The Effect of Microchannel Geometries on Dispersing Solute Asymmetries

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INTRODUCTION: Characterizing the behavior of dispersing chemicals is of value in microfluidics for applications such as drug delivery. It is now known that a simple change in a microchannel's cross-sectional geometry has a significant impact on asymmetries in the Taylor Dispersion process[1].

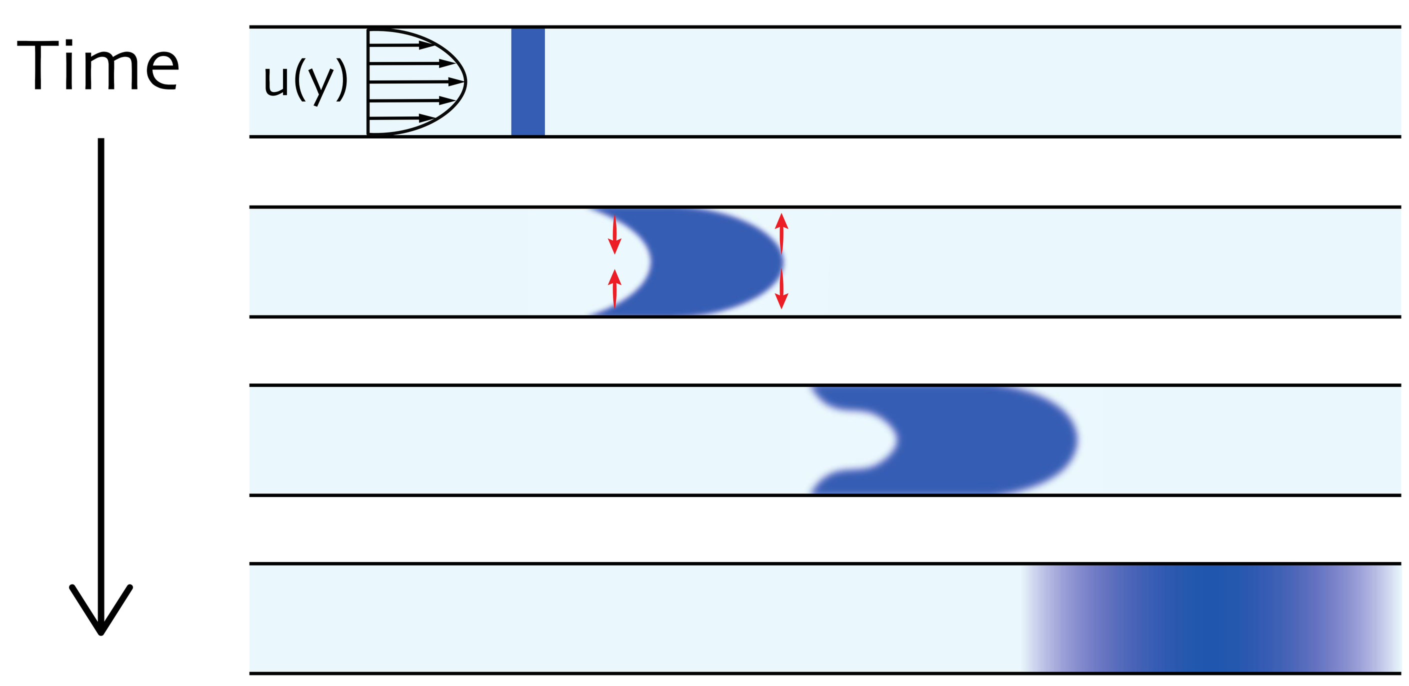


Figure 1. Taylor dispersion of a solute patch in Poiseuille flow.

COMPUTATIONAL METHODS: "Transport of Diluted Species" physics with a time-dependent study simulates translating and diffusing solute within a microchannel. The species concentration, C, is governed by the advection-diffusion equation, shown here in non-dimensional form:

$$\frac{\partial C}{\partial \tau} + Pe\ \tilde{u}(y, z)\ \frac{\partial C}{\partial \tilde{x}} = \nabla^2 C$$

Non-dimensionalized by:

- t = Time
- a = Channel half-height
- κ = Species diffusivity
- U = Initial velocity

$$\tilde{u} = \frac{u}{U} \qquad \tau = \frac{t\kappa}{a^2}$$

$$\tilde{x} = \frac{x}{a} \qquad Pe = \frac{Ua}{\kappa}$$

Along with no-flux conditions along the channel walls and an initial Gaussian distribution centered at starting position $\tilde{x}_m$. The non-dimensional quantity 'Pe' is the Peclet number, which is a ratio of convective to diffusive effects.

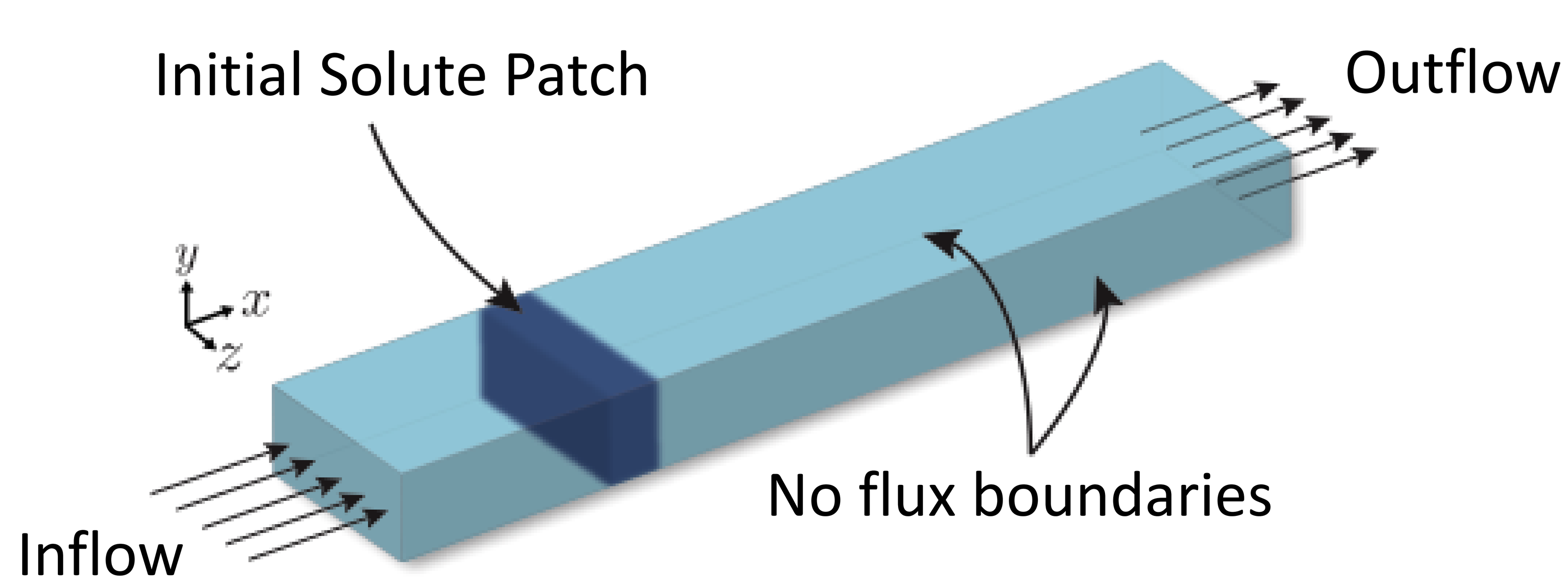


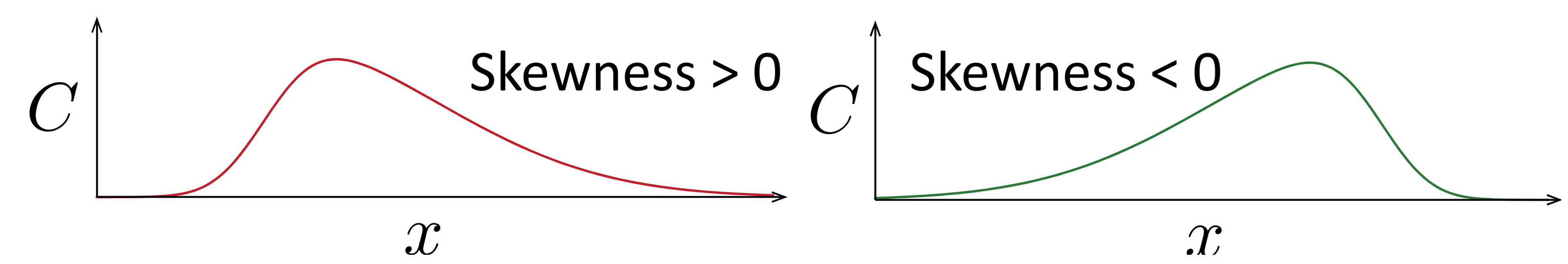
Figure 2. "Transport of Diluted Species" boundary conditions.

To account for creeping flow through the channel, the exact flow solution of the Stokes' Equations is entered directly into the 'velocity field' parameter for this physics. This allows the solute to be redistributed by influence of a steady background creeping flow, as well as molecular diffusion. A linear projection function computes the cross-sectional average of solute concentration, $\bar{C}(\tilde{x}, \tau)$.

Meshing: We completed 2D and 2D Axisymmetric simulations. For both, a free-triangular mesh was used with 100 elements spanning the height of each channel.

RESULTS: We are interested in longitudinal asymmetries in the solute distribution. Thus, we consider the second and third centered moments, M_2 and M_3 respectively, as well as the skewness. These quantities are defined as follows:

$$M_n = \frac{1}{\int_{-\infty}^{\infty} \bar{C}(\tilde{x}, \tau)\, d\tilde{x}} \int_{-\infty}^{\infty} (\tilde{x} - \tilde{x}_m - \tau)^n\ \bar{C}(\tilde{x}, \tau) d\tilde{x}$$



$$Skewness = \frac{M_3}{M_2^{3/2}}$$

Figure 4. Positive skewness generally describes a "back-loaded" distribution (left). While a curve exhibiting negative skewness will typically be "front-loaded" (right).

Our simulation results show that a 2D channel exhibits an asymmetric solute distribution with negative skewness. Conversely, the 2D Axisymmetric channel drives the solute curve to positive skewness.

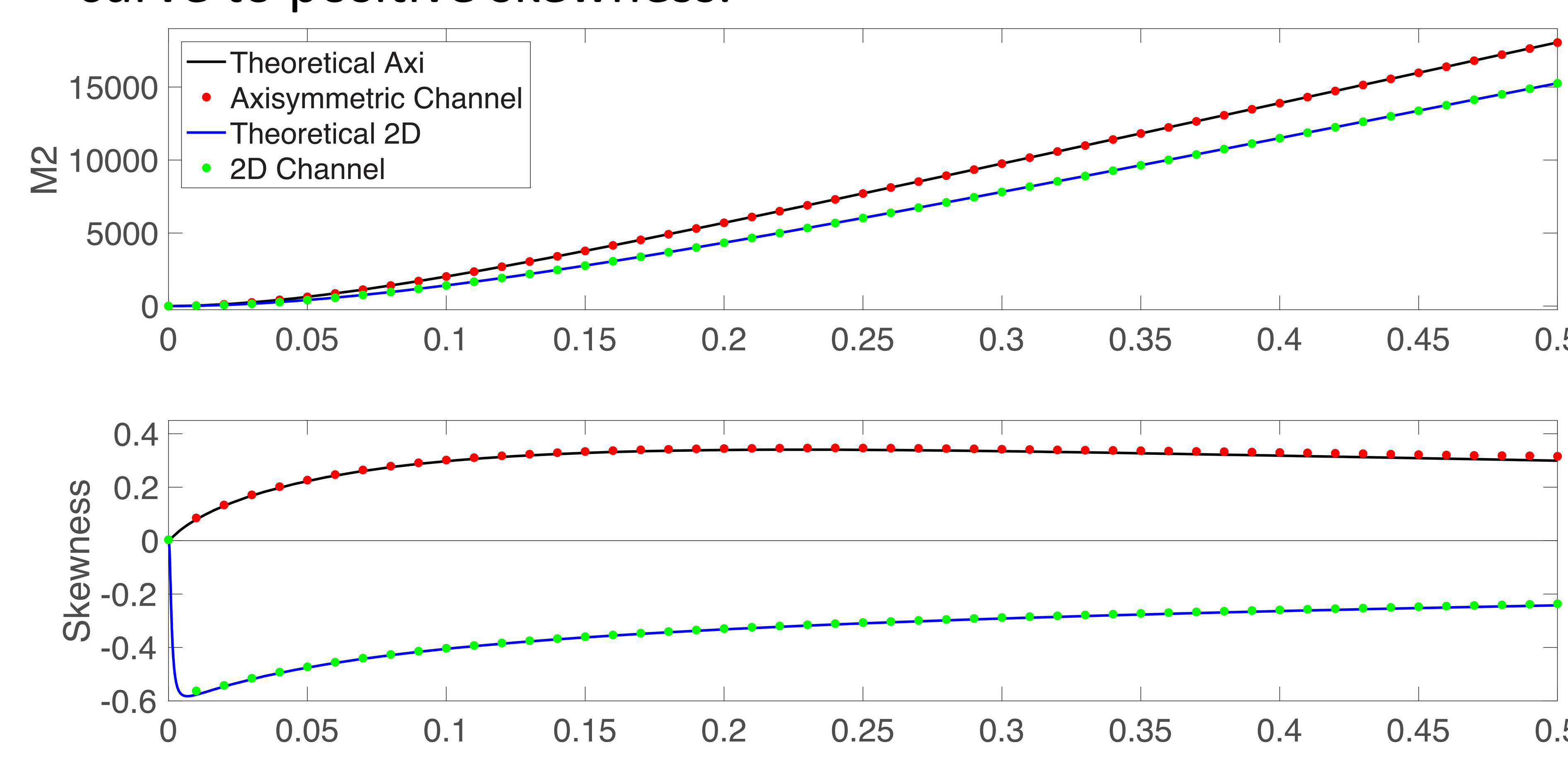


Figure 5. Normalized M_2 and skewness quantities derived from simulation results are superimposed with their corresponding mathematical predictions[2] for both a 2D and 2D Axisymmetric channel. Pe = 1000 for both simulations. The initial Gaussian distribution has standard deviation $\frac{\sigma}{a} = 4$.

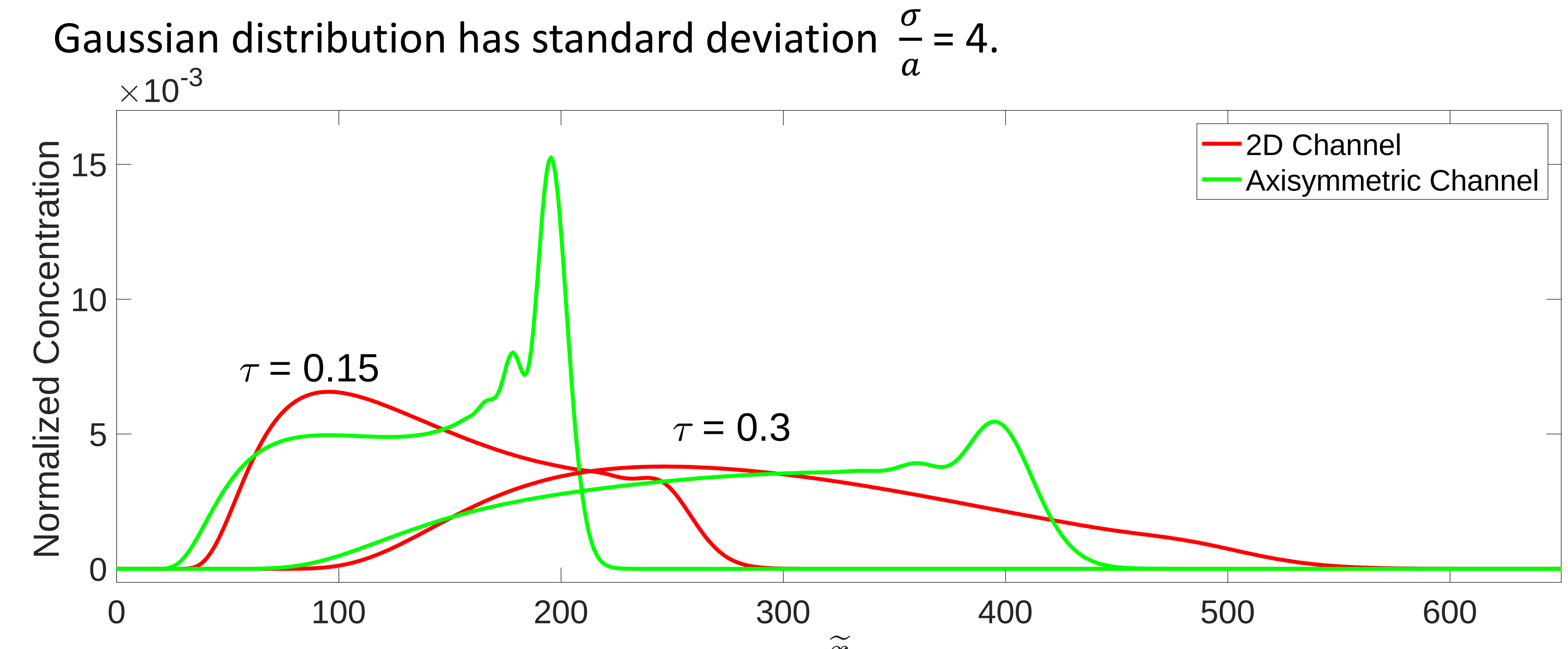


Figure 6. Normalized concentration plots of the 2D and 2D Axisymmetric channels show different asymmetries during a transitional time regime.

CONCLUSIONS: This research impacts microfluidic designs by offering a simple way to influence concentration distribution within a channel. These benchmarking results also illustrate that COMSOL Multiphysics® is effective in accurately modeling these types of microfluidic dispersion problems. In the future, we wish to compare experimental results and consider more complex geometries.

REFERENCES:

1. M. Aminian, F. Bernardi, R. Camassa, D. Harris, R. McLaughlin, How boundaries shape chemical delivery in microfluidics, Science, Vol. 354, No. 6317, pp.1252-1256, (2016)
2. F. Bernardi, Space/Time Evolution in the Passive Tracer Problem, 2018, PhD Thesis, University of North Carolina, Chapel Hill, NC