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Dispersion and Straining Behaviors of Non-Spherical Suspended Particles in Saturated Randomly Packed Beads: A Numerical and Theoretical Study

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Understanding the transport of particles in porous media, including dispersion and straining, plays a pivotal role in optimizing various engineering processes, such as drug delivery, wastewater treatment, and fracking proppants displacement. While prior numerical endeavors have significantly expanded our understanding of the microscopic behavior of particles within porous media, they have frequently overlooked the shape anisotropy of particles. When particles are non-spherical, such as pills, bacteria, and microplastics, the shape anisotropy of particles may determine their dispersion and straining behaviors in porous media, even in weakly heterogeneous environments like beadpacks.

To bridge this knowledge gap and evaluate our hypothesis, we simulated the Lagrangian transport of 3-D non-spherical particles through a 3-D porous network generated by a randomly sedimented, saturated bead pack, employing a computational fluid dynamics-discrete element method (CFD-DEM) approach. To account for the particles' asphericity as well as its impact on particle transport, we modeled the particles as superquadrics of varying asphericities and implemented a particle-fluid two-way coupling algorithm, where the fluid flow influences particles' motion, and conversely, particles also affect the fluid streamlines.

Our results suggest that, compared to spherical particles, highly aspherical particles tend to migrate along streamlines more readily, resulting in a higher mean dispersivity; such particles also tend to sweep a larger volume of the pore space, leading to a more uniform spatial distribution of retained particles. To support our numerical observations, we report a particle velocity probability distribution function that encompasses the impact of particles' asphericity on their dispersion and straining behaviors. Said function compiles all numerical observations and distinguishes between the straining and dispersion characteristics. We also deliberate on the similarities and differences between this new function and the function applicable to spherical particles, as previously reported [1]. The presented function can be useful in designing particle topology to achieve specific velocity distributions or mean dispersivity of interest.

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References

[1] Fan, Dian, Ronny Pini, and Alberto Striolo. "A seemingly universal particle kinetic distribution in porous media." *Applied Physics Letters* 119.13 (2021).

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