COMPUTATIONAL STUDY OF INERTIAL MIGRATION OF PROLATE PARTICLES IN A STRAIGHT RECTANGULAR CHANNEL

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ABSTRACT
Inertial migration of spherical particles has been investigated extensively using experiments, theory, and computational modeling. Yet, a systematic investigation of the effect of particle shape on inertial migration is still lacking. Herein, we numerically mapped the migration dynamics of a prolate particle in a straight rectangular microchannel using smoothed particles hydrodynamics (SPH). For the first time, we identified a new logrolling behavior of a prolate ellipsoidal particle in the confined channel. Our findings are especially relevant to the applications where particle shape and alignment are used for sorting and analysis, such as shape-based enrichment of microalgae, bacteria, and chromosomes.

KEYWORDS: Microfluidics, Inertial, Prolate, Computational

INTRODUCTION
The majority of studies on inertial migration have focused on spherical particles, and there is a lack of experimental and computational studies on shaped particles due to the associated technical challenges. To the best of our knowledge, only one systematic computational investigation for ellipsoidal particles in a microchannel has been published [1], but it was limited to oblate particles. Prolate particles have been investigated even less than oblate particles.

We not only studied how the focusing position changes for prolate particles of different sizes and aspect ratios, but also examined the rotational behavior, angular velocity, focusing length, and migration trajectory, mapping their migration dynamics. For the case of highly confined particles, we observed the logrolling motion of prolate ellipsoids in our simulations, for the first time. This new predicted result was confirmed by our microfluidic experiments on cell aggregates with similar shape aspect ratio and confinement ratio.

THEORY
SPH is a mesh-free Lagrangian method, originally designed for astrophysical problems, but it is also widely employed for various fluid mechanics problems. [2] The fluid domain is represented with Lagrangian particles, i.e. SPH particles. Each of these particles has its own mass, velocity, energy, and other properties. Navier-Stokes equations are discretized using SPH particles and a set of field variables, such as density and velocity, are interpolated by means of a kernel function, which decays to zero within a range of the smoothing length h.

EXPERIMENTAL
Microchannels were designed in a L-shape, so that cross-sectional imaging orthogonal to the flow direction can be setup without difficulty. The microchannel was placed on the stage of an inverted and images of cell aggregates inside the microchannel were acquired using a high-speed camera. Non-small-cell-lung cancer cell line was used and cell aggregates were formed in the low attachment plates, which were made by coating 12-well plate with anti-adherence solution.

RESULTS AND DISCUSSION
We first compared values of orbit period with the Jeffery's theory [3]. Jeffery's theory shows that an ellipsoidal particle, in an unbounded linear shear flow, rotates along the so-called Jeffery orbits: a set of infinite orbits that depend on the initial particle orientation. The time required to complete one orbit, the period of rotation, is given in Jeffery's formula (1) as:

$$T = \frac{2\pi}{\gamma}\left(\frac{1}{\lambda} + \lambda\right) \quad (1)$$

Our results in **Figure 1A** are in agreement with the theoretical values. We also validated our model against an existing numerical study for oblate particles, that employs an immersed boundary method (IBM) in square and rectangular microchannels17. We investigated 3 different cases, to test our model in capturing the characteristic behaviors observed in the study. The trajectory of the migration of the center of mass and the final rotational behavior well agrees with the reference work.

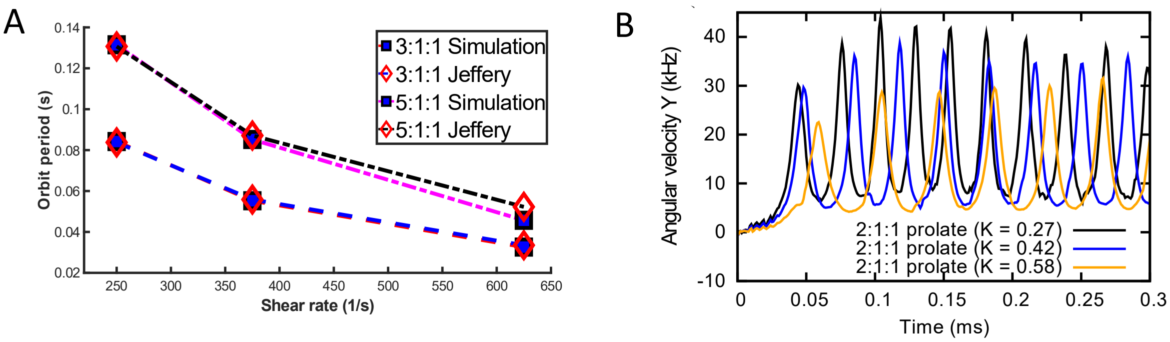

Figure 1- (A) Orbits period from Jeffery's formula13 (red diamonds) and the result from our SPH simulations in a simple shear flow (blue squares). Higher aspect ratios prolate particles rotate slower, namely 5:1 prolates exhibits higher periods of rotation than the 3:1's. (B) The maximum value of angular velocity reached during the rotation is higher for smaller particles, which are also characterized by a higher frequency of rotation. Only a part of the simulation is plotted, but the same trend also extends for the rest of the simulation.

Then, we focused on the transient migration behavior of prolate particles in a straight channel. We found that the parameter mainly responsible for the log rolling mode is the confinement ratio, defined as the ratio between the largest particle dimension and the channel height. We identified the threshold value of confinement ratio of 0.72 for the logrolling to occur, assuming that the particle is sufficiently distant from the center. We observed a higher period of rotation for higher aspect ratios particles and also for increasing values of confinement ratio, with a fixed aspect ratio. However, the magnitude of this difference is greater for distinct aspect ratios and the size contributes to minor changes. Moreover, a particle that is logrolling rotates about 3 times faster than a particle with the same volume that is tumbling. We found that within the same aspect ratio, smaller particles show higher peaks for the maximum angular velocity, as shown in **Figure 1B**.

CONCLUSION

Shape-based separation is a powerful tool, but the main limiting factors are the lack of a general framework to study the shape effects and the absence of systematic work in the literature to address the multiple variables that can affect the migration dynamic [4]. This approach can be extended to different channel cross-sections and particle shapes to provide some design basis for shape-based separation and interrogation platforms and help their integration into Lab-on-Chip devices.

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