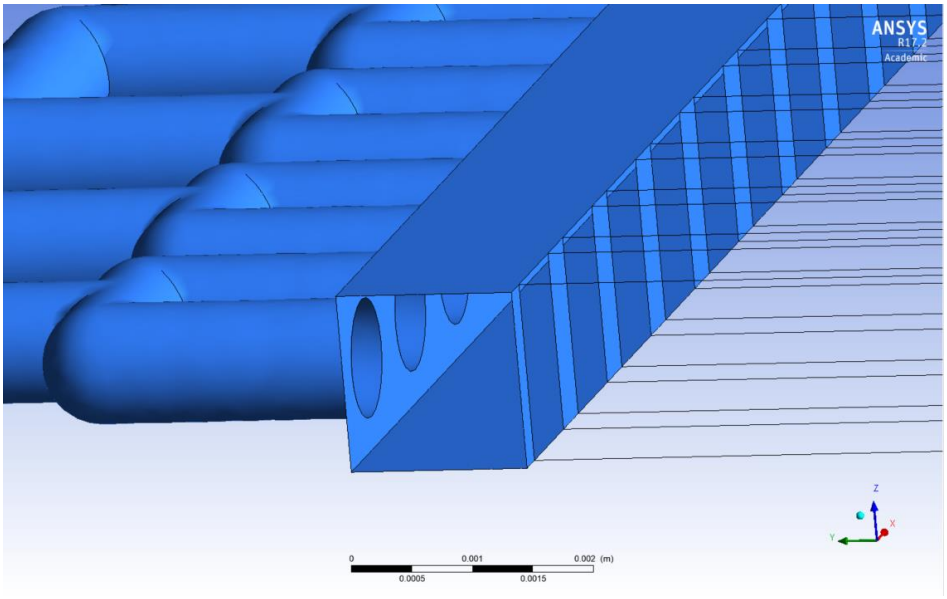

Figure 1S. A zoom-in of the design used for the simulation. The walls of the distributor and the ^{1}D channel are with blue, while the walls of the ^{2}D channels are shown as a wireframe.

For the calculation of the variance at the computational setup, the mass fraction of dye over time was extracted as an area weighted average at two control planes parallel to the ^{1}D channel, one at the start (CP1) and one at the end of the ^{2}D area (CP2). For the experimental setup, the band variance in the time domain was calculated at two control lines corresponding to the position of the control planes in the simulation setup (CL1 and CL2 respectively). The variance at CP1 and CL1 was then subtracted from the variance at CP2 and CL2. The position of CP1-2 and CL1-2 is shown in Figure 2S.

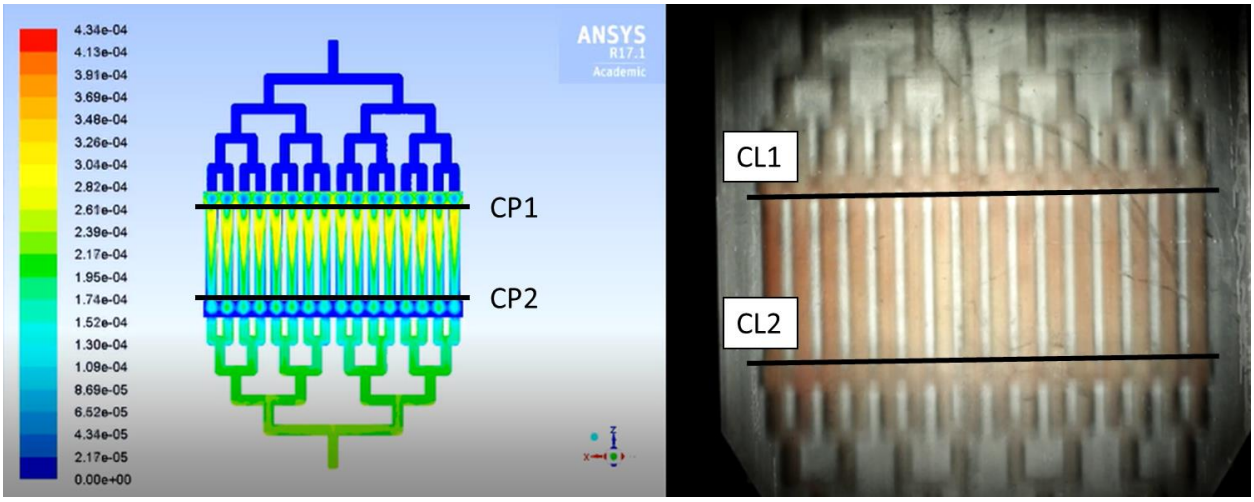

Figure 2S. Left: the profile of the mass fraction of dye calculated via computational fluid dynamics (CFD), right: the red dye migrating in the device.

In both cases, equations [1S] and [2S] were used for the calculation of the variance.

$$\bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt} \qquad [1S]$$

$$\sigma^2 = \frac{\int_0^\infty t^2 Cdt}{\int_0^\infty Cdt} - \bar{t}^2 \qquad [2S]$$

The difference in variance corresponding to that case was 403.6776 s^2 while from the simulations it was 77.3717 s^2. This discrepancy could be due to the differences in recording the variance between the simulation and experiment. In the simulation, the concentration over time was extracted as the average for the two cutoff planes while in the experiment it was extracted from the top view. Additionally it could be caused by differences between the 3D-printed part and the design.