A chip system for hydrodynamic chromatography
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CHAPTER 5

Design of a Low Dispersion Outlet for a Flat Conduit with Pressure-Driven Flow

Flow and dispersion of species has been studied in differently shaped outlets for a flat, shallow and wide microfluidic channel. The aim is the coupling of such channel, used as an analytical separation column, to a narrower detection channel or cell. Two general small-volume designs - a flat nozzle and a transversal slit - are suggested. For each, an optimized form is derived using geometric and fluidic considerations. Simulations by 3D computational fluid dynamics are performed for all structures and the results are converted into general transfer functions for concentration. The contribution to the second moment of a species zone is calculated. The dispersion in the optimized outlets is found to be the lowest.

Introduction

Extracolumn zone broadening becomes the limiting factor for the performance of analytical separation methods when the efficiency of the column itself is high enough. Besides the contribution from the injection this zone broadening is generated in the connection to the detector and in the detection cell. The latter is the more difficult to suppress, because the sensitivity of a detector in general increases with the cell volume or the cell optical path length. A general rule¹ states that extracolumn fluidic structures should be small in volume and streamlined in geometry in order to maintain the zone integrity.

In analytical microdevices created on a microfluidic chip,² high efficiencies can be achieved by reducing the column dimensions and by integrating the system components on a small area. For pressure-driven separations, plain conduits of a large-aspect-ratio cross-section³ offer the advantage of both a sufficient loadability and smaller dispersion as compared to the use of cylindrical channels. Such shallow wide channels are, however, mostly not suitable for a direct integration with a microdetector, except perhaps with electrochemical or evanescent light techniques.⁴ For example, in classical optical detection principles based on absorption or deflection of an excitation beam (e.g. UV absorption,
fluorescence, classical refractive index detectors), the aligning of the excitation beam with the channel plane would be very difficult if not impossible, especially when the channel depth approaches the wavelength of the light.\textsuperscript{5} The alternative configuration with the beams perpendicular to the shallow channel plane would not profit from a larger width, however. A low-dispersion transition into a narrower deeper channel is then a potential solution. In addition, via confining the flow into a narrow outlet channel measurable pressure drops\textsuperscript{6} can be created and used for viscometric detection of macromolecules. An outlet cross-section close to that of cylindrical microcapillaries would allow the use of already developed coupling techniques to e.g. mass spectrometry.\textsuperscript{7} In addition, a low dispersion coupling is needed when two or more channels are used in series with alternating orientation to fit a longer column onto a chip. Simple U-turns would cause a large dispersion, for similar reasons as in electrodriven devices, where this effect has been studied in detail.\textsuperscript{8}

Here, we present a study of various outlet designs for a 1 \( \mu \text{m} \) deep and 500 \( \mu \text{m} \) wide microchannel with pressure driven flow, which is suitable for on-chip liquid chromatography (LC), specifically hydrodynamic chromatography (HDC) of macromolecules and particles.\textsuperscript{3} The results may also be helpful in the design of larger scale channels e.g. for Flow- or Thermal Field-Flow Fractionation\textsuperscript{9} (FFF) or elsewhere when uniform collection of flow from a flat tube is required.

\textit{Theory}

\textbf{Governing equations}

In microdevices, flow of liquids is dominated by viscosity, because of the small dimensions (Re \( << 1 \)). For this special form of laminar flow, called creeping flow,\textsuperscript{10} the inertia term in the momentum equation can be neglected. The Navier-Stokes equations then become linear. For incompressible stationary creeping flow

\begin{align}
\nabla \cdot \mathbf{u} &= 0 \quad \text{(1a)} \\
\eta \nabla^2 \mathbf{u} &= \nabla p \quad \text{(1b)}
\end{align}
Here, \( u \) is the velocity field, \( p \) the pressure profile and \( \eta \) the dynamic viscosity. The accuracy of the flow equations for dimensions of \( \sim 1\,\mu\text{m} \) or smaller has been questioned in literature. The authors have observed deviations from the predicted pressure drops and attribute this to the molecular effects on viscosity near the channel walls. However, experiments supporting the validity of the equations in this small scale were also reported. In this study we assume that the equations (1) hold for channel dimensions down to \( 1\,\mu\text{m} \).

The transport of non-reacting species is governed by the convection-diffusion equation

\[
\frac{\partial c}{\partial t} = D \nabla^2 c - \mathbf{u} \cdot \nabla c
\]

(2)

where \( t \) is time \( c \) is the concentration profile and \( D \) the diffusion coefficient. A specific solution of (2) in dimensionless form applies to all cases of the same Peclet number \( Pe = ud/D \) and Strouhal number \( St = d/ut \), where \( u, d, \) and \( t \) are respectively a characteristic velocity, geometric dimension and time in the system. When the cases differ in velocity field however, this difference has to be uniform in space i.e. \( u_2(x,y,z) = au_1(x,y,z) \). This is strictly possible only when the Navier-Stokes equations become linear i.e. in the creeping flow regime, the present situation.

Analytical solution of eqn's (1) and (2) is possible only for simple cases. However, the state-of-the-art 3D Computational Fluid Dynamics (CFD) provides accurate numerical solutions in virtually any geometry, if sufficient computer power is available.

Although specific conditions have to be selected for the simulation, generally applicable results are obtained here, because the above mentioned invariance of (2) applies also for the scaling in chromatographic separation channels. In addition, independence on the injected zone profile can be achieved by converting the results into transfer functions.

Chromatographic zone dispersion

The sample moves through the system subject to convection and diffusion. This leads to zone dispersion and determines, together with the differential migration achieved in the separation column, the resolution of the method. The dispersion is characterized by the
second moment $\sigma^2$ of the zone concentration profile, formed by contributions from the separation column and the external components:

$$\sigma^2 = \sigma^2_{\text{col}} + \sum \sigma^2_{\text{ex,i}}$$

(3)

Here $\sigma$ is the standard deviation of the zone.

In a properly designed system $\sigma_{\text{col}}$ is the only major contribution to the dispersion, while other contributions should together cause less than $\sim 10\%$ of the final peak width. (In this case $\sigma_{\text{ex}} < 0.3 \sigma_{\text{col}}$). $\sigma_{\text{col}}$ depends on the column Peclet number, also called reduced velocity $v$. For a flat channel $v = \langle u \rangle h_c/D$ where $\langle u \rangle$ is the average fluid velocity and $h_c$ the channel height. An optimum value $v = v_{\text{opt}}$ exists for which the dispersion in the column is minimal, and thus the highest separation resolution is obtained. For an unretained zone in a flat channel $v_{\text{opt}} = \sqrt{210}$. The optimum velocity and the minimum dispersion (in length units) are then

$$\langle u \rangle_{\text{opt}} = \sqrt{210}D/h_c$$

(4)

$$\sigma^2_{\text{col.min}} = 2\sqrt{2/105Lh_c}$$

(5)

where $L$ is the column length.

In this study we assume this kinetic optimum situation. For the channel depth of 1 $\mu$m, the theoretical $\sigma_{\text{col.min}}$ is 150 $\mu$m (i.e. 75 pL for a 500 $\mu$m wide channel) for the 8 cm long channel used in the HDC chip prototype. However, a good separation was observed already in a much shorter length of this channel, viz $\sim 2$ cm. A channel of this length may thus be preferred in some cases, because of smaller pressure drops. For the shorter channel $\sigma_{\text{col.min}}$ would be 75 $\mu$m (37.5 pL at a 500 $\mu$m width).

In size-separation methods such as HDC, where the individual constituents differ in diffusion coefficient substantially because of the different size, the velocity can be optimized for species of an intermediate size resp. diffusion coefficient. In our device the velocity of $\sim 0.5$ mm/s is a good trade-off between the speed and resolution. This velocity is the optimal one for a diffusion coefficient of $3.5 \times 10^{-11}$ m$^2$/s$^{-1}$. These values are therefore
used in this study. It is stressed however, that the results, expressed in volume units, hold for all cases of the same reduced velocity $v$, in this case $v_{opt}$. This is because the scaling of the flow separation column according to $D$ is accompanied by the same, uniform scaling of the flow in the outlet (in view of the incompressible creeping flow regime at hand), and thus constant $Pe$ there.

**Transfer function**

The effects of various parts of a fluidic system on the transported zones of species can be described in more detail by a transfer function for concentration $h(t)$.$^{16,17}$ This is, under certain conditions, independent of the injected zone length and profile in time. A sufficient condition is a uniform distribution of the concentration over the inlet section. The transfer function can be obtained by deconvoluting the input function (initial profile) $f(t)$ from the output function (the resulting profile) $g(t)$ of the system, obtained either from an experiment or a simulation. The deconvolution is performed using Fourier transforms$^{18}$ (FT, and inverse the transform $FT^{-1}$) as illustrated below

```
\[
\begin{align*}
    f(t) & \quad \text{FT} \quad F(\omega) \\
    \text{fluidic structure} & \quad \text{CFD or experiment} \\
    g(t) & \quad \text{FT} \quad G(\omega) \\
    \end{align*}
\]
```

The transfer function has the same shape as would have a response function of the system to an input concentration Delta-pulse. A response function for an arbitrary $f(t)$ can then be obtained by convolution with $h(t)$.

**Alternative Geometries**

**Flat nozzle**

The simplest small-volume transition from a wide to a narrow channel is a flat nozzle with equal depth (Figure 1). This can be made as plain or alternatively with splitting features$^{19}$
which should more or less equalize the times the sample travels from different positions over the channel width to the end orifice. This should minimize the zone dispersion and distortion. In our case, the nozzle has to couple the above mentioned channel to a narrow measuring channel of a microviscodetector\textsuperscript{6} which is 20 μm wide x 1 μm deep.

The dispersion of a sample in a plain nozzle used as an inlet for a FFF channel has been experimentally studied by Giddings.\textsuperscript{9} Flow in a flat nozzle is also studied in.\textsuperscript{20} According to Giddings, both the longer path and lower velocity along the sides of the nozzle (as compared to the middle) result into some peak distortion and dispersion. In a plain nozzle, the angle of the converging walls is the only parameter to choose. With smaller angles, the differences in length decreases but the nozzle allocates more space. For this study, an angle of 90 ° was used.

![Diagram of flat nozzle outlet](image)

**Figure 1:** The design of a flat nozzle outlet. Plain nozzle (solid line) and the optional splitting features (hatched) used to equalize the path lengths (dashed line).

The splitting features were designed as shown in Figure 1, but other configurations with different number, size and position of the splitting features are certainly possible.

**Transversal slit**

Another small-volume outlet can be formed as a deeper slit, spanning across the width of the channel at the end of it. In microdevices, such slits can be created using the reactive ion
etching (RIE) technology. The simplest design is a slit of constant cross-section and positioned perpendicular to the channel axis. This form, however, is likely to cause a large dispersion.

An optimal shape for the transversal slit can be derived from the following constraints for time $t$, pressure $p$ and volumetric flow rate $F$ (see also Figure 2)

\[
\begin{align*}
\Delta t_1 &= \Delta t_0 \\
\Delta p_1 &= \Delta p_0 \\
F_1(z) &= \frac{z}{w} F_0
\end{align*}
\]

(6a) (6b) (6c)

where $w$ is the total width of the flat channel and indices 0 and 1 refer to a traveled path (Figure 2) in the flat channel region (B to C) and in the slit (A to C) respectively. Condition (6a) ensures that at every position along the slit the sample is eluting from the flat channel at the right moment when the already collected sample is passing by. Conditions (6b) and (6c) represent the continuity of pressure and mass.

![Figure 2: The scheme for the design of an optimized slit outlet.](image)

The conditions (6a-c) should ideally be satisfied all over the channel width i.e. $z \in (0,w)$. However, one can expect mathematical problems in the starting location, because there the slit width has to approach the depth of the channel, otherwise dead volumes and
nonuniformities would result. Therefore we examine the constraints for \( z \in (\xi, w) \) where \( \xi \) is the smallest \( z \) for which a consistent solution exists.

The relation between the pressure drop \( \frac{dp}{dl} \) and the flow rate for a conduit with an arbitrary cross-sectional shape is \(^{22}\)

\[
\frac{dp}{dl} = K \frac{F \eta}{qd^4}
\] (6d)

where \( d \) is the conduit characteristic cross-sectional dimension, \( \eta \) is the fluid dynamic viscosity and \( K \) and \( q \) are geometrical factors. The factor \( q \) relates \( d \) and the cross-sectional area \( S = qd^2 \). For rectangular cross-section, the smaller dimension \( b \) is taken as \( d \). Then \( q \) is the channel aspect ratio \( (q > 1) \). For lower aspect ratios \( K \) varies between 12 and 25. For wide shallow channels \( K = 12 \), \( d = h \) and \( q = w/h_r \).

The shape of the slit is defined by two functions. An "external shape" function \( a(z) \) describes the curvature of axis of the slit in the channel plane, while an "internal shape" function \( b(z) \) describes the variation in the cross-sectional dimension of the slit. An analytically tractable situation is obtained when a condition is imposed that the flow in the shallow part is parallel to \( x \) and constant in \((x, z)\). Then (6a) can be expressed for \( a(z) \) and its derivative to \( z \), \( a'(z) \) as

\[
\frac{a(z) - a(\xi)}{u_0} = \frac{1}{u_1(z)} \int_{\xi}^{z} \sqrt{1 + a'^2(z)} \, dz
\] (7a)

and the combination of (6b) and (6d) together with \( F_0 = u_0 h \) gives

\[
\frac{12u_0}{h^2} [a(z) - a(\xi)] = \frac{1}{\xi} \int_{\xi}^{z} K F_1(z) \, dz
\] (7b)

Taking \( \xi \) constant, using \( F_1(z) = Su = q b^2(z) u_1(z) \), differentiating to \( z \) and rearranging we get from (7a) and (7b)
Optimized Outlet

\[ u_1(z) = u_0 \sqrt{1 + \frac{1}{a'^2(z)}} \]  

(8a)

\[ \frac{12u_0}{Kh^2} = \frac{u_1(z)}{b^2(z)} \sqrt{1 + \frac{1}{a'^2(z)}} \]  

(8b)

The condition (6c) can be expressed as

\[ b^2(z)u_1(z) = \frac{hu_0}{q} z \]  

(9)

Combining (8a) and (9) we obtain one relation between the internal and the external shape of the slit

\[ \frac{h}{q} z = b^2(z) \sqrt{1 + \frac{1}{a'^2(z)}} \]  

(10a)

and combining (8b) and (9) we have another relation

\[ \frac{12}{Kh^2} = \frac{1}{b^2(z)} \left( 1 + \frac{1}{a'^2(z)} \right) \]  

(10b)

From equations (10a) and (10b) the internal slit shape \( b(z) \) can be obtained as

\[ b(z) = b_{\text{out}} \left( \frac{z}{w} \right)^{1/3} \]  

(11a)

\[ b_{\text{out}} = \left( Kh^4w^2/12q^2 \right)^{1/6} \]  

(11b)
The internal shape is thus fully constrained, starts from \( b(0) = 0 \) and ends with size \( b_{\text{out}} \), which is prescribed once a certain geometry and aspect ratio of the slit cross-section is chosen.

For the external shape \( a(z) \) we get from (10a) and (10b) after integration

\[
a(z) = \frac{3\ln\left(\sqrt{Az^{2/3}} - 1\right) + z^{1/3}}{2A^{3/2}} + \frac{3z^{1/3}\sqrt{Az^{2/3}} - 1}{2A} \\
A = \left(\frac{12}{Kqh}\right)^{2/3}
\]

(12a)

(12b)

where an integration constant was is set to 0, because it only represents shifting of the shape along the channel length. The function \( a(z) \) exists for \( z > (1/A)^{3/2} = Kqh/12 \), because the conditions cannot be satisfied in a small starting length of the slit, where its dimensions are smaller or comparable to the depth of the shallow channel. In addition, the initial part of the function is almost parallel to \( x \), because its shape is to a large extent determined by the logarithmic part. A practical option is to take \( z > (2/A)^{3/2} = Kqh/6 \), which assures that the logarithm in (12a) is positive and its slope deviates sufficiently from the parallel direction.

For the simulation we have extrapolated the function to \( z = 0 \) by a groove of a small constant cross-section. As shown in the results, this practically does not influence the flow in the structure.

Taylor dispersion\(^{23}\), which may be important in the broader parts of the slit, is not considered in this derivation. Accounting for this effect would require a complex iterative optimization procedure. Because Taylor dispersion decreases monotonously with a conduit cross-section, a slit, narrower than what equation (11) suggests, may perform even better, provided it does not deform the flow in the shallow part too much.

For the considered application for \( 500 \mu m \times 1 \mu m \) channel and e.g. a rectangular slit of aspect ratio \( q = 2 \), the geometrical factor \( K = 17.49^{22} \). The shape function exist and is positive for \( z > 5.8 \mu m \) and the outlet dimensions result as \( 6.7 \mu m \times 13.4 \mu m \). These dimensions can be achieved with the RIE technology\(^{21} \) and are close to the dimensions of cylindrical capillaries used in open tubular liquid chromatography where coupling to MS has been achieved\(^{7} \). The aspect-ratio of the slit cross-section produced by RIE is however
not constant due to the so-called RIE-lag effect\textsuperscript{21} and the presented shape functions may have to be corrected for this.

The straight slit, included in this study for later comparison has a uniform cross-section identical with the end cross-section of the optimized slit.

\textbf{Adaption for an optical cell}

In the considered application with the 500 $\mu$m $\times$ 1 $\mu$m separation channel, the end-orifice (6.7 $\times$ 13.4 $\mu$m) of the optimized slit is too small in cross-section to form an optical detection cell with practical detection limits. A change in an aspect ratio or geometry of the slit cross-section would not increase the cross-sectional area substantially (cf. eq. 11). With respect to this the slit is not much different from the flat nozzle where the end-orifice cross-section is limited by the shallow depth. In contrast, an optical cell should be at least a few tens of $\mu$m deep to create sufficient path length for e.g. UV absorption (perpendicular detection) and also a few tens of $\mu$m wide to allow alignment of external optical components e.g. fibers and apertures.\textsuperscript{24} A solution could be to couple a simple cell in a form of a larger groove right to the outlet designed either as the flat nozzle or the optimized slit as shown above. In this way dead volume would still be small. A large step increase in the cross-section may however result in trapping of bubbles or particulate material in the dead corners. A short and smooth expansion of the width may be used in the case of the optimized slit. For the coupling of the optical cell to the flat nozzle, a similar transition in the perpendicular direction would be desirable, but cannot be achieved with the RIE technology. An alternative would be the use of the above mentioned RIE-lag effect\textsuperscript{21}. The transition could be divided into several short narrow diverging slits, the depth of which would gradually increase with the width because of this effect. A brief study of such a structure, we call it a "beak" structure, is presented below.

A more extensive study would be necessary to find the proper cell dimensions. The contribution of the cell to the zone width due to the averaging over its volume is $\sim$ 5\%, when its volume is $V = \sigma_{v,\text{cell}}$.\textsuperscript{1} However, when the cell is formed by a groove of a large cross-section, the Taylor dispersion may increase the dispersion substantially. In this study we select a groove of 30 $\mu$m $\times$ 30 $\mu$m. The first 40 $\mu$m resp. 80 $\mu$m of its length can be used as a detection cell for the 2 cm resp. 8 cm long separation channels.
**CFD Setup**

For the CFD simulations the FLUENT™ software package (version 5.5.14) was used. The computation domain geometry was created and meshed in the default pre-processor GAMBIT™ (version 1.3.0). The numerical simulations were performed on a PC platform. All flows are pressure driven, laminar (Re~10^3–10^4) and modeled as stationary. The creeping flow approximation is not available in the software, therefore the more general laminar incompressible flow model was used. The flow calculations and species transport calculations were decoupled. First, the Navier-Stokes equations were solved for the carrier liquid to obtain the flow field. This field was then fixed and the time-dependent solution of the convection-diffusion equation was performed for an analyte, specified by a diffusion coefficient and initial concentration in boundary conditions.

As some of the considered structures are likely to influence the flow profile also in the final part of the separation channel, a 100 μm long straight inlet part is included in all the cases. The contribution of this part to the dispersion is negligible. The shape of the optimized outlet slit edges is approximated by 6 points and a "NURB" (software feature) polynomial fit. A large number of computation volume elements is necessary because of the large aspect ratios of the domain. Because of symmetry, in the case of the nozzles only a quarter and in the case of the detection cell only a half of the domain has do be modelled. A time step of 10^{-3} sec was used in all species transport simulations.

As the boundary condition, the velocity on the inlet boundary is set to be the velocity of 0.5 mm/s as valid in the separation channel. The carrier liquid is water at 293 K and the sample is a mixture of water and "analyte" with a diffusion coefficient \( D = 3 \times 10^{-11} \text{ m}^2\text{s}^{-1} \). The analyte is either introduced at \( t = 0 \) as a narrow (50 μm long) rectangular plug of mass fraction 0.001, or for a quantitative study, as a Gaussian profile in time on the inlet boundary, with standard deviation 75 ms, corresponding to 37.5 pL in volume. This zone profile enables an accurate simulation and postprocessing because it is long enough and thus smooth with respect to the grid spacing (1-3 μm) and still sufficiently influenced by the structures.
**Figure 3:** The meshed CFD domains for the nozzle with splitting structures (above) and the beginning part of optimized slit (below).

Higher order numerical schemes and double precision were used as recommended for large aspects ratio problems involving long thin conduits. The solutions are practically independent on the spatial and temporal discretization with the grids and the time step used. The amount of analyte, as reported by integration on the boundaries, corresponds to the amount introduced to the domain within ~ 0.5%.

The Fourier transformation was performed using standard modules in Mathematica (version 2.0).

**Results and Discussion**

Here we compare the results for the four suggested outlet geometries with the following dimensions of the end orifice: 20 x 1 \(\mu\)m both for the plain nozzle (a) and the nozzle with splitting structures (b) and 6.7 x 13.4 \(\mu\)m both for the straight (c) and the optimized (d) slit.
The contours of static pressure obtained in the flow simulation (Figure 4) show that the flow is most uniformly distributed both in the optimized slit and in the nozzle with structures. As seen, the flow pattern in the optimized slit is practically ideal despite of the shape extrapolation for the beginning part, for which the function (12) does not exist. Because of linearity of the creeping flow, the same flow distribution but of opposite sign would be obtained if the structures were used as inlets i.e. with reversed flow on the boundaries.

Figure 4: The flow simulation. The contours of the static pressure are plotted for the plain nozzle (a), nozzle with structures (b), straight slit (c) and the optimized slit (d).

The optical cell is flushed better when the beak-structures are used, compared to the step transition (Figure 5).

A practical illustration of the outlets performances is the simulation of the transport of a narrow rectangular zone of diffusing species (Figure 6). The dead volume in the bottom of the straight slit and the zone bending in the plain nozzle are likely to cause peak
broadening. In contrast, the optimized-shape slit or the splitting structures in a flat nozzle keep the zone more compact.

Figure 5: The profiles of the velocity magnitude in the depth transition for an optical cell. Only velocities lower than 0.4 mm/s are plotted. The transition with beaks (above) results in a more uniform flow in the beginning part of the cell than the step transition (below). The end orifice dimensions are 30 x 30 μm in both cases.

In order to obtain a more quantitative characterization of the outlets, the species simulation is performed for a broader, Gaussian input profile in time and the mass fraction is monitored as an average at the outflow boundary. From the deconvolution of the input and the response functions the transfer function is obtained as explained (Figure 7). Its second moment is equal to the contribution of the structure to the total second moment. This is however obtained more directly and accurately from the moments of the input and output function, using eq. (3). The zone broadening in the different outlet structures and its relative importance for separation columns of different lengths are summarized in Table 1.
Figure 6: The simulation of the transport of a narrow zone of species through the different outlet designs. The plain nozzle (a), nozzle with structures (b), straight slit (c) optimized slit (d). The original species zone is rectangular, 50 μm long, with a uniform mass fraction 0.001.

Figure 7: The calculated transfer functions for the concentration of species for the different outlet structures. The plain nozzle (A), nozzle with structures (B), straight slit (C), optimized slit (D) and the depth transition with beaks (E). The original functions are shifted in volume so that their first moments are approximately aligned and shapes can be compared.
Table 1: The peak broadening caused by the studied outlet structures.

<table>
<thead>
<tr>
<th>structure</th>
<th>$\sigma_{xx1}$ (pL)</th>
<th>increase in the total peak $\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$L_{col} = 2$ cm</td>
<td>$L_{col} = 8$ cm</td>
</tr>
<tr>
<td>straight slit</td>
<td>55</td>
<td>80 %</td>
</tr>
<tr>
<td>optimised slit</td>
<td>11</td>
<td>5 %</td>
</tr>
<tr>
<td>plain nozzle</td>
<td>24</td>
<td>20 %</td>
</tr>
<tr>
<td>nozzle with structures</td>
<td>12</td>
<td>5 %</td>
</tr>
<tr>
<td>beaks</td>
<td>20</td>
<td>14 %</td>
</tr>
</tbody>
</table>

As can be seen from Figure 7 and Table 1, the straight slit causes a large peak broadening and also tailing. The plain nozzle performs much better. Both the optimized slit and the nozzle with structures cause an even smaller dispersion, negligible for the 8 cm long channels.

The adaption with beaks adds some extra volume to the outlet, but the calculated transfer functions and the contribution to sigma is quite acceptable for the longer channels. These results on the adaption for the optical cell are however only illustrative. A somewhat wider cell (combined with a wider flat nozzle) may be preferred in actual practice. A simultaneous optimization of the nozzle and the cell dimensions and shapes would be needed, but this is an extensive task beyond the scope of this paper. Tracer experiments are also needed in order to find out whether the step structure indeed causes problems with bubbles or particles, and whether the beaks would then offer a real improvement without complicating the fabrication process too much.

The presented results also demonstrate that it is difficult to make conclusions about the species transport and dispersion only from the flow profiles or the volumes of the structures. For example, the contours of pressure are much more deformed by the plain nozzle, but this shows lower species dispersion than the straight slit, as is apparent from the transfer functions or the standard deviations. The optimal-slit outlet, which performs the best, has surprisingly the largest volume (~120 pL).

Although the flat nozzle design was motivated by the use with the microviscometer, in microdevices it may be the preferred structure in general because its fabrication would be
easier than the fabrication of the optimized slit. However, the latter together with its mirror image would allow easy coupling of two channels of opposite orientation.

In the larger sized FFF devices where the channel is defined as a space cut-off in a spacer layer clamped in-between a top and a bottom plate, the optimized slit shape could be easily machined in the plates, while the splitting structures would be difficult to implement. As was discussed above, reversed flow in the optimized structure would possess the same uniformity. The optimized structures are therefore also suitable as low-dispersion inlets. A modified, symmetric form, obtained by using the shape on each half of the channel sharing the end-orifice in the middle can also be suggested.

Conclusions

The flat nozzle with splitting structures and the specifically shaped transversal slit both lead to a negligible zone or peak dispersion as was demonstrated by the presented CFD simulations. The designs can be scaled for the use with channels of different dimensions, and can be applied in miniaturized on-chip liquid chromatography or in larger sized systems for field-flow fractionation.

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