Particle-based, direct simulation of transport and reactions along micro-plastic synthetic fibers: Assessing the role of agglomeration on mass transfer and contaminant accumulation

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Introduction

Particle based methods for simulating reactive transport have notably advanced in recent years and now allow complex geochemical processes to be modeled accurately in a mesh-free framework [1,2]. One recent variation on this is termed complex reactions on particles, which discretizes a multi-component solute mass onto an ensemble of particles that interact with each other using a kernel based mass exchange algorithm. Transport is simulated as a random walk and arbitrarily complex reactions are then evaluated locally on each particle in an operator splitting approach framework [3]. One of the main advantages of this approach is that it explicitly separates mixing and spreading, which is more difficult in an Eulerian model, but the particles are discrete objects and this is a complication of the method, particularly when comparisons are made to continuous fields. However, the discrete nature of the method is a natural fit for a different class of transport problems involving individual, neutrally buoyant objects, which broadly includes the mobility of micro-plastic synthetic fibers (MSFs). MSFs are discrete by definition and little is known about the details of their transport dynamics, despite being a known emerging contaminant. This presentation explores how these fibers can be modeled as freely-jointed chains [4,5] using a two-step predictor/corrector approach for the fiber motion. The same basic algorithm from the reactive particle methods is adapted to determine the inter-particle distances along a fiber, which are maintained as a constraint on the motion, and inter-fiber distances to influence how the fibers and interact. Simple models of electrical interaction are included as are mass transfer models allowing sorbed solutes to migrate along and between fibers. These physically based models are allowing hypothesis testing of the aggregation mechanisms for MSFs suspended in water. Agglomeration is thought to be a major factor in the potentially irreversible trapping of plastics in porous media and the subsequent concentration of the contaminants that tend to sorb to the fibers. The lack of physical models to describe these phenomena are a major limitation to understanding fiber transport at macro-scales and this ongoing work is helping to realize that goal.

References

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