Simulations of solid–liquid mass transfer in fixed and fluidized beds

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HIGHLIGHTS

- Particle-resolved simulations of mass transfer in liquid–solid fixed and fluidized beds.
- Well resolved mass transfer boundary layers through Coupled Overlapping Domains.
- At moderate density ratios, fluidized beds exhibit less mass transfer than fixed beds.
- Schmidt to the power one-third behavior of Sherwood numbers recovered.

GRAPHICAL ABSTRACT
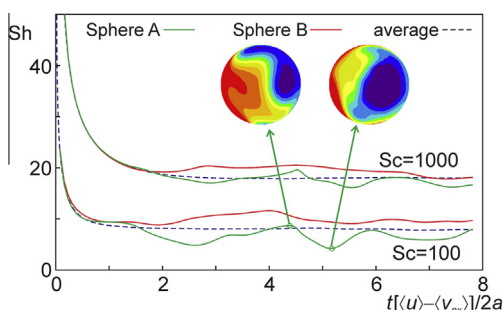
ABSTRACT

Solid-to-liquid mass transfer as a result of liquid flow through static and dynamic assemblies of mono-sized solid spheres has been simulated. The three-dimensional, transient simulations fully resolve the flow of liquid in the interstitial space between the spheres by means of a lattice-Boltzmann scheme. For the mass transfer process, a finite volume method on Coupled Overlapping Domains (CODs) is used. Spherical grids around the particles allow for resolving the thin scalar concentration boundary layers that are the result of high Schmidt numbers (Sc up to 1000). The spherical grids – one for each sphere – are coupled to an outer cubic grid. Particle-based Reynolds numbers are in the range 1–10; solids volume fractions are 0.15–0.40. The results demonstrate the validity of the COD approach for multi-particle systems, and provide insight in the dependencies of the Sherwood number on the solid–liquid system characteristics. It is shown that for moderate solid-over-liquid density ratios, fluidized particle assemblies have lower Sherwood numbers than fixed beds.

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1. Introduction

Mass transfer between a solids phase and a liquid phase is at the heart of many natural and technological processes. In engineering, the applications and their scale of operation are very diverse: detection of biological and biochemical agents in medical diagnostics through particle-based receptors in microfluidic devices [1], formation of solids in crystallization processes for a myriad of products (from fine chemicals and pharmaceuticals to bulk materials) [2], heterogeneous catalysis in slurry reactors, and wastewater treatment in large-scale municipal facilities are just a few exam-

ples. Equipment sizes range from micrometers in micro-fluidics, to multiple meters in large industrial vessels. Since mass transfer requires interfacial area and is enhanced by relative motion between solid and liquid, suspending the solids phase as small particles in the liquid phase is a practical way to stimulate it (1 ml of solid spheres with a diameter of 1 micron in random close packing has a surface area of approximately 3.6 m^2). Typical for mass transfer in liquid–solid systems is the low diffusivity of almost any species (but specifically those consisting of large molecules) dissolved in the liquid. Hence, there is the necessity for convection (and thus relative motion of liquid and solid) to transport species towards and/or away from the interfaces, since diffusion can hardly take care of this. The above notions have implications for reactor design

and operation with respect to – for instance – choice of particle size and solids loading; the denser the suspension (i.e. the higher the solids loading) the larger the surface area per unit volume. At the same time, dense suspensions are limited in flowability and do not necessarily allow for strong relative motion between the particles and the interstitial liquid.

Clearly, the dynamics of solid–liquid suspensions are determinant for their mass transfer capabilities. The hydrodynamics of suspension is an active field of research, with review papers summarizing the state of the art [3–7]. Some research trends in the field of dense suspensions are towards highly resolved simulations and the development of closure relations for coarse-grained descriptions [8], connecting the micro-structure with rheological behavior [6], hydrodynamic (self) diffusion of particles [9], and the effects of the shape of particles on their collective behavior [7,10,11]. A significant portion of that research is done in a computational manner with various numerical methods being employed, and a wide spectrum of length scales being considered. The length scales relevant to non-Brownian, inertial suspensions (particles not having vanishingly small Stokes numbers) typically range from the roughness of particle surfaces to the overall sizes of industrial vessels and reactors (from approximately 10^{-7} m to 10 m). Capturing this full spectrum in a single numerical simulation is impossible and therefore simulations usually focus on a subrange of the full spectrum. In simulations on the equipment scale, most often the objective is to assess overall solids distributions and solids and liquid fluxes [12]. In such simulations, it is unpractical and unnecessary to treat the particles as individual entities. Instead, the collection of particles is treated as a continuous phase having its own transport and constitutive equations that interacts with the liquid phase (Euler–Euler simulations). In Lagrangian simulations, individual particles or groups of particles (parcels) are being tracked through the liquid with the latter solved in an Eulerian manner. For computational and modeling reasons, Lagrangian simulations have mainly been used for dilute systems where collisions between particles are relatively scarce and might be less critical for the behavior of the suspension [13]. Recently, however, much progress has also been reported in utilizing Euler–Lagrange approaches to simulations of large volumes and under dense, suspended conditions [14]. Where in the majority of Euler–Lagrange simulations the flow around particles or parcels is unresolved (i.e. particles are smaller than the width of the Eulerian mesh for the continuous phase; they are treated as "points"), this is not the case in *resolved*-particle simulations [15–17]. By making the mesh finer than the size of the particles, and imposing no-slip conditions at the actual solid–liquid interfaces, a realistic dynamic

solid–liquid coupling can be achieved. Hydrodynamic forces on particles are then determined directly, i.e. do not need to be derived from empirical correlations as is done in point-particle approaches. No need to explain that the price for resolving the particles is a strong reduction in the number of particles that can be dealt with in a simulation (order 10^7 with point particles [18], order 10^4 with resolved particles [16]).

The lattice-Boltzmann method [19,20] in combination with various ways of imposing no-slip at solid surfaces (link-bounce-back [15], immersed boundary method [21], forcing [22]) has been extensively employed for particle-resolved simulations of suspensions. However, also finite volume discretizations have been reported [16,23].

In the present paper, an attempt is made to include liquid–solid mass transfer in particle-resolved suspension simulations. The short diffusion distances in liquids are the key challenge in this respect. Length scales of mass transfer are smaller by a factor $\sqrt{Sc}$ than the fluid-dynamic length scales, with $Sc \equiv \nu/\Gamma$ the Schmidt number, ν the kinematic viscosity of the liquid, and Γ the mass-diffusivity. In liquids, $Sc = O(10^3)$. Therefore, a computational grid that is sufficiently fine for resolving the hydrodynamics is not necessarily fine enough for mass transfer. In a recent paper [24], we have proposed a computational method to overcome this resolution challenge for mass transfer of a *single* spherical particle immersed in a liquid that undergoes laminar and also turbulent flow. The method is based on the notion that the need for a very fine grid to resolve scalar concentration is mostly restricted to a thin layer adjacent to the solid surface where steep concentration gradients normal to the solid–liquid interface exist. In [24], scalar concentration fields were solved on Coupled Overlapping Domains (COD's). One (inner) domain is a spherical shell around the particle and moving with the particle. It has fine radial grid spacing. The other (outer) domain is static and is discretized with a uniform cubic grid. The COD approach has been illustrated in Fig. 1 (left panel). The concentration fields in the domains are coupled through interpolation; in addition, the velocity field in the spherical shell is imposed by the flow as resolved in the outer domain. The consistency of the coupling between the domains was demonstrated in [24], and good results were achieved for simple mass transfer benchmarks, with Schmidt numbers up to 10^3, and Peclet numbers up to order 10^4.

Extending the COD approach as applied to one spherical particle to a dense suspension of many – in our case – uniformly sized spherical particles is not straightforward, the major issue being the occasional, however inevitable, overlap of the shells surrounding each particle in the suspension (as schematically shown in
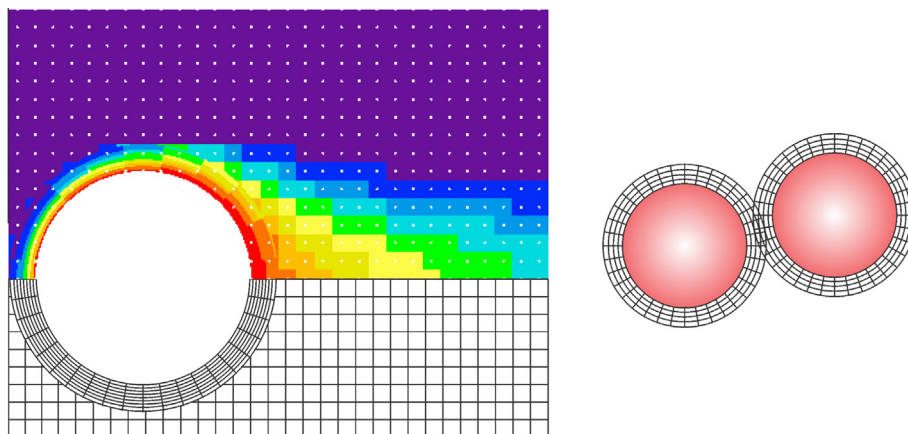

Fig. 1. Left: schematic of Coupled Overlapping Domains for a single sphere: a spherical shell with a grid in spherical coordinates interacts with an outer uniform cubic grid. Right: cartoon of overlapping spherical grids of two closely spaced spheres.