Modelling of Diffusiophoretic Motion for Microplastic Filtration in Microchannel Flows.

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Methodology

- Definition of relevant parameters and design criteria for diffusiophoresis.
- Generation of simplified 2D flow model.
- Iteration of designs using MATLAB.

Background

Water Resources:

- 29% (2.2 billion) of the world population lacks safe drinking water resources [1].
- Microplastics like polystyrene are found commonly in wastewater effluent [2] and in concentrations of 1,280 particles per square foot in river sediment [3].

Diffusiophoresis:

Definition

"Migration of a colloidal particle in a solution in response to the macroscopic concentration gradient of a molecular solute that interacts with the surface of the particle" [4]

In this study:

Dissolution of CO_2 forms gradient across a microchannel to induce diffusiophoresis, which comprises of 2 components:

Chemiphoretic Velocity:

- Caused by the concentration gradient.
- Direction is opposite to gradient.

Electrophoretic Velocity:

- Caused by diffusion of mobile ions.
- Magnitude and direction depends on ion species' reduced diffusivity difference.

Together, both phenomenon act on colloidal particles (microplastics) to produce a net diffusiophoretic velocity, $\boldsymbol{V_{dp}}$ **[5]**

$$V_{dp} = (\Gamma_{electrophoretic} + \Gamma_{Chemiphoretic}) * \Delta\ln(\frac{Ci/Cs}{X})$$

This velocity is proportional to the particle's mobility, Γ, as well as the natural log of the solute gradient, and is perpendicular to the flow velocity as the particles advect with the fluid.

Total mobility is described by [5]:

$$\Gamma_{total} = \underbrace{\frac{\epsilon}{2\eta}\left(\frac{k_BT}{Ze}\right)^2}_{\text{A coefficient}} [\underbrace{2\beta\frac{Ze\zeta}{k_BT}}_{\Gamma_{electrophoretic}} + \underbrace{8\ln\cosh\left(\frac{Ze\zeta}{4k_BT}\right)}_{\Gamma_{chemiphoretic}}]$$

Which depends largely on the:

- Particle Surface Charge, ζ
- Reduced Ion difference of the ions, β

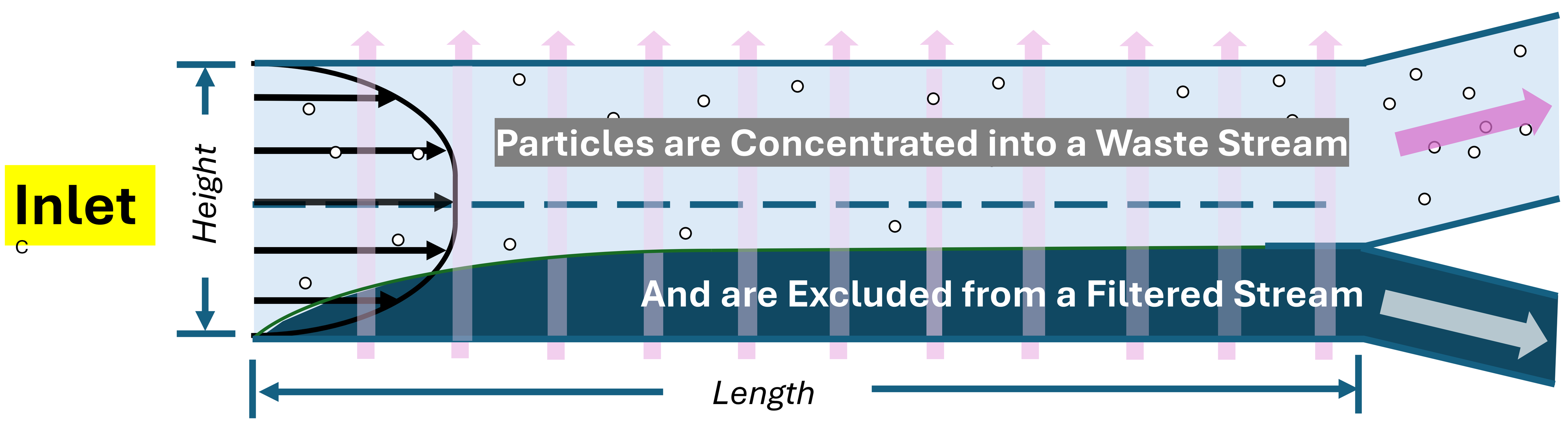
Overview:

This research develops microchannel designs for water filtration by harnessing diffusiophoresis, which induces particle motion using an electrolyte solute gradient in a cross-flow orientation.

Diffusiophoresis shows potential to provide a decentralized and low-cost water filtration technology to separate micrometer sized colloids such as microplastics from raw water.

Microchannel Design:

Using the Influence of a Solute Gradient:



- A chemical gradient causes diffusiophoresis to force particles upwards.
- Produced by diffusing CO_2 through a semipermeable membrane.

Final Results:

Filtration Performance of an Optimized Design

Final Channel Design	
Height, um	150
Width, um	8,000
Length, cm	30
Flow Velocity, mm/s	5

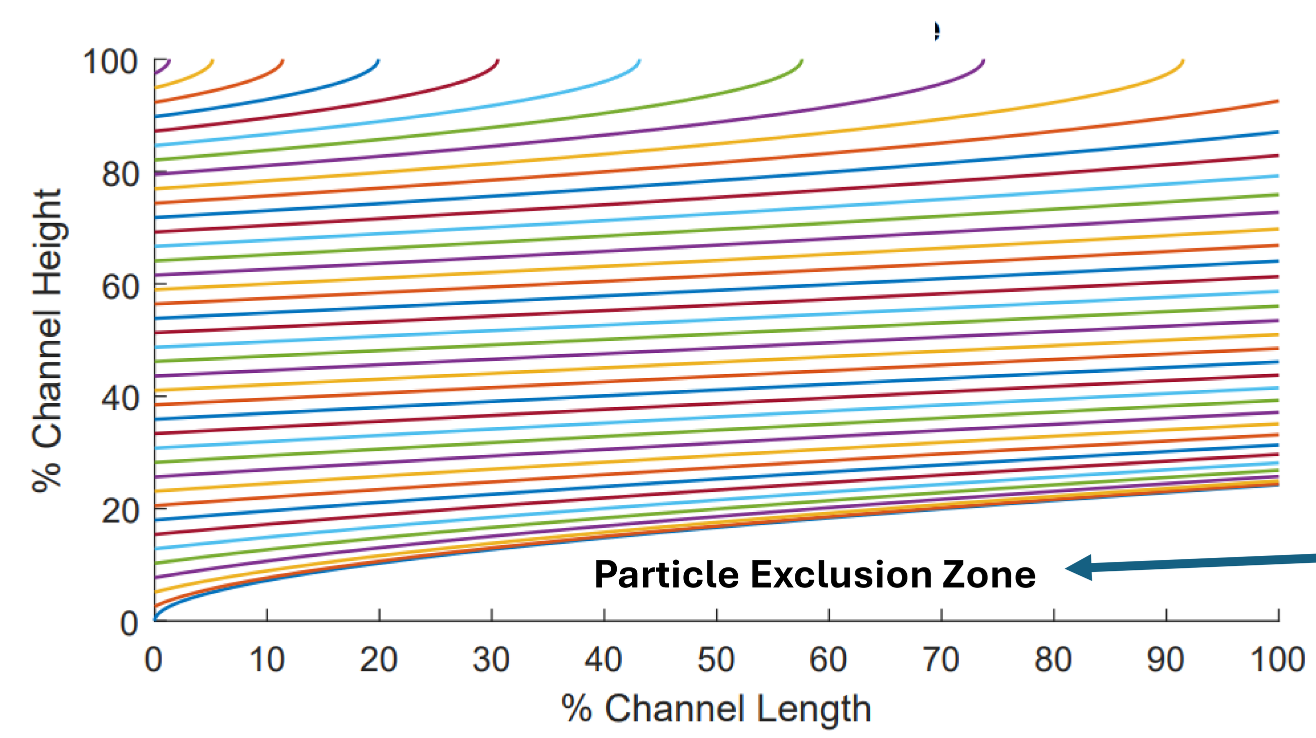


Figure shows tracking of particles as pathlines from inlet to outlet, showing development of a particle exclusion zone towards outlet.

Filtration Effect:

- 7.4 mL/hr. filtered stream

Pressure Required:

- 12.7 cm water column

Channel Internal Volume:

- 360 mm^3

Particle Exclusion:

- 26% of channel height

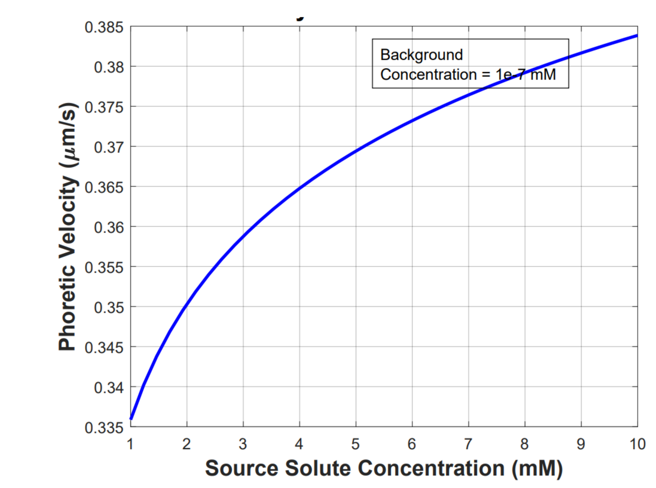
Diffusiophoretic Velocity:

- 0.37 um/s

Future Work: Developing a genetic algorithm to optimize channel design.

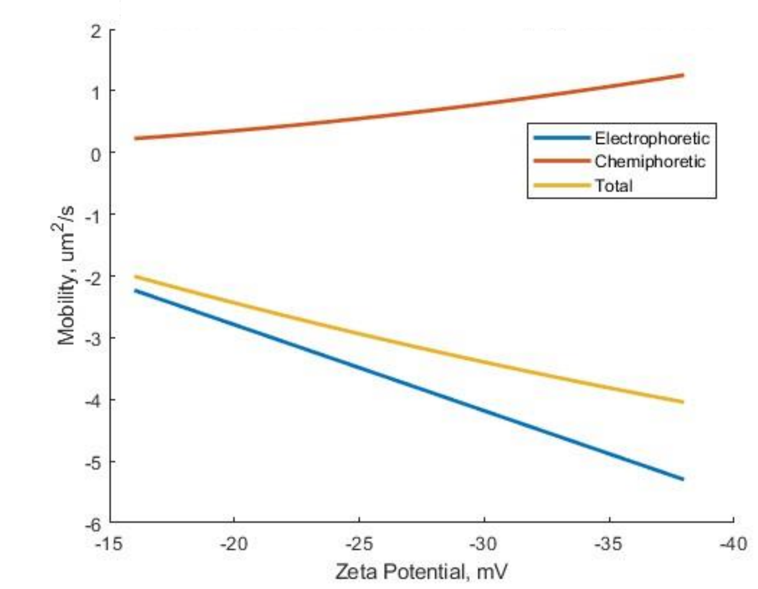
Intermediate Results

Phoretic Velocity vs CO_2 Solute Concentration



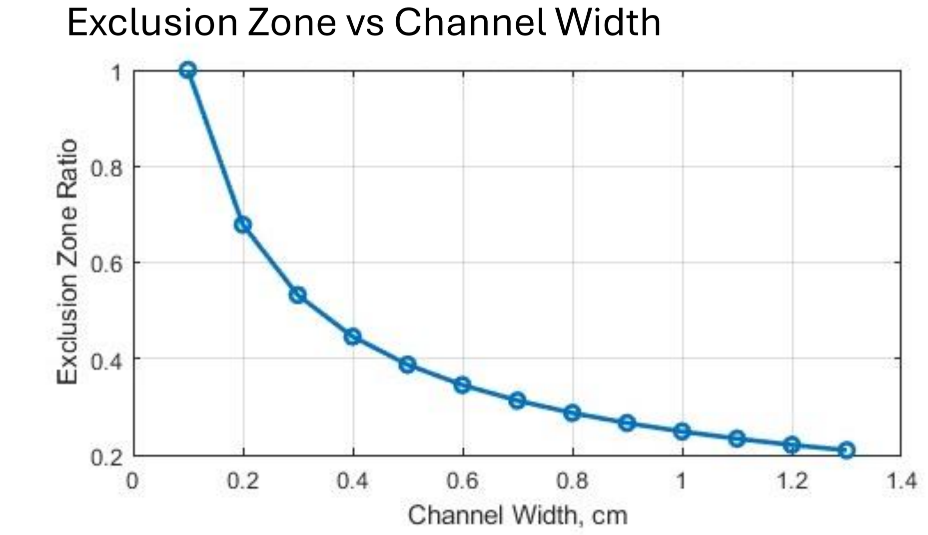
Diffusiophoretic velocity for any channel design is enhanced by higher solute concentrations.

Phoretic Mobility vs Surface Charge, ζ



Total particle mobility increases with its surface charge, with chemiphoresis dominating.

Exclusion Zone vs Channel Width



The exclusion zone is sensitive to the channel's width dimension, and the exclusion zone is affected by wall shear stress.

Implications:

There are several competing factors for design optimization:

- Large average flowrates and exclusion zones compete against the pressure head required, Reynold's number, and wall shear rate
- Reducing channel height to increase the chemical gradient and reducing average wall shear stress to increase exclusion height are competing factors.

Multiple designs can achieve similar filtered water flowrates but have unique drawbacks.

[1] United Nations, "SDG Indicators - Clean Water and Sanitation," *unstats.un.org*. https://unstats.un.org/sdgs/report/2020/goal-06/ (accessed Oct. 11, 2024).
[2] United States Geological Survey, "Microplastics in our Nations's waterways," *labs.waterdata.usgs.gov*. https://labs.waterdata.usgs.gov/visualizations/microplastics/index.html
[3] A. A. Koelmans, N. H. Mohamed Nor, E. Hermsen, M. Kooi, S. M. Mintenig, and J. De France, "Microplastics in freshwaters and drinking water: Critical review and assessment of data quality," *Water Research*, vol. 155, no. 1, pp. 410–422, May 2019, doi: https://doi.org/10.1016/j.watres.2019.02.054.
[4] H. J. Keh, "Diffusiophoresis," *Springer eBooks*, pp. 365–369, Aug. 2008, doi: https://doi.org/10.1007/978-0-387-48998-8_328.
[5] S. Shin *et al.*, "Size-dependent control of colloid transport via solute gradients in dead-end channels," *Proceedings of the National Academy of Sciences*, vol. 113, no. 2, pp. 257–261, Dec. 2015, doi: https://doi.org/10.1073/pnas.1511484112.