# Taylor dispersion in arbitrarily shaped axisymmetric channels
## Supplementary Information

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CONTENTS



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## A. Intermediate steps in deriving Eq. 2.19

In Eq. 2.18 of the main manuscript we derived an expression of $c'(x,r,t)$ in terms of $\frac{\partial\langle c\rangle}{\partial x}$. We here present some details of the derivation. The followings are expressions for each of the terms in Eq. 2.11:

$$\frac{\mathrm{d}U}{\mathrm{d}x} = U_0 a_0^2 \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{a^2}\right) = -2U_0 a_0^2 \frac{\beta}{a^3} = \frac{-2Ua^2\beta}{a^3} = \frac{-2U\beta}{a} \tag{S1}$$

$$c'|_{r=a} = \frac{1}{24}\frac{Ua^2}{D}\frac{\partial\langle c\rangle}{\partial x} + \frac{1}{4}\beta a \frac{\partial\langle c\rangle}{\partial x} \tag{S2}$$

$$\begin{aligned}\frac{\partial c'}{\partial x} &= \left\{\frac{U\beta}{2aD}\left(-r^2 + \frac{r^4}{a^2}\right) + \left(-\frac{\beta^2 r^2}{2a^2} + \frac{\gamma r^2}{2a} - \frac{1}{4}\gamma a - \frac{1}{4}\beta^2\right)\right\}\frac{\partial\langle c\rangle}{\partial x} \\ &+ \left\{\frac{U}{D}\left(\frac{r^2}{4} - \frac{r^4}{8a^2} - \frac{a^2}{12}\right) + \left(\frac{\beta r^2}{2a} - \frac{\beta a}{4}\right)\right\}\frac{\partial^2\langle c\rangle}{\partial x^2}\end{aligned} \tag{S3}$$

$$\begin{aligned}\int_0^a c'\mathrm{d}r &= \int_0^a \left[\frac{\partial\langle c\rangle}{\partial x}\frac{U(x)}{D}\left(\frac{r^2}{4} - \frac{r^4}{8a^2} - \frac{a^2}{12}\right) + \left(\frac{\beta r^2}{2a} - \frac{1}{4}\beta a\right)\frac{\partial\langle c\rangle}{\partial x}\right]\mathrm{d}r \\ &= -\frac{1}{40}\frac{Ua^3}{D}\frac{\partial\langle c\rangle}{\partial x} - \frac{1}{12}\beta a^2 \frac{\partial\langle c\rangle}{\partial x}\end{aligned} \tag{S4}$$

$$\left.\frac{\partial c'}{\partial r}\right|_{r=a} = \frac{U}{D}\left(\frac{a}{2} - \frac{a}{2}\right)\frac{\partial\langle c\rangle}{\partial x} + \beta\frac{\partial\langle c\rangle}{\partial x} = \beta\frac{\partial\langle c\rangle}{\partial x} \tag{S5}$$

$$\begin{aligned}\frac{\partial}{\partial x}\left(a\ c'|_{r=a}\right) &= \frac{\partial}{\partial x}\left(\left(\frac{1}{24}\frac{U_0 a_0^2}{D}a + \frac{1}{4}\beta a^2\right)\frac{\partial\langle c\rangle}{\partial x}\right) \\ &= \left(\frac{U_0 a_0^2\beta}{24D} + \frac{\gamma a^2}{4} + \frac{\beta^2 a}{2}\right)\frac{\partial\langle c\rangle}{\partial x} + \left(\frac{Ua^3}{24D} + \frac{\beta a^2}{4}\right)\frac{\partial^2\langle c\rangle}{\partial x^2}\end{aligned} \tag{S6}$$

$$\begin{aligned}\left\langle u_r'\frac{\partial c'}{\partial r}\right\rangle &= \frac{2}{a^2}\int_0^a r\left(2\beta U\left(\frac{r}{a} - \frac{r^3}{a^3} - \frac{4}{15}\right)\left[\frac{U}{D}\left(\frac{r}{2} - \frac{r^3}{2a^2}\right) + \frac{\beta r}{a}\right]\frac{\partial\langle c\rangle}{\partial x}\right)\mathrm{d}r \\ &= \frac{4\beta U}{a^2}\frac{\partial\langle c\rangle}{\partial x}\left(\frac{11}{3600}\frac{Ua^3}{D} - \frac{\beta a^2}{180}\right)\end{aligned} \tag{S7}$$

$$\begin{aligned}\left\langle u_x'\frac{\partial c'}{\partial x}\right\rangle &= \frac{2}{a^2}\int_0^a U\left(1 - \frac{2r^2}{a^2}\right) \\ &[\left\{\frac{U\beta}{2aD}\left(-r^2 + \frac{r^4}{a^2}\right) + \left(\frac{-\beta^2 r^2}{2a^2} + \frac{\gamma r^2}{2a} - \frac{\gamma a}{4} - \frac{\beta^2}{4}\right)\right\}\frac{\partial\langle c\rangle}{\partial x} \\ &+ \left\{\frac{U}{D}\left(\frac{r^2}{4} - \frac{r^4}{8a^2} - \frac{a^2}{12}\right) + \left(\frac{\beta r^2}{2a} - \frac{\beta a}{4}\right)\right\}\frac{\partial^2\langle c\rangle}{\partial x^2}]r\mathrm{d}r \\ &= \frac{U}{12}(\beta^2 - a\gamma)\frac{\partial\langle c\rangle}{\partial x} - \frac{a^2U^2}{48D}\frac{\partial^2\langle c\rangle}{\partial x^2} - \frac{Ua\beta}{12}\frac{\partial^2\langle c\rangle}{\partial x^2}\end{aligned} \tag{S8}$$

Substituting each term into Eq. 2.11 and we arrive at Eq. 2.19 of the main manuscript.

## B. Derivation of the dominant error term in Eq. 2.31

As stated in the main manuscript, the ODE for the dynamics of $\sigma_x^2$ can be written as $\frac{\mathrm{d}\sigma_x^2}{\mathrm{d}t} = 2Ua^2\left[\overline{\frac{x}{a^2}} - \overline{x}\,\overline{\frac{1}{a^2}}\right] + \frac{U^2a^4}{24D}\overline{\frac{1}{a^2}} + 2D + 4D\overline{\frac{\beta}{a}(x-\overline{x})}$. The dominant error term listed in Eq. 2.31 comes from the first term $2Ua^2\left[\overline{\frac{x}{a^2}} - \overline{x}\,\overline{\frac{1}{a^2}}\right]$. Taylor expansion of this term according to Eqs. 2.26 and 2.29 yields:

$$
\begin{aligned}
\left[\overline{\frac{x}{a^2}} - \overline{x}\,\overline{\frac{1}{a^2}}\right] &= \overline{\overline{x}\widetilde{a^{-2}}} + \overline{(x-\overline{x})(\overline{x}\widetilde{(a^{-2})'} + \widetilde{a^{-2}})} + \overline{(x-\overline{x})^2\left(\frac{1}{2}\overline{x}\widetilde{(a^{-2})''} + \widetilde{(a^{-2})'}\right)} \\
&\quad + \overline{\frac{1}{6}(x-\overline{x})^3\left(\overline{x}\widetilde{(a^{-2})'''} + 3\widetilde{(a^{-2})''}\right)} - \overline{x}\widetilde{a^{-2}} - \overline{(x-\overline{x})\widetilde{(a^{-2})'}} \\
&\quad - \overline{\frac{1}{2}(x-\overline{x})^2\widetilde{(a^{-2})''}}\overline{x} - \overline{\frac{1}{6}(x-\overline{x})^3\widetilde{(a^{-2})'''}}\overline{x} + O(\sigma_x^4\mathrm{Kurt}_x\widetilde{(a^{-2})'''}) \\
&= \sigma_x^2\widetilde{(a^{-2})'} + \frac{1}{2}\sigma_x^3\mathrm{Skew}_x\widetilde{(a^{-2})''} + O(\sigma_x^4\mathrm{Kurt}_x\widetilde{(a^{-2})'''}) \\
&= -2\sigma_x^2\widetilde{a^{-3}\beta} + \sigma_x^3\mathrm{Skew}_x\frac{\widetilde{3\beta^2 - a\gamma}}{a^4} + O(\sigma_x^4\mathrm{Kurt}_x\widetilde{(a^{-2})'''}).
\end{aligned}
\tag{S1}
$$

Here $(\cdot)' = \frac{\mathrm{d}(\cdot)}{\mathrm{d}x}$; $\mathrm{Skew}_x$ is the axial skewness of the solute zone, defined as $\mathrm{Skew}_x = \overline{(x-\overline{x})^3}/\sigma_x^3$; $\mathrm{Kurt}_x$ is the axial kurtosis of the solute zone, defined as $\mathrm{Kurt}_x = \overline{(x-\overline{x})^4}/\sigma_x^4$. The second term gives rise to the error listed in Eq. 2.31 of the main manuscript.

Table S1. Parameters for Brownian dynamics simulation.

**- Shared parameters:**
$U_0 = 1$, $a_0 = 1$, $D = U_0 a_0 / Pe_{a_0}$.
Time step $\mathrm{d}t = Pe_{a_0}/40$. Number of timesteps = $40Nt_0 + 1$.
Number of points = 5000.
All simulations repeated with random seed 0 - 4.

**- Figure 3:**
diverging: $a(x) = a_0 + \beta x$, $a_0 = 1$, $\beta = 10^{-3}$.
$Pe_{a_0} = 10$, $Nt_0 = 500$, $\sigma^2_{x0} = 10$
converging: $a(x) = a_0 + \beta x$, $a_0 = 1$, $\beta = -10^{-3}$.
$Pe_{a_0} = 10$, $Nt_0 = 26$, $\sigma^2_{x0} = 10$

**- Figure 4-6, S1:**
$a(x) = 1 + 0.2\sin(x/400)$, $Nt_0 = 500$, $\sigma^2_{x0} = 10$
Figure 4: $Pe_{a_0} = 10$
Figure 5: $Pe_{a_0} = 100$
Figure 6: $Pe_{a_0} = 1000$

**- Figure 7:**
$\lambda = 200$, $\delta = 0.05$, $Nt_0 = 500$, $\sigma^2_{x0} = 10$
$Pe_{a_0} = 0.1, 1, 10, 100, 1000$
Left: $1 + \delta\sin(2\pi x/\lambda)$
Middle: $1 + \frac{3\delta}{2\lambda}\mathrm{mod}(x,\lambda) - \frac{9\delta}{2\lambda}(\mathrm{mod}(x,\lambda) - \frac{2}{3}\lambda)H(\mathrm{mod}(x,\lambda) - \frac{2}{3}\lambda)$
Right: $\frac{\delta}{e}\exp(\sin(2\pi x/\lambda)) + (1 - \frac{\delta}{e})$

**- Figure 8:**
$a(x) = 1 + 0.2e^{-(x-500)^2/8000} + 0.1e^{-(x-800)^2/20000} + 0.2e^{-(x-2000)^2/100000} - 0.1e^{-(x-3500)^2/2000000}$
$Pe_{a_0} = 10$, $Nt_0 = 500$, $\sigma^2_{x0} = 10$

**- Figure 9:**
constant axial variance:
$Pe_{a_0} = 10$, $Nt_0 = 120$,$\sigma^2_{x0} = 300$
$A = \frac{D}{2\sigma^2_{x0}U_0 a_0^2}$, $B = \frac{U_0 a_0^2}{96\sigma^2_{x0}D}$, $c_1 = \frac{48\sigma^2_{x0}D}{U_0 a_0^2}\ln\left(\frac{a_0^2}{(B + \frac{D}{2\sigma^2_{x0}U_0})}\right)$
$x(a) = \frac{1}{2B}\ln\left(\frac{a^2}{Aa^2 + B}\right) - c_1$
sinusoidal axial variance:
$Pe_{a_0} = 10$, $Nt_0 = 120$,$\sigma^2_{x0} = 300$.
$\delta = 50$, $\lambda = 600$, $\sigma^2_x(\overline{x}) = 300 + \delta\sin(2\pi\overline{x}/\lambda)$.
Solve Equation 2.35.

## C. Summary of simulation parameters

This section lists the parameters used for the Brownian dynamics simulations in the main manuscript.

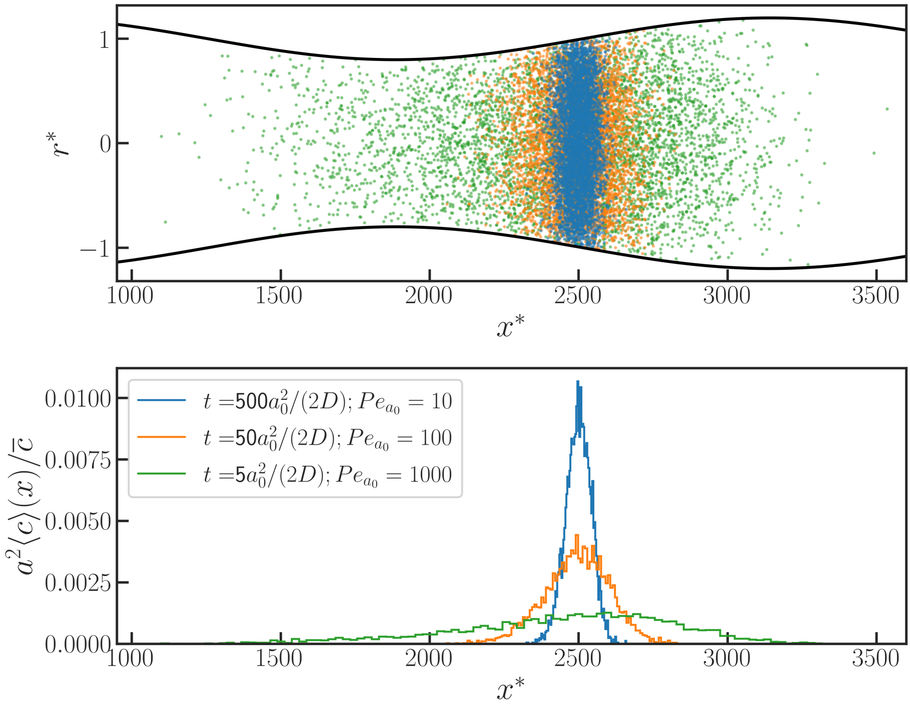


Figure S1. Taylor-Aris dispersion in a channel with a sinusoidal (periodic) radius distribution, $a(x)$. The channel is the same as that of Figure 4-6, with initial Peclet numbers $Pe_{a_0}$ of 10 (blue, $t = 500a_0^2/(2D)$), 100 (orange, $t = 50a_0^2/(2D)$) to 1000 (green, $t = 5a_0^2/(2D)$). The top plot shows results from a Brownian dynamic simulation. The bottom plot shows the concentration distribution normalized by local cross-sectional area. For a fixed distance of travel, the solute zones subjected to greater Peclet numbers disperse faster and the solute distribution becomes more skewed.

## D. Supplementary figures

Figure S1 shows plots of the Brownian dynamics simulations (top) and the concentration distribution weighted by local cross-sectional area (bottom) for the channel with a sinusoidal radius distribution (the same channel as in Figure 4-6), with initial Peclet number $Pe_{a_0}$ varying from 10, 100 to 1000 and the mean axial location $\bar{x}$ the same. As expected, the solute zone subjected to a higher Peclet number spreads faster, and the axial concentration distribution is more skewed.

## E. Comparison of effective dispersion coefficient in periodic channels with solutions by Adrover et al.

Adrover et al. comprehensively analyzed effective dispersion coefficient in a wide range of wavelengths for a periodic channel with a specific radius $R(x) = R_0(1+\delta \sin(2\pi x/(\lambda R_0)))$ (Adrover *et al.* 2019). For our current model, the Taylor dispersion analysis requires that the flow field in the channel be well approximated by lubrication theory. This constraint in turn requires the ratio ($\lambda$) of the channel wavelength to channel radius be significantly greater than unity. In this limit, Adrover et al. provided the following asymptotic formula for the effective dispersion coefficient in the axisymmetric sine-wave channel as

$$\begin{aligned} D_{\text{eff}}^{\infty *} &= D_0^* + \epsilon^2 D_1^* + \epsilon^4 D_2^* + \dots \\ \lim_{Pe_\lambda \to \infty} D_0^* &= \frac{16 + 120\delta^2 + 90\delta^4 + 5\delta^6}{16(1+\delta^2/2)} \\ D_1^* &= \frac{Pe_\lambda^2}{48} \frac{(1+3\delta^2+3\delta^4/8)}{(1+\delta^2/2)^3} \\ D_2^* &= Pe_\lambda^2 \frac{43\pi^2\delta^2(1+3\delta^2/2+\delta^4/8)}{480(1+\delta^2/2)^3} \end{aligned} \qquad \text{(S1)}$$

Here, $\epsilon^2 = \lambda^{-2}$ and $Pe_\lambda = \lambda \frac{UR_0}{D}$ is the Peclet number defined based on wavelength.

## REFERENCES

Adrover, Alessandra, Venditti, Claudia & Giona, Massimiliano 2019 Laminar dispersion at low and high Peclet numbers in a sinusoidal microtube: Point-size versus finite-size particles. *Physics of Fluids* **31** (6), 062003.