Numerical study of acoustic streaming on the reduction of Taylor-Aris dispersion for chromatographic applications

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ABSTRACT

Recently methods based on acoustics and AC electroosmotic induced vortices have been introduced by our group to reduce dispersion in chromatographic devices. In this work a numerical model has been applied and evaluated to gain deeper insight on the effect of lateral flows on dispersion for chromatographic applications.

KEYWORDS: Taylor-Aris dispersion, Acoustic streaming, Chromatography

INTRODUCTION

To allow for a further fundamental improvement of chromatographic separations, Taylor-Aris dispersion, related to slow mass transfer in the parabolic flow profile, needs to be targeted. Recent experimental work actively induced flows perpendicular to the axial direction to reduce Taylor-Aris dispersion. Lateral flow were introduced either by applying an oscillating electric field or by generating a standing pressure wave across the width of the channel[1,2]. To steer future developments, further investigation of channel geometry, diffusion coefficients, axial and lateral flows on dispersion is needed. In this work we numerically apply the general dispersion theory to evaluate the effect of lateral vortices on Taylor-Aris dispersion. This is performed in the context of analytical separations.

THEORY

The general dispersion theory (GDT), developed by Howard Brenner, uses a conditional probability density for finding a Brownian 'tracer' particle in the global and local space, respectively Z and z at time 't'[3]. We are often interested in the average velocity of the probability density distribution, $\overline{U}$, and its dispersion, $D_{ax,}$ with:

$$\bar{Z} = \overline{U} * t \tag{1}$$

$$\overline{(Z - \bar{Z})^2} = 2D_{ax}t \tag{2}$$

where $\bar{z}$ represents the mean global position of the probability density distribution and $\overline{(z - \bar{z})^2}$ is the variance on the probability density functions. Using the method of moments $\overline{U}$ and D_{ax} can be described as:

$$\overline{U} = \int P_0^{\infty} U(z) dz \tag{3}$$

$$D_T = \int P_0^{\infty} B\ U(z)\ dz \tag{4}$$

$$D_{ax} = D_T + D_m \tag{5}$$

with P_0^{∞} the zeroth moment, which represents the distribution of probability that a particle would have a certain position in the z-space, and the B-term expressing the difference between the first moment the probability density and the first moment at a specific location.

In the present work, acoustic streaming was chosen for the lateral flow. This is a phenomenon arising from viscous dissipation of a standing pressure wave in the boundary layer of the liquid[2].

EXPERIMENTAL

The GDT model was implemented in COMSOL Multiphysics (version 5.5). The Poiseuille flow in the axial direction was represented by the reduced Navier-Stokes equation with a no slip boundary condition on the channel walls. The lateral acoustic streaming flow was implemented using the numerical procedure proposed by Muller *et al*[4]. P_0^{∞} and the B-term were determined by solving the convection-diffusion equation with a no flux boundary condition through the channel walls. Finally, axial dispersion could be determined using Eqs. (4) and (5). To determine the validity of the GDT model in an experimental setting, a comparison with our experimental data[2] was performed. Next, the effect of channel size, molecular diffusion coefficient and lateral velocity, at a fixed axial velocity of 520 µm/s, on the Taylor-Aris dispersion was evaluated.

RESULTS AND DISCUSSION

Figure 1 (left) displays the reduced plate height (a measure of dispersion) at different flow velocities. As can be noticed, the dispersion coefficient is reduced with a factor of 2. This is in good agreement with the expected value based on the general dispersion theory, confirming, that the model can be used to predict how lateral mixing can reduce the dispersion in real applications. Figure 1 (right) shows the effect of increasing lateral flow on the reduction of the Taylor-Aris dispersion coefficient. As can be observed, the effect of lateral flow is much more pronounced on dispersion of large molecules as lateral transport is dominated by the applied flow and not diffusion. To evaluate the potential of lateral flow in a chromatographic context, the channel size needs to be scaled down to the micron scale. At a streaming velocity ratio of 0.5, a performance gain of a factor of 10 or more is generally obtained, confirming that vortex chromatography can further increase the efficiency of analytical separations.

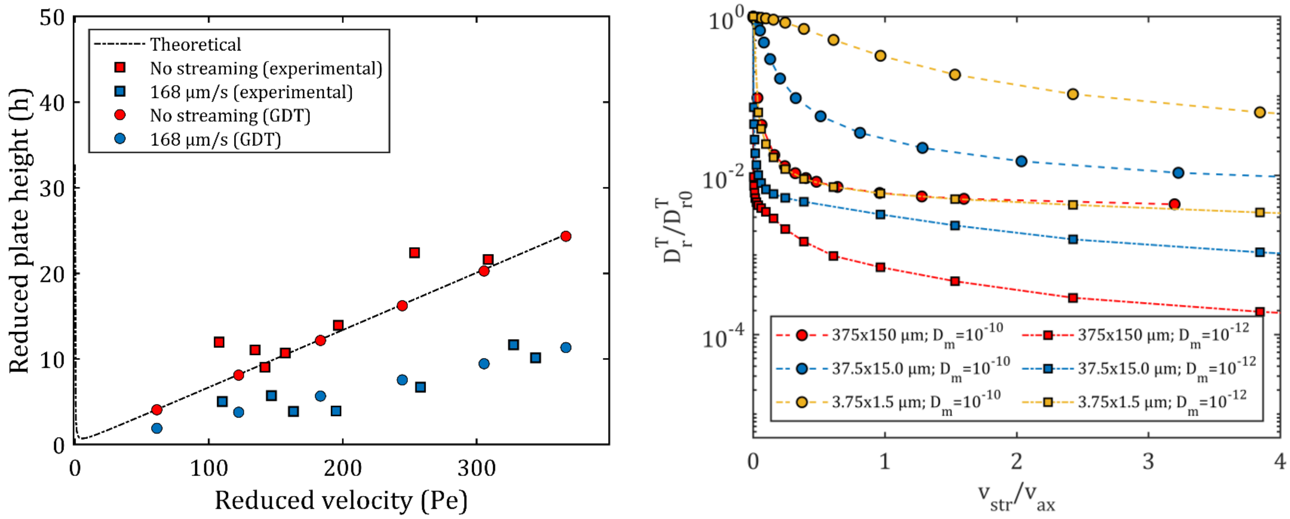

Figure 1: Left: Comparison of the GDT model and experimental data obtained for channels with a cross section of 375 x 33 µm. Right: Effect of absolute size and diffusion coefficient (m²/s) on the relative Taylor-Aris dispersion coefficient as a function of different velocity ratios of the lateral and axial velocity fields.

CONCLUSION

This work describes the application of the GDT to evaluate the potential of lateral vortices on dispersion for chromatographic purposes. We have validated the model and have shown that lateral flow can improve Taylor-Aris dispersion by a factor of 10 or more in analytical separations.

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