Self-diffusion of spherocylindrical particles flowing under non-uniform shear rate

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This work numerically studies the self-diffusion of spherocylindrical particles when flowing down an inclined plane. This system is challenging due to particles being non-spherical and because they are subjected to a non-uniform shear rate. We perform simulations for several aspect ratios and inclination angles, tracking the particle trajectories. Using the simulation data, we compute the diffusion coefficients D, and a coarse-graining methodology allowed accessing the shear rate spatial profiles $\dot{\gamma}(z)$. It enables us identifying the spatial regions where the diffusivity fully correlates with the local shear rate $\dot{\gamma}(z)$. Introducing an effective particle size $d_\perp$, we propose a well-reasoned scaling law between D and $\dot{\gamma}$. Our analysis also identifies specific locations where the diffusivity does not correlate with the shear rate. This observation corresponds to zones where $\dot{\gamma}(z)$ has non-linear spatial variation, and the velocity probability density distributions exhibit asymmetric shape. Moreover, examining the velocity correlations, we obtain that the correlation length l_ξ is not constant, resulting shorter l_ξ values close to the bottom plane and higher l_ξ close to the free surface. Although our scaling analysis does not involve the particle correlation length l_ξ, our finding suggests that collective movement might play a crucial role in the self-diffusive dynamics.

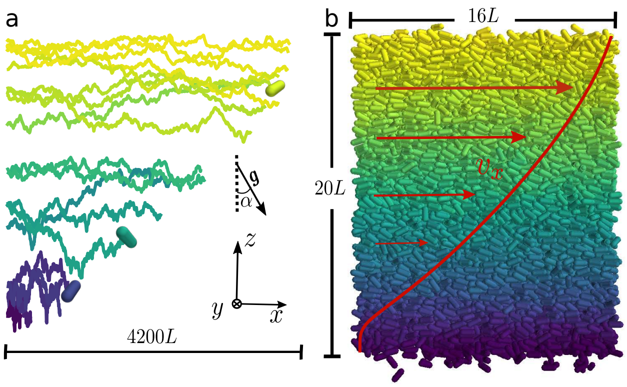

Fig. 1. a) Trajectories of twenty randomly chosen particles after reaching the steady regime. b) Snapshot of the numerical setup; the red curve indicates the mean value of the x-component of the velocity profile along the z-direction, $\bar{v}_x(z)$. The figures correspond to the case $\xi = 2.5$ and $\alpha = 31.0$ degrees. The color of the particle quantifies the magnitude of its v_x. Note that gravity has an angle α to the vertical direction, representing a slope with an angle of elevation of α degrees.

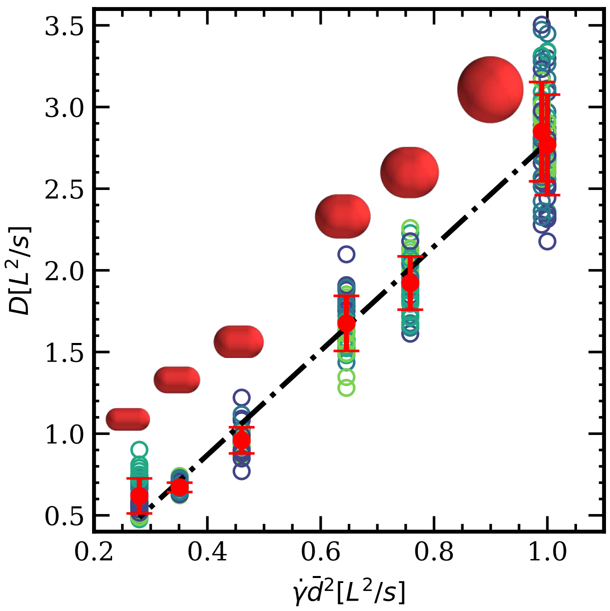

Fig. 2. Ratio of diffusion coefficient and shear rate, $D/\dot{\gamma}$, plotted against the square of the characteristic particle length $d_\perp^2$ for all inclinations α and elongations ξ. The red points are the mean values of all $D/\dot{\gamma}$ for each ξ, and the error bars indicate the standard deviation thereof. The black line represents the resultant linear fit. For all ξ values, a representation of the particle is illustrated.

[1] R. C. Hidalgo, B. Szabó, K. Gillemot, T. Börzsönyi, and T. Weinhart, "Rheological response of nonspherical granular flows down an incline" *Phys. Rev. Fluid.* 3, 074301 (2018)

[2] D. Hernández-Delfin, T. Weinhart and R.C. Hidalgo "Self-diffusion of spherocylindrical particles flowing under non-uniform shear rate" submitted to *Soft Matter*, (January 2022)