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Consistent closures for Euler-Lagrange models of bi-disperse gas-particle suspensions derived from particle-resolved direct numerical simulations

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ABSTRACT

Particle-Resolved Direct Numerical Simulation (PR-DNS) is employed to simulate momentum and energy transport in bi-disperse gas-solid suspensions by means of a novel hybrid immersed-boundary/fictitious domain (HFD-IB) method. First, we demonstrate the accuracy of the new HFD-IB method against several verification tests. Subsequently, we simulate momentum and energy transfer in bi-disperse suspensions in the limit of high Stokes number, and the predicted flow and temperature fields are used, in conjunction with the open-source parallel data processing library CPPPO (Municchi et al., 2016), to assess the validity of existing closures for momentum and heat transfer in the frame of Particle-Unresolved Euler-Lagrange (PU-EL) models. We propose a correction to the drag force model proposed by Beetstra et al. (2009) which consistently takes into account the pressure contribution to the total fluid-particle interaction force in PU-EL models. Also, we propose a stochastic closure model for the per-particle drag coefficient based on a modified log-normal distribution. Finally, we assess the existence of an analogy between the particle-based drag coefficient and the conditionally-averaged Nusselt number. Indeed, our PR-DNS data indicates that a stochastic closure similar to that for the drag can be used to close the particle-based Nusselt number in dense bidisperse suspensions.

1. Introduction

Numerical simulations of large scale particle flows, which are widely encountered in industrial applications, are normally performed using averaged equations of motion. In these descriptions the solid and fluid phases are modeled as interpenetrating continua [3]. These models are normally based on the kinetic theory of granular flows [4] and contain unclosed terms that have to be modeled somehow. In a multi-scale approach [5,6], these models can be derived from more detailed simulations where particles are described as a discrete phase. In particular, in case the trajectory of each particle is tracked and collisions are resolved, one obtains the so-called Computational Fluid Dynamics-Discrete Elements Method (CFD-DEM) that, in case fluid cells are larger than particle diameters, can also be referred to as the Particle-Unresolved Euler-Lagrange approach (PU-EL) [7–13]. However, even PU-EL equations have several unclosed terms, like the interphase transport coefficients, that account for, for example, fluid-particle heat and momentum transfer. Following the multi-scale paradigm in our present contribution, we seek to obtain certain closures from fully resolved simulations, i.e., where the detailed flow and temperature (or concentration) fields are resolved on a sub-particle level. This latter approach can be denoted as Particle-Resolved Euler-Lagrange (PR-EL), or Particle-Resolved Direct Numerical Simulation (PR-DNS) if turbulence models are used or not, respectively. PR-DNS has already been extensively used to derive closures for the drag coefficient in mono- and bi-disperse suspensions [14,2,15], or for the Nusselt/Sherwood number in mono-disperse suspensions [16–20]. However, almost the totality of this previous work focused on closures for Euler-Euler-based simulations in a coarse scale. Naturally, the question arises of the same closures can be used for PU-EL simulations, and we will demonstrate that indeed this is not the case.

1.1. Upscaling and closure development strategies

A major difference between closures for Euler-Euler and PU-EL models is that the latter require a particle-based description of the interphase transfer processes, while the former (i.e., EE models) require average exchange coefficients. Thus, particle-based models are affected by per-particle fluctuations that arise simply due to the random arrangement of individual particles, and occur even in low-Reynolds number flows. When developing closures for continuum formulations, these quantities, are obtained from averages

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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

α	log-normal standard deviation [–]
β	log-normal lower bound [–]
η	particle diameter [–]
γ	correction function
κ	tortuosity [–]
Λ	interphase saturation coefficient [–]
λ_o	characteristic fluid-particle system length [–]
ν	fluid kinematic viscosity [m^2/s]
Ω	computational domain
ω	relaxation factor [–]
ϕ	volume fraction [–]
Φ_m	marker field
Φ_s	sampled field
ρ	phase density [kg/m^3]
σ	scaled standard deviation [–]
Θ	saturation margin [–]
θ	fluid temperature [–]
ϱ	filter size [–]

Latin characters

$\boldsymbol{f}$	total interphase force [–]
$\boldsymbol{u}$	velocity field [–]
C^i	ensemble conditional averaging Kernel [–]
M	coefficient matrix [–]
U	discrete binning set [–]
$\mathcal{P}$	modified log-normal distribution
A	surface [m^2]
A_p	specific exchange surface [1/m]
c_p	fluid thermal capacity [J/kg K]
d	particle diameter [m]
d_{cs}	distance between cell c and particle surface [m]
F	interphase drag coefficient [–]
F_B	Beetstra interphase drag coefficient [–]
F_{corr}	corrected interphase drag coefficient [–]
h	CFD cells per particle diameter [–]
I	indicator function [–]
K	kernel function
k	heat conductivity [W/mK]
N_p	number of particles [–]
Nu	Nusselt number [–]
Nu_{bi}	bi-disperse Nusselt number [–]
p	pressure [–]
Pe	Peclet number [–]
Pe_L	longitudinal Peclet number [–]
Pr	Prandtl number [–]
Q	interface heat transfer rate [–]
r	radial coordinate [m]
Re	Reynolds number [–]
s	HFD-IB interpolation distance [m]
T	temperature [K]
t	temporal coordinate [–]
U_s	superficial velocity [m/s]
v	particle velocity [m/s]
V	CFD cell volume [m^3]
x, y, z	cartesian coordinates [–]

Subscripts/superscripts

$(cons)$	consistent
$\odot$	evaluated from the HFD-IB algorithm
$\Phi_{m,j}$	evaluated using discrete marker field at j
$Deen, Gunn, Sunn$	refers to one of these correlations
F	relative to the drag force
G	global quantity
mix	relative to the homogeneous mixture
Nu	relative to the Nusselt number
$*$	dimensional quantity
0	reference value
32	mean Sauter quantity
∇p	contribution from pressure gradient
Φ_m	evaluated using marker field
b	bulk quantity
c	property related to CFD cell c
d	contribution from drag
f	property related to fluid phase
g	quantity related to the whole domain (global)
I	imposed value
i	property related to particle number i
k	property related to particles specie k
M	property related to particles with the largest radii
m	property related to particles with the smallest radii
n	quantity at time step n
p	property related to particle phase
$P1, P2$	property interpolated at point $P1$ or $P2$
s	property evaluated at particle surface
sat	value at saturation

Averaging/filtering operators

$\langle(*)\rangle$	ensemble average
$\langle(*)\rangle_\Phi$	ensemble average conditional on Φ
$\overline{(*)}$	volume average
$\widehat{(*)}$	flux average
$\widetilde{(*)}$	Favre average

within each realization, so that the fluctuations in the particle population are lost and the final standard deviation is calculated based on the ensemble of realizations. On the contrary, closures for PU-EL models are based on the whole studied population and thus, they may require stochastic models to take into account the single particle variability [14,21].

The process of upscaling of fluid quantities that we adopted is known as (spatial) filtering or coarse-graining [22]. The local domain where this operation is performed (in PR-DNS) can be identified with a fluid cell used in PU-EL. In general, closure models derived using this approach have a functional dependence on the filter size, i.e., the support of the filtering kernel or, in other words, the size of the coarse-grained cell [8]. Moreover, while the velocity field is statistically homogeneous in homogeneous particle configurations, the temperature field is generally inhomogeneous [19,20]. This is in contrast with the assumption of separation of scales required for the development of continuum formulations, e.g., Euler-Euler models, and poses a challenge also in the development of particle-based models such as PU-EL-based models. In the present work we refer to this issue as *saturation*, since this term does reflect the physical process that is behind.