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Momentum, heat and mass transfer simulations of bounded dense mono-dispersed gas-particle systems

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ABSTRACT

Particle Resolved Direct Numerical Simulation (PR-DNS) is employed to study momentum, heat and mass transfer in confined gas-particle suspensions. In this work, we show that the presence of wall boundaries induces an inhomogeneous particle distribution, and as a consequence continuous phase fields exhibit peculiar profiles in the wall-normal direction. Therefore, we first propose a correlation for the particle volume fraction as a function of the distance from the wall and the bulk particle concentration. Secondly, we quantify wall effects on flow field and interphase transfer coefficients (i.e., the flow field, a scalar field, as well as the Nusselt number and drag coefficient). We show that these effects do not depend significantly on the Reynolds number in case an appropriate scaling is applied. Finally, we propose correlations to reconstruct the continuous phase fields in the proximity of adiabatic walls. Also, we provide interpolation tables for the correction to the drag force and the Nusselt number that are helpful in unresolved Euler–Lagrange simulations.

1. Introduction

Confined suspensions are a topic of active research since they are of use in a wide range of industrial processes like energy storage, heterogeneous catalytic reactors, pulp fibers, separation in micro-channels, or the petroleum industry. Other applications include blood flow in the human body, sediment transport in river beds and pyroclastic flows from vulcanos. Current developments indicate that the confinement effect in suspension flows becomes even more important: for example, so-called ‘3D printing’ technology aiming on producing materials capable to be used at high temperatures (e.g., metals or ceramics) is already reality [1]. This enables the use of complex geometries with characteristic dimensions closer to that of the suspended particles. In such systems wall effects will play a central role. In addition, the accurate modeling of momentum, heat and mass transport in dense gas-particle systems is of pivotal importance for designing chemical reactors [2,3], and many other systems, e.g., future solar-thermal systems [4,5].

Again, the effect of confinement plays a central role in most of these applications, and is potentially becoming more important. However, most of the studies regarding wall effects in fluid-particle systems are devoted to the study of packed beds in cylindrical containments. In contrast, investigations on suspensions bounded by one or more flat walls were performed only recently [6–8,3,9]. This is despite the obvious importance of near-wall treatment when modeling suspension flows: For example, it was shown that (in dilute suspensions under turbulent flow conditions) particles tend to migrate towards (flat) walls due to a phenomenon named *turbophoresis* [10]. Another example is the peculiar effect that walls have on the particle arrangement in dense suspensions and packed beds as discussed in Section 1.1.

Thanks to the continuous increase in the availability of computational resources, hybrid Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) simulations have become a tool for studying such dispersed multiphase systems [11]. A specific example is the so-called Particle-Unresolved Euler–Lagrange (PU-EL) formulation in which each particle trajectory is followed and particle–particle interactions are resolved. The governing equations for describing continuous phase flow are formulated at a length scale larger than the particle characteristic length. Therefore, one has to solve coarse-grained equations for the continuous phase. Unlike the Euler-Euler (EE) formulation where the dispersed and continuous phases are described as interpenetrating continua, PU-EL formulations allow to directly study intra-particle transport phenomena. This is possible because PU-EL formulation still retains the definition of single particles as separate discrete entities, allowing to track the internal state of each particle, e.g., intra-particle temperature profiles. Thus, PU-EL simulations are best suited for studying complex systems of chemically reacting

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Nomenclature

Abbreviations

CFD	computational fluid dynamics
DEM	Discrete Element Method
DNS	Direct Numerical Simulation
EL	Euler–Lagrange
HFD-IB	hybrid fictitious-domain/immersed-boundary
PR	particle-resolved
PU	particle-unresolved

Greek characters

ϕ	particle volume fraction $[-]$
Γ	boundary
λ	fluid heat conductivity [W/mK]
μ	dynamic viscosity [Kg/ms]
Ω	domain
η	particle diameter $[-]$
ρ	phase density [kg/m^3]
θ	scalar field $[-]$
ϱ	filter size $[-]$
ζ	wall normal correction

Latin characters

$\boldsymbol{u}$	velocity field $[-]$
c	concentration [m^{-3}]
C_p	fluid thermal capacity [J/kg K]
d_p	dimensional particle diameter [m]
F	interphase drag coefficient $[-]$
f	interphase force $[-]$
h	size of a CFD cell [m]
N_p	number of particles $[-]$
Nu	Nusselt number $[-]$
p	pressure $[-]$
Pe	Peclet number $[-]$
Pr	Prandtl number $[-]$
Q	interface scalar transfer rate $[-]$
Re	Reynolds number $[-]$
t	temporal coordinate $[-]$
U_s	streamwise velocity $[-]$
x, y, z	Cartesian coordinates $[-]$

Subscripts/superscripts

$'$	field in the induced boundary layer
ℓ	refers to the induced boundary layer
$Deen, DS$	refers to a correlation
F	relative to the drag force
Nu	relative to the Nusselt number
$\star$	dimensional quantity
b	bulk quantity
f	property related to fluid phase
i	property related to particle number i
p	globally averaged quantity
ref	reference value

Averaging/filtering operators

$\langle(*)\rangle$	ensemble average
$\langle(*)\rangle_{xy}$	average over a layer
$\overline{(*)}$	volume average
$\widetilde{(*)}$	Favre average

particles for which it is difficult (or even impossible) to formulate a continuous dispersed phase model with the desired accuracy. Similarly, modeling systems comprised of non-spherical particles is most natural, and pheraphs successful, when using a EL-based model.

However, coarse grained equations in PU-EL formulations have several unclosed terms (e.g., the drag coefficient, the pseudo-turbulent stress, or the interphase heat and mass transfer coefficients) for which one has to provide suitable expressions. In our previous work [12] we showed how such models can be constructed from Particle-Resolved Euler–Lagrange (PR-EL) simulations by means of volume averaging in a way that is consistent with the PU-EL formulation. It was shown that when the filter size is small (i.e., in the order of two times the particle diameter) significant differences arise with respect to EE closures due to local inhomogeneous structures. In other words, EE-based closures cannot be simply used in PU-EL-based simulation models. Furthermore, PU-EL models perform often poorer compared to EE-based models: inaccuracies caused by the interpolation and mapping scheme used to calculate the local voidage may deteriorate the fidelity of PU-EL models [13]. Particularly interesting aspects surface in case walls are present in the region to be modeled:

- the presence of walls induces an inhomogeneous distribution of particles which affects the flow field and the interphase transfer coefficients. This effect is not accounted for in the totality of closures currently used in EE and PU-EL models.
- since the details of the flow field near the wall are not known, typically the slip condition for the fluid is employed in EE and PU-EL models. This leads to significant uncertainties when interpolating the fluid velocity at the particle position near walls. This issue is especially relevant for size-polydisperse suspensions.
- for PU-EL models, the issue of insufficient mesh resolution in case heterogeneous particle structures exist has been systematically explored only in unbounded domains [14]. One would expect that similar issues arise in case the suspension is confined by walls. Conceptually, one could envision treating such wall effects similar to what is done in wall-bounded turbulent flows (e.g., one could employ wall functions). Unfortunately, such concepts are currently not available for dense fluid-particle flows.

A first step to systematically investigate the above aspects would be to quantify wall effects in an isolated fashion, i.e., separate them from the curvature effect that is typically included in the analysis (see Theuerkauf et al. [15], or van Antwerpen et al. [16]). Also, little is known for more dilute and intermediately dense suspensions, since most previous work explored packed beds only. Considering a wider parameter space is, however, essential when building a robust, generally-applicable simulation model. In our present contribution we indeed show that the particle concentration has a pronounced effect on both the velocity and temperature (as a proxy for any scalar) field. This is even the case for the simplest situation of adiabatic walls. We will start our analysis by considering the origin of these effects, namely the particle distribution near the wall.

1.1. Particle distribution in wall bounded domains

Extensive studies have been dedicated to the prediction of particle volume concentration of packed beds in the near wall region. In packed beds, the first layer of spherical particles in contact with the walls is characterized by having a well ordered distribution. Most of these near-wall particles are indeed in contact with the wall. Such ordering is progressively lost in the subsequent layers