**UNIVERSITY OF SÃO PAULO
SÃO CARLOS SCHOOL OF ENGINEERING**

Joseph Mouallem

**Effects of sub-grid gas turbulence on the meso-scale
hydrodynamics of fluidized gas-solid flows**

São Carlos

2018

Joseph Mouallem

**Effects of sub-grid gas turbulence on the meso-scale
hydrodynamics of fluidized gas-solid flows**

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Supervisor: Prof. Dr. Fernando E. Milioli

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**São Carlos
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Joseph Mouallem

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gás-sólido**

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*“He who would learn to fly one day
must first learn to stand and walk and run and climb and dance;
one cannot fly into flying.”*

Friedrich Nietzsche

ABSTRACT

MOUALLEM, J. **Effects of sub-grid gas turbulence on the meso-scale hydrodynamics of fluidized gas-solid flows.** 2018. 162p. Thesis (Doctor of Science) - São Carlos School of Engineering, University of São Paulo, São Carlos, 2018.

Filtered two-fluid models used to perform large scale simulations of gas-solid fluidized flows of industrial risers require closures for filtered parameters such as filtered and residual stresses, and interphase interaction forces mainly effective drag. Closure models for those filtered parameters may be derived by averaging over results of highly resolved simulations with microscopic two-fluid modeling. This work is a contribution in that context. Recent models for filtered parameters have been written as functions of filter size, filtered solid volume fraction, and filtered slip velocity. A recent study showed that macro-scale variables like domain average solid volume fraction and gas Reynolds number also significantly affect the filtered parameters. In the current work, in addition to these filtered and macro-scale variables, the effects of two new variables over the filtered parameters are investigated: filtered solid kinetic energy and sub-grid gas turbulence. It is shown that the filtered solid kinetic energy should be accounted for in the concerning correlations, thereby improving accuracy. Regarding gas turbulence, literature shows it has no significant effects on the motion of high Stokes particles. Extending on literature, this work investigates the sub-grid gas turbulence effects on meso-scale structures formed of high Stokes particles. Results showed that sub-grid gas turbulence has no significant effects on the meso-scale structures and corresponding filtered parameters. The open source code MFIX was used for all simulations. Ranges of dilute concentration of solid and gas Reynolds number typical of riser flow regimes were considered. A modified two-fluid model with microscopic formulation was used. The sub-grid gas turbulence was generated by means of a forcing function procedure which was implemented in the physical space, over the gravitational term of the momentum conservation equation of the gas phase. First, numerical simulations of the gas phase alone were performed, accounting for literature available data, in order to set a turbulent gas field and calibrate the turbulence intensity. Then, the forcing function was introduced in to the two-fluid model and various gas-solid flows were simulated. While the current results show the necessity of accounting for additional variables in the filtered parameter correlation, they also make it clear the necessity of further developments that are required in the search for better accuracy.

Keywords: Two-fluid modeling. Sub-grid modeling. Highly resolved simulation. Gas-solid flow. Fluidization. Turbulence.

RESUMO

MOUALLEM, J. **Efeitos da turbulência sub-malha do gás sobre a hidrodinâmica de meso-escala de escoamentos fluidizados gás-sólido.** 2018. 162p. Tese (Doutorado) - Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos, 2018.

Modelos filtrados de dois-fluidos usados em simulações de grandes escalas de escoamentos fluidizados de gás-sólido de risers industriais exigem fechamentos para parâmetros filtrados tais como as tensões filtradas e residuais, e forças interativas interfases, principalmente arrasto efetivo. Modelos de fechamento para estes parâmetros filtrados podem ser gerados a partir de procedimentos de média aplicados sobre resultados de simulações altamente resolvidas com modelagem microscópica de dois-fluidos. Este trabalho é uma contribuição neste contexto. Modelos de fechamento recentes para parâmetros filtrados tem sido formulados em função de tamanho de filtro, fração volumétrica de sólido filtrada, e velocidade de deslizamento filtrada. Estudo recente mostrou que variáveis de macro-escalas como fração volumétrica de sólido e número de Reynolds de gás médios no domínio também afetam significativamente os parâmetros filtrados. No presente trabalho, além dessas variáveis filtradas e de macro-escala, os efeitos de duas novas variáveis sobre os parâmetros filtrados são investigados: energia cinética filtrada do sólido e turbulência sub-malha do gás. Em relação à energia cinética filtrada do sólido, mostra-se que a sua consideração refina as correlações em questão, contribuindo assim para melhor acuracidade. Com relação à turbulência do gás, a literatura mostra que não tem efeitos significativos no movimento de particulados de elevados números de Stokes. Acrescentando à literatura, este trabalho investiga os efeitos da turbulência sub-malha do gás sobre estruturas de meso-escala formados de particulados de elevados números de Stokes. Os resultados mostraram que a turbulência sub-malha do gás não tem efeitos significativos sobre estruturas de meso-escalas e parâmetros filtrados correspondentes. O código aberto MFIX foi usado para todas as simulações. Faixas de concentração diluída de sólido e número de Reynolds típicos de escoamentos em risers foram considerados. Um modelo modificado de dois fluidos com formulação microscópica foi utilizado. A turbulência sub-malha do gás foi gerada por meio de um procedimento de 'forcing function' que foi implementado no espaço físico, sobre o termo fonte gravitacional da equação de momentum da fase gás. Primeiramente, simulações numéricas da fase gás foram realizadas separadamente, levando-se em conta dados disponíveis na literatura, a fim de gerar um campo de gás turbulento e calibrar a intensidade de turbulência. Posteriormente, a 'forcing function' foi introduzida no modelo de dois-fluidos e vários escoamentos de gás-sólido foram simulados. Enquanto os resultados obtidos mostram a necessidade de consideração de variáveis adicionais para correlação de parâmetros filtrados, também deixam claro a necessidade de desenvolvimentos mais aprofundados na busca de melhor acuracidade.

Palavras-chave: Modelagem de dois fluidos. Modelagem sub-malha. Simulação altamente resolvida. Escoamento gás-sólido. Fluidização. Turbulência

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LIST OF ABBREVIATIONS AND ACRONYMS

ACFB	Atmospheric Circulating Fluidized Bed
CFB	Circulating Fluidized Bed
CFD	Computational Fluid Dynamics
DEM	Discrete Element Method
DNS	Direct Numerical Simulation
DOE-USA	United States Department of Energy
FCB	Fluidized Bed Combustion
FCC	Fluid Catalytic Cracking
HIT	Homogeneous Isotropic Turbulence
HRS	Highly Resolved Simulation
IEA	International Agency Energy
KTGF	Kinetic Theory of Granular Flows
LBM	Lattice Boltzmann Method
LES	Large Eddy Simulation
LSS	Large Scale Simulation
MFIX	Multiphase Flow with Interphase eXchange
MPPIC	Multi-phase Particle in Cell Method
NETL	National Energy Technology Laboratory
NS	Navier-Stokes
OU	Ornstein-Uhlenbeck
PTE	Pseudo-Thermal Energy
SIMPLE	Semi-Implicit Method for Pressure Linked Equations
TFM	Two-Fluid Model
TVD	Total Variation Diminishing

TKE Turbulent Kinetic Energy

VPF Volume Body Force

LIST OF SYMBOLS

$\mathbf{B}'_{gs}$	Nm^{-3}	Fluctuation of gas-solid buoyancy force
c	—	Turbulence constant multiplier or forcing coefficient
C_D	—	Single particle drag coefficient
d_p	m	Particle diameter
e	—	Restitution coefficient for particle-particle collisions
f	—	Forcing function discrete value
Fr_{d_p}	—	Particle size based Froude number
$\mathbf{g}, g$	ms^{-2}	Acceleration of gravity
$\mathbf{g}_0$	—	Radial distribution function
H	—	Drag coefficient correction
$\mathbf{I}$	—	Unit tensor
$\mathbf{J}_{coll}$	$Jm^{-3}s^{-1}$	Rate of dissipation of granular energy by collisional damping.
$\mathbf{J}_{vis}$	$Jm^{-3}s^{-1}$	Rate of dissipation of granular energy by viscous damping.
k	$m^{-2}s^{-2}$	Kinetic energy
L	m	Characteristic length
$\mathbf{M}$	Nm^{-3}	Interface force
P	Nm^{-2}	Pressure
R_G	—	Random number
Re	—	Reynolds number
$\mathbf{s}$	s^{-1}	Strain rate tensor due to viscous plus pressure effects
St	—	Stokes number
t	s	Time
T	K	Temperature
u'	ms^{-1}	Velocity fluctuation in the horizontal direction
v'	ms^{-1}	Velocity fluctuation in the vertical direction
$\mathbf{v}$	ms^{-1}	Velocity vector
v_t	ms^{-1}	Terminal settling gas velocity
W	—	Wiener stochastic process
X	—	Mass fraction
y	m	Vertical (axial) Cartesian coordinate

Greek letters

β	$kgm^{-3}s^{-1}$	Micro-scale gas-solid drag coefficient
Γ_{slip}	$Jm^{-3}s^{-1}$	Rate of production of granular energy by gas-particle slip
Δ_f	m	Filter size

Δt	s	Time step
ϵ_p	—	Particle sphericity
Θ	$m^2 s^{-2}$	Granular temperature
κ_s	$kgm^{-1}s^{-1}$	Granular thermal conductivity
λ	Nsm^{-2}	Bulk viscosity
μ	Nsm^{-2}	Dynamic viscosity
ρ	kgm^{-3}	Density
σ	Nm^{-2}	Deviatoric stress tensor
σ	ms^{-1}	Root mean square velocity
τ'	Nm^{-2}	Reynolds-like stress tensor
τ	s	Response time
τ^*	s	Lagrangian integral timescale
ϕ	—	Volume fraction

Subscripts

eff	Effective, or meso-scale related
f	Fluid
fil	Filtered
g	Gas phase
i	Horizontal direction
I	Interface
j	Vertical direction
ℓ	A generic phase, either s or g
max	Maximum
p	Particle
r	Relative
res	Residual, or meso-scale related
s	Solid phase
$shear$	Related to the shear components
$slip$	Slip
$susp$	Suspension

Other symbols

—	Filtered or volume averaged
*	Dimensionless parameter
$\sim$	Favre or mass weighed average, $\tilde{f} = \frac{\overline{\phi f}}{\overline{\phi}}$
$\langle \ \rangle$	Domain volume average

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1 INTRODUCTION

1.1 Overview

Multiphase flow processes are widespread among pharmaceutical, chemical, petrochemical, agriculture, biochemical, food, power generation, metallurgical and consumer products industries. Prosperetti and Tryggvason (2007, p. 3) reported: "It is estimated that over half of anything which is produced in a modern industrial society depends to some extent on a multiphase flow process". Multiphase flows also occur in the environment: snow, sand, waves, mud slides, weather systems, oceanic circulation, coastal processes, rivers, overland flows, lake and estuary dynamics, groundwater flow, and geophysical fluid dynamics. Due to the high occurrence of multiphase flows in nature and industry, the necessity of understanding the underlying physics becomes one of the main interest of modern research which, in its turn, aims to ultimately explore the concerning applications in the most efficient manner.

As an example, let's briefly consider the relevance of multiphase processes in the energy generation sector. Over the last decade, renewable energy started to gain popularity up to a level where people considered it as a revolution or a new era in the energy sector. Moreover, renewable energy was expected to replace fossil fuel energy; however, U.S Energy Information Administration (2018) reported that the fossil fuel energy will be the first and biggest part of energy source for at least the 35 years to come, as can be seen in Figure 1. Due to the projected increase of energy consumption up to 2050, more in-depth studies

Figure 1: The fuel sector mix of energy consumption changes over the projected period in the Reference case

Source: U.S Energy Information Administration (2018)

should be conducted in order to develop efficient ways to explore and use these energy sources. [Figure 2](#) shows the world energy investment for 2016 ([IEA, 2017](#)). A total of \$1.8 trillion has been invested in 2016 only. It is worth noticing that fossil fuel energy industry is still getting very high levels of new capital investments, but faces several challenges. The following passage was taken from the workshop report on multiphase flow research attended by the most reputable scientists in the field ([DOE-US; NETL, 2006](#), p. 19):

To get a sense of the magnitude of the challenges faced by the fossil fuel industry, we will use clean coal technology as an example. To meet the demand for power in the United States, projections call for the construction of 87 GW of new coal-based power plants in the next 20 years. That corresponds to 174 new 500-MW power plants, which requires an investment of over \$100 billion. The new plants will deliver power worth over \$250 billion in the next 20 years. The clean coal technology roadmap has set aggressive targets for efficiency, plant availability, capital cost, and cost of electricity. Furthermore the targets must be achieved with near-zero emission of pollutants including CO₂ and multiphase flow systems such as gasifiers form the centerpiece of clean coal technology. Therefore, the opportunity to address the multiphase flow challenges in fossil fuel industry is indeed a large one. Addressing those challenges themselves would lead to great economic benefits. The above example considers only new power generation in the United States. The opportunities are enormous when innovations in existing plants and power generation for the entire world are considered.

Among the widespread multiphase flows of industrial interest are gas-solid flows. Gas-solid flows developed in risers are the main concern of the present research work, especially, the ones related to petroleum catalytic cracking and thermoelectric power generation. In order to improve the efficiency and performance of these industrial processes, we need to develop a better understanding of their respective flow hydrodynamics.

As an example of this kind of effort, let's consider the Nucla power plant project which was part of the US department of energy "Clean Coal Tecnology Demonstration Program". The Nucla atmospheric circulating fluidized-bed (ACFB) was scaled from small industrial units to a 110-MWe (total electric output) utility power plant. It is the largest demonstration project of its kind in the world. The following passages are taken from the Nucla Project performance summary ([NUCLA, 1999](#), p. 3, 12):

Department of Energy (DOE), Electric Power Research Institute, and Technical Advisory Group (potential users) interest and participation in the project was on the basis of evaluating ACFB potential for broad utility application through a comprehensive test program. Over a 2½ year period, 72 steady state performance tests were conducted and 15,700 hours logged.

The final capital costs associated with the engineering, construction, and start-up of the Nucla ACFB system were \$112.3 million (construction started in November 1984 and was completed in May 1987). This represented a capital cost of \$1,123/net kW. Total power costs associated with plant operations between September 1988 and January 1991 were approximately \$54.7 million.

On average, 43 staff were required on site to operate the Nucla ACFB system during the demonstration project. Adjusting for the demonstration program would result in a staffing requirement of 41 under normal utility operating conditions.

In summary, experiments for plant development of industrial size fluidized beds are too expensive: At first, a large investment of money is required for the construction process, then a second large investment is necessary to cover the expenses of the plant operations. In addition, these tasks necessitate a lot of time and manpower.

One can argue that experimental data can be obtained from pilot plant studies on smaller scales such as laboratories experiments. It has been shown that such approach is not practical due to the non-linear scale-up of the multiphase reactors design. The scale-up factor can vary in the interval 50-100 for fluidized beds and up to 10 000 for other types of reactors! (PANGARKAR, 2015). To sum up, empirical equations obtained under laboratory conditions can not predict accurately the fluidized beds behavior at industrial scales.

Mathematical modeling is an alternative to experimental development. CFD is a cheap and valuable tool currently used to expand and extend our knowledge on multiphase flows. For instance, Hydro-Quebec Canada developed a CFD study of an hydroturbine to increase its efficiency by 1.6 %, consequently, increased its revenue sales by \$3.2 million per year (BISH, 2001). Another example, an engineering company concluded that the benefits accrued from the use of CFD resulted in a six-fold return on the total required CFD investments (DAVIDSON, 2002). In conclusion, conventional laboratory experiments can be replaced by numerical simulations. Henceforth, to make CFD a trustworthy tool, the current mathematical models must be improved. The current work is a contribution in that direction.

1.2 Gas-solid flows

Gas-solid flows in general and fluidized beds in particular are key elements in several industrial applications. Fluid Catalytic Cracking (FCC) and Fluidized Bed Combustion (FCB) are two important processes in the petroleum and energy industries. Figure 3 is a simplified schematic of a Circulating Fluidized Bed (CFB). The main component of a CFB where all the chemical reactions take place is the riser. Gas is blown over solid particles leading to a process named fluidization, which will be shown in details in

Figure 2: World energy investment by sector in 2016

Source: IEA (2017)

the next section. The hydrodynamics of fluidized gas-solid flows present very complex behavior and characteristics. This raises the challenge for modelers to try to 'decipher' these phenomenons. The traditional method to develop CFB reactors consists of conducting experiments on multiple scales. These experiments are very time consuming, expensive and difficult to handle as discussed in [section 1.1](#). Recently, CFD has emerged as a cheap and practical alternative to the traditional experimental approach, for requiring much less capital investment and offering results in a much short period of time. CFD developments allow an easy and fast manipulation of the simulations, testing of many variations until reaching an optimal result, besides eliminating pollution and any kind of danger caused by real experimentation (power plants can explode, putting the life of people in danger, even on small scales).

On the other hand, numerical simulations require accurate modeling, and the latter requires a sound physical understanding of the gas-solid flows in question. Due to the large size of risers, numerical simulations performed on such scales are called Large Scale Simulations (LSS). Mathematical models and equations used for LSS require constitutive closures. Due to the current computational limitations, only coarse grids are viable for LSS. The effects that occur on a scale lower than the grid size are lost. These effects are called sub-grid effects. Disregarding the sub-grid effects will yield low accurate results. These sub-grid effects are usually recovered through the constitutive closures for the LSS. Generating closures for LSS becomes of utmost relevance for modelers, since the LSS are tremendously affected by the accuracy of such closures. One way to generate closures is through filtered results from Highly Resolved Simulations (HRS).

Figure 3: Simplified diagram of a CFB

Source: elaborated by the author

1.3 Fluidization

The fluidization process consists of imposing appropriate conditions over a number of solid particles to make them behave as a fluid. Figure 4 represents different fluidization regimes. The first state at the left represents a fixed bed where particles in a tube or column are at rest. This condition happens when the fluid blows from below in an upward direction, exerting a drag force which is not enough to suspend the particles. When the gas velocity increases, the drag exerted on the particles increases. When the drag force on the particles overcomes the gravity force, the particles enter the fluid-like state of motion. By increasing the gas velocity, different fluidization regimes can be achieved as shown in Figure 4 from left to right.

The main concern in this work are gas-solid flows in fluidized beds. In most industrial applications, gas is usually used as the acting fluid on solid particles, and the fluidization runs above the turbulent fluidization regime, usually in the fast fluidization regime. Fluidized beds present various advantages (GELDART, 1987):

- Easy handling of the system due to the fluid-like flow of particles

Figure 4: Different fluidization regime with increasing gas velocity

Source [Kunii and Levenspiel \(1991\)](#)

- Radial and axial isothermal condition due to the rapid mixing of solid particles
- Suitable for large scale applications
- Improved heat and mass transfer rates between phases
- Possibility to add or remove large quantities of heat due to particle circulation
- Huge area of contact between the fluid and solid phase (1 m^3 of $100 \mu\text{m}$ has a surface area of about $30,000 \text{ m}^2$), highly improving the heterogeneous chemical reactions.

However, some disadvantages also exist:

- Difficulty to describe the system due to complex flow hydrodynamics
- High rate of erosion of the reactor
- Nonuniform residence times of solid particles in the reactor
- Agglomeration and sintering¹ can possibly occur in some process which change the flow behavior
- Bubbles can prevent gas-solid contact
- Particle entrainment² and attrition³

In essence, the advantages outweigh the disadvantages, making fluidized beds reactors widely used in the industry.

¹ Coalesce of a powdered material into a solid

² Ejection of particles from the surface of a bubbling bed and removal of particle from the unit

³ Particle wear off into fine powders

1.4 Fluidized beds modeling

Several lines of research exist for fluidized beds modeling. Most models employ either Euler-Euler or Euler-Lagrange formulations. The gas phase is considered as a continuum (Euler approach). The solid phase can be treated as a continuum (Euler) or as discrete particles (Lagrange). The Navier-Stokes equations are used for the continuum formulations. If the particle is treated as a discrete phase, Newton's second law is used to determine the forces acting on each particle and therefore its motion. If it is considered as a continuum, NS equations are used instead.

The Euler-Lagrange method has the potential for providing more accurate predictions since the continuum approach of discrete particulates is avoided (it should be noticed, however, that all complexities related to gas-particle and particle-particle interactions, which are major causes of inaccuracy, are present in any modeling approach, Euler-Euler or Euler-Lagrange). Despite its advantages, the conventional Euler-Lagrange method is very time-consuming, since it requires to compute the equation of motion of each particle individually. Therefore, this method becomes impractical for large systems where a huge number of particles is present, which is the case of usual industrial gas-solid riser flows. However, it is valuable, because it provides a detailed description of particle movements for smaller systems where the number of particles does not exceed a thousand or for relatively larger ones with a very dilute concentration of solid. Some Euler-Lagrange like formulations are: Discrete Element Method (DEM), Lattice Boltzmann Method (LBM) and Multi-Phase Particle in Cell Method (MPPIC).

On the other hand, the Euler-Euler approach treats the two phases as interpenetrating continuum. Particles of same diameters and densities are considered as a single continuum phase. If the diameter of a particle or its density, or both change, we may consider multiple solid phases in the system. The Euler-Euler approach is computationally cheaper than that of Euler-Lagrange. The formulation requires closures which are of three types: topological laws, constitutive laws, transfer laws. Topological laws describe the spatial distribution of phase-specific flow quantities or variables. Constitutive laws describe the physical properties of different phases using axioms or experimental data. Transfer laws are equations that describe different interactions between phases at the interface. To close the set of equations, these laws must satisfy certain principles in order to successfully solve the problem. These principles were discussed by [Drew and Lahey \(1993\)](#), [Arnold et al. \(1990\)](#). The formulation known as Two-Fluid Model, which is applied in the present work, follows the Euler-Euler approach. The closure laws of interest in this work are the constitutive and transfer laws. Since, fine grids are practiced, all heterogeneities of the solid phase are expected to be captured, and no additional closures related to topology are required. Examples of constitutive laws are the closure equations for the solid phase stresses, involving the definition of solid phase pressure and viscosity. The drag force

Figure 5: Multiscale two-fluid modelling

Source: Elaborated by the author

closures constitute the most relevant of the transfer laws.

1.5 Multi-scale analysis

From the two-fluid modeling perspective, the micro-scales of a gas-solid flow are defined as those below which the flow is completely homogeneous, so that no coherent structures are observed. Otherwise, the meso and macro-scales of the flow are quite heterogeneous and fully characterized by coherent structures. The macro-scales are all the scales that can be captured in large scale simulations (LSS). The meso-scales are all the scales that are filtered in large scale simulations, and can be captured in highly resolved simulations (HRS).

Usually, in gas-solid riser flows, the relevant length scales are:

- Micro-scale - Order of the usual grid size in HRS (mm)
- Meso-scale - Order of meso-scale structures captured in HRS (cm)
- Macro-scale - Order of macro-scale structures captured in LSS ($dm - m$)

Large scale simulations are usually performed for real industrial risers using a filtered two-fluid formulation. Coarse grids are used under these conditions. These grids are usually of the order of centimeters. Hence, by performing LSS, only the macro-scale structures are being resolved. It has been shown that meso-scale structures affect the flow considerably (AGRAWAL et al., 2001). However, since they are smaller than the LSS grid size, they are

not resolved in LSS and their effects are filtered. To recover the effects of the meso-scale structures, highly resolved simulations are performed. The grid size in these simulations are of the order of millimeters, so that the meso-scale structures are resolved. HRS are performed using the two-fluid model with microscopic closures. [Figure 5](#) summarizes the relationship between HRS and LSS. On the right, a LSS is shown where the filtered TFM is used. On the left, a HRS is shown where the TFM with microscopic closures is used. By averaging over an area of an HRS (this filtering procedure will be explained in details in the following sections), one can produce meso-scale closures to be used in LSS. Therefore, by performing LSS with closures generated at the meso-scale level, by filtering over HRS, the accuracy of the LSS results is considerably improved.

The current work is a contribution to the development of sub-grid closures to LSS by applying HRS with microscopic two-fluid modeling. In special, two aspects are analyzed, one related to the marker correlation issue, the other related to the gas turbulence filtering in HRS. The concerning literature is revised next.

1.6 Literature review

1.6.1 HRS under microscopic two-fluid modeling

Two-fluid models including suitable filtered closures represent the most promising next generation models for multiphase reactors and, in this context, the formulation of realistic filtered models is a great challenge ahead ([SUNDARESAN, 2000](#)). This particular issue has been addressed by a number of researchers on the basis of HRS experiments with microscopic two-fluid modeling (see [Agrawal et al. \(2001\)](#), [Andrews et al. \(2005\)](#), [Igci et al. \(2008\)](#), [Igci and Sundaresan \(2011\)](#), [Parmentier et al. \(2012\)](#), [Ozel et al. \(2013\)](#), [Milioli et al. \(2013\)](#), [Agrawal et al. \(2013\)](#), [Schneiderbauer and Pirker \(2014\)](#), [Sarkar et al. \(2016\)](#)). Besides making it clear the real necessity for filtered models, those works suggest that filtered models so produced from highly resolved computational experiments do require continuous improvement as more and more realistic approaches are pursued. The filtered models are also called meso-scale models since they are generated from computational experiments under grid refinements that are expected to capture all the solid phase scales of the flow, so that filtered meso-scale data can be derived. In most cases, reduced domains are considered, which are extracted from the free stream in the core of the flow field, and periodic boundaries are applied. As periodic boundaries are applied, an extra gas phase pressure gradient is imposed in the vertical direction in order to impose a flow driving force. It is usual to consider an extra gas phase pressure gradient to exactly compensate the gravity acting on the gas-solid mixture. This idea is brought from fundamental studies on the instabilities that develop in gas-solid flows owing to inter-particle inelastic collisions, which ultimately lead to clustering ([GOLDHIRSCH et al., 1993](#)). While those studies are valid for quasi-static conditions, where the particulate arranges itself in low velocity

suspensions, it has been commonly assumed that the cluster formation mechanism that prevails is also relevant to any flow topology, from bubbling, to turbulent, to rapid gas-solid flows.

Following the above basic approach, [Agrawal et al. \(2001\)](#), [Andrews et al. \(2005\)](#), [Igci et al. \(2008\)](#), [Igci and Sundaresan \(2011\)](#) developed highly resolved simulations aiming for filtered correlations for the effective pressure and viscosity of the solid phase, and for the effective drag coefficient. [Agrawal et al. \(2001\)](#) characterized the meso-scale of the gas-solid flow as comprised of solid coherent structures with dimensions from 10 to 100 times the particulate size. From their predictions the authors analyzed the effective drag coefficient, and the effective dynamic viscosity and pressure of the solid phase. As observed by [Vanderhoef et al. \(2006\)](#), [Agrawal et al. \(2001\)](#) showed that grid refinements of the order of 10 times the particulate size provided grid independent predictions for a particular case. They also showed that vertical boundary conditions of free slip, partial slip and periodic, do produce similar flow topologies. [Andrews et al. \(2005\)](#) explicitly proposed ad hoc closures for the effective drag, viscosity and pressure of the solid phase. [Igci et al. \(2008\)](#) further extended the previous works of [Agrawal et al. \(2001\)](#), [Andrews et al. \(2005\)](#), and showed that the filtered predictions depend on the sub-grid filter size. A posterior work by [Igci and Sundaresan \(2010\)](#) also showed the filtered predictions to depend on the distance from walls. Further extending the work reported in [Igci et al. \(2008\)](#), [Igci and Sundaresan \(2011\)](#) produced correlations for the filtered effective drag, pressure and viscosity of the solid phase, as a function of filter size and filtered solid volume fraction. The effective drag coefficient was expressed in the form of a drag coefficient correction relating the actual effective drag coefficient to the filtered micro-scale drag coefficient, as previously done, for instance, by [Zhang and VanderHeyden \(2002\)](#). [Igci et al. \(2012\)](#) tested the correlations presented in [Igci and Sundaresan \(2011\)](#), including the wall corrections proposed in [Igci and Sundaresan \(2010\)](#), in coarse grid simulations of a riser flow. The comparisons against empirical data showed qualitative agreement, while quantitative differences still remained.

Following the same basics of the previous works, [Parmentier et al. \(2012\)](#) proposed a similar approach to deal with the filtered effective drag, except they did not apply periodic boundaries but a small 2D bubbling bed configuration. Their correlations for the effective drag correction were alike those proposed in [Igci and Sundaresan \(2011\)](#), except for the inclusion of a macro-scale length scale in the filter size dependence of the drag coefficient correction. They also included a coarse grid dynamical adjustment analogous to the dynamic correction usually applied in large eddy simulation of turbulent flows. A test of their drag correction correlation in a coarse grid simulation of a bubbling bed set up recovered the correct bed expansion which came out from a highly resolved simulation. The model remained to be tested for more dilute flow configurations such as circulating fluidized beds. [Ozel et al. \(2013\)](#) extended the work of [Parmentier et al. \(2012\)](#) by incorporating vertical periodic boundaries over 3D bubbling bed conditions, and also by

extending the development to include stresses analyses as done by [Agrawal et al. \(2001\)](#). Their conclusions were similar to those of [Parmentier et al. \(2012\)](#).

In the above works [Agrawal et al. \(2001\)](#), [Andrews et al. \(2005\)](#), [Igci et al. \(2008\)](#), [Igci and Sundaresan \(2011\)](#), [Parmentier et al. \(2012\)](#), [Ozel et al. \(2013\)](#), filtered parameters have been correlated to filter size and filtered solid volumetric fraction. It so happens that different patterns, ranging from very homogeneous to very heterogeneous, may occur for any particular values of filter size and filtered solid fraction. In order to account for the heterogeneity of the flow, [Milioli et al. \(2013\)](#) introduced an additional independent variable in filtered parameter correlation (named 2nd marker, while the solid volume fraction was named 1st marker). Models for effective pressures and viscosities were proposed in analogy with the Smagorinsky's turbulence viscosity model, thereby introducing the filtered scalar shear rate as 2nd marker. Also, a model for the effective drag coefficient correction was proposed including the filtered slip velocity as a 2nd marker. [Ozarkar et al. \(2015\)](#) applied the sub-grid models of [Milioli et al. \(2013\)](#) to a large scale simulation of a bubbling fluidized bed, and compared results to experiment. They found a very good agreement between experiment and predictions for both bed expansion and pressure drop through the height of the bed. [Schneiderbauer and Pirker \(2014\)](#) followed the same path as [Milioli et al. \(2013\)](#), and found similar results. [Agrawal et al. \(2013\)](#) extended the work of [Milioli et al. \(2013\)](#) by also proposing filtered models for the mass/heat diffusivity coefficient and for the inter-phase mass/heat transfer coefficient; respectively accounting for the filtered scalar shear rate and the filtered slip velocity as 2nd marker.

[Sarkar et al. \(2016\)](#) developed new sub-grid models following the work of [Milioli et al. \(2013\)](#), except that based on 3D highly resolved simulations. Similar behavior of the effective drag coefficient correction and effective pressures and viscosities were observed, with some quantitative differences. Regarding the effective pressures and viscosities, a correlation to the filtered velocity as 2nd marker was also observed which was not seen on the previous results of [Milioli et al. \(2013\)](#). In addition to sub-grid model proposition, [Sarkar et al. \(2016\)](#) also developed a validation step by comparing predictions of a large scale simulation against experiment for a bubbling bed situation. A very good agreement between predictions and experiment was found for both bed expansion and pressure drop through the height of the bed.

The majority of the studies mentioned above have been carried out under suspension like conditions in periodic domains, where a pressure gradient matching the weight of the gas-solid mixture is imposed in the vertical direction. Scale separation hypothesis is supposed to be fulfilled. In other words, macro-scale flow parameters should not affect the meso-scale parameters. [Mouallem et al. \(2018a\)](#) and [Mouallem et al. \(2018b\)](#) questioned this assumption by investigating two macro-scale parameters, the domain average gas Reynolds number and solid volume fraction. The authors performed HRS, imposing a wide

range of domain average gas Reynolds numbers and solid volume fractions typical of riser flows. Instead of following the typical 'enforced pressure gradient approach', they imposed domain average gas velocities to cover different fluidization regimes up to conditions close to pneumatic transport. They found that higher domain average solid volume fractions give rise to denser and thicker clusters of particles, while higher domain average gas Reynolds numbers elongate the clusters in the vertical direction and make the flow more homogeneous. These two parameters were shown to affect the drag coefficient correction, residual and filtered stresses, significantly. The marker issue is reassessed in the current research having in view the new scenario where the macro-scale effects also come to play a role.

1.6.2 Turbulence in gas-solid fluidized flows

[Sinclair and Jackson \(1989\)](#) observed that, in gas-solid flows, turbulent vortexes uniformly disperse finer particles, which follow the gas stream, and non-uniformly disperse coarser particles, whose inertia allows them to break through the vortexes. However, they notice that the effect of the particles over the turbulent structure of the gas is not known; and the velocity fluctuations of the gas induced by velocity fluctuations of the particles, and vice-versa, are also not known. They observed that a realistic model for a turbulent gas-solid flow must account for drag between phases owing to differences on their average velocities, and also for effects of velocity fluctuations in each phase over its own average motion defining apparent stresses. The development of turbulent structures is little known owing to a lack of knowledge on these issues, which imposes considerable arbitrariness over current modelling efforts. [Hrenya and Sinclair \(1997\)](#) observed that the currently available models for describing solid phase turbulence are of a somewhat speculative nature in view of the lack of information on this issue, and [Hrenya et al. \(2008\)](#) even questioned the capability of the usual Navier-Stokes equations for dealing with granular flows. The more recent literature did not report any major evolution on any of the previous issues. In spite of this scenario, [Gidaspow \(1994\)](#) observed that the coupled equations of momentum for fluid and particulate phases of the two-fluid models seem to correctly predict, in a qualitative way, the turbulence of two-phase flows.

Studies of turbulence in gas-particle flows usually seek for two different goals: i. to model the effects of the particulate over the fluid phase turbulence, i.e. to model fluid phase modulation; ii. to model the effects of the fluid phase turbulence over the particulate behaviour. The former is of higher interest here, since the current main concerns mostly regard the effective meso-scale hydrodynamics of solid phases. The effects of fluid sub-grid turbulence on the motion of particles remains as an open issue and a modelling challenge for researchers (see [Sinclair and Jackson \(1989\)](#), [Yamamoto et al. \(2001\)](#), [Fede and Simonin \(2006\)](#)).

Literature shows that the Stokes number (ratio between the response time of particles to a fluid flow and a turbulence time scale of the fluid) establishes boundaries defining whether a particulate is significantly affected or not by the fluid turbulence. The coarser and the heavier the particulates the higher the Stokes numbers result. For very small Stokes numbers (finer and lighter particles) the particulate is supposed to follow the fluid turbulent eddies just like a tracer; turbulence uniformly disperses the particles which are dragged into the eddies and simply follow the flow stream. For high Stokes numbers (coarser and heavier particles), otherwise, the motion of the particles is expected not to be significantly affected by the turbulent eddies in the fluid; fluid turbulence non-uniformly disperses the particles whose inertia makes them able to break through the eddies. Experiment in this field is regarded as both limited and uncertain (WANG et al., 2000). Comparisons between modelling predictions and experiment are reputed to be misleading owing to a lack of well-controlled experiments. Most of the relevant studies found in literature are either theoretical or based in computational experiments, a sample of which is briefly reviewed next in the light of the current interest, namely the evaluation of carrier fluid turbulence effects over carried high Stokes number particulates.

In the concerning field different theoretical approaches are practiced, ranging from statistical to Lagrangean and Eulerian modelling, mostly applying either DNS or LES. The main practical objectives of research are frequently related to establishing particle collision rates, rates of particle deposition, or sub-grid data to be applied in multi-scale approaches of real flows (VANDERHOEF et al., 2006). The statistical analysis of Abrahamson (1975) under isotropic turbulence showed the velocities of colliding particles in a turbulent air stream to be uncorrelated for particles of 2000 kg/m^3 density larger than $10 \mu\text{m}$ size, so that those high Stokes number particles result little affected by the turbulent field. Continuing researches in this line produced similar results, as reported by Zaichik et al. (2009), who also accounted for anisotropic turbulence. While the statistical analyses have been restricted to uniformly distributed particles in uniformly sheared flows, they stand for high Reynolds numbers realistic to real particle-laden flows. The uniformity restrictions of the statistical analyses have been removed by various researchers who practiced various different lines of modeling (CROWE et al., 1996). A very promising modeling direction consists of applying DNS for the carrier fluid coupled with Lagrangean approaches for the particulate motion (see Sundaram and Collins (1997), Wang et al. (2000), Zhou et al. (2001), Fevrier et al. (2005), Fede and Simonin (2006)). In all of those studies the authors found little effect of gas turbulence over the behavior of high Stokes number particulates.

While the DNS/Lagrangean approaches do provide a complete description of fluid turbulence down to the micro scales of Kolmogorov, they are still limited to low Reynolds numbers owing to computational limitations. Some authors practiced LES for the fluid phase coupled with Lagrangean particle calculations (see Wang and Squires (1996), Yamamoto et al. (2001), Fevrier et al. (2005), Yamamoto and Okawa (2009)). Wang and

Squires (1996) studied particle deposition in a vertical channel flow applying LES/Lagrange, neglecting inter-particle interactions. They observed that sub-grid velocity fluctuations did not have a large effect on particle deposition even for low Reynolds numbers, which was in reasonable agreement with previous DNS/Lagrange predictions. Yamamoto et al. (2001) also performed LES/Lagrange simulations, but accounting for inter-particle inelastic collisions. They considered vertical low Reynolds air flows transporting particulates in a very wide range of Stokes numbers (particles of 7 to 90 μm diameter, 700 to 8800 kg/m^3 density). LES were carried out for the gas flow, and the Lagrangian particle calculations were performed for air flow fields filtered at different extents. The authors found the filtering not to affect the particulate motion for high Stokes numbers. They also found that accounting for inelastic inter-particle collisions improved the predictions in comparison to experiment. Following the same line, Yamamoto and Okawa (2009) showed the Reynolds number of the gas flow to considerably affect the lateral motion of the particulate even for large Stokes numbers (90 μm diameter, 2500 kg/m^3 density). Fevrier et al. (2005) applied both the approaches, DNS/Lagrange and LES/Lagrange for ranges of low Reynolds and low Stokes numbers. Their results support previous observations that sub-grid velocity fluctuations in the fluid should have a negligible effect over the statistics of high Stokes number particulates.

Concerning fluidized gas-solid flows, there are no literature reported works applying continuum models under DNS since its implementation remains unrealistic for domains of practical interest (scale of centimetres, at least). Instead, HRS (highly resolved simulations) are practiced, which allow for the capture of even the smallest scales of particulate (see Agrawal et al. (2001), Andrews et al. (2005), Igci et al. (2008), Igci and Sundaresan (2011), Parmentier et al. (2012), Ozel et al. (2013), Milioli et al. (2013), Agrawal et al. (2013), Schneiderbauer and Pirker (2014), Sarkar et al. (2016)). In those works, however, no assessment has been attempted on the effects of gas turbulence over clusters, which is one of the propositions of the current research.

1.7 Objective

The objective of this work is to extend the previous study of [Mouallem et al. \(2018a\)](#) and [Mouallem et al. \(2018b\)](#) by:

- Investigating the effects of the flow macro-scale over meso-scale filtered parameters in gas-solid riser flows
- Investigating the necessity of inclusion of a third marker for better correlating relevant filtered parameters.
- Assessing the effects over relevant filtered parameters, of the gas turbulence usually filtered in HRS

A third marker, the filtered solid kinetic energy, for the drag coefficient correction and residual stresses is investigated in order to assess its suitability to catch the variation of the filtered parameters of interest for a wide range of domain average gas Reynolds numbers and solid volume fractions typical of riser flows.

It is well known that the effects of gas turbulence over the motion of high Stokes particles are negligible. Otherwise, such effects over clusters of particles remain unknown, and therefore also unknown are the effects over filtered parameters. In traditional HRS, the numerical grids are not refined enough to allow for DNS of the gas phase. We then artificially introduce turbulence in the gas phase at scales smaller than the grid size by applying a forcing function method.

2 METHODOLOGY

In what follows the TFM formulations are presented. First the TFM with microscopic closures is presented which is applied to HRS. Then the filtered TFM is presented in order to define the meso-scale closures to be derived from HRS results. Gas and particulate are treated as inter-penetrating continuum phases in thermodynamic equilibrium (see [Anderson and Jackson \(1967\)](#), [Gidaspow \(1994\)](#), [Enwald et al. \(1996\)](#), [Ishii \(1976\)](#), [Delhayé \(1974\)](#), [Drew \(1971\)](#), [Drew \(1983\)](#)). The hydrodynamic two-fluid models consist of a set of equations for each phase. Mass and momentum equations are resolved for the gas and solid phases. The derivation of these equations is not presented here and can be found in literature (see [Anderson and Jackson \(1967\)](#), [Gidaspow \(1994\)](#), [Enwald et al. \(1996\)](#)). Closures are needed for the stress tensors of both phases and for interface interaction forces.

2.1 Microscopic Two-Fluid model

The conservation equations of continuity and momentum for both phases are:

$$\frac{\partial}{\partial t} (\rho_g \phi_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g) = 0 \quad (2.1)$$

$$\frac{\partial}{\partial t} (\rho_s \phi_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s) = 0 \quad (2.2)$$

$$\frac{\partial}{\partial t} (\rho_g \phi_g \mathbf{v}_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g \mathbf{v}_g) = -\phi_g \nabla \cdot \boldsymbol{\sigma}_g - \mathbf{M}_I + \rho_g \phi_g \mathbf{g} \quad (2.3)$$

$$\frac{\partial}{\partial t} (\rho_s \phi_s \mathbf{v}_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \mathbf{v}_s) = -\nabla \cdot \boldsymbol{\sigma}_s - \phi_s \nabla \cdot \boldsymbol{\sigma}_g + \mathbf{M}_I + \rho_s \phi_s \mathbf{g} \quad (2.4)$$

The terms that need closures in the momentum equations are the solid phase stresses σ_s and the term $\mathbf{M}_I$ which represents interaction forces between the two phases. As pointed out in the previous section, constitutive laws stand for determining the stress terms, while transfer laws stand for determining the interaction forces between the gas and the solid, which is reduced mainly to the drag force (Other forces such as virtual mass, lift and history forces are usually lower order and are disregarded).

2.1.1 Solid phase stresses microscopic closures

The gas-solid two-fluid model presents various closure relations for the solid phase ([SYAMLAL et al., 1993](#)). In this study, the micro-scale closures for the solid phase are established by applying the kinetic theory of granular flows (KTGF) (see [Bagnold \(1954\)](#),

Gidaspow (1994), Jenkins and Savage (1983), Lun et al. (1984)), where solid phase micro-scale properties are derived as a function of a granular temperature determined from a pseudo thermal energy (PTE) balance. The conservation equation of granular energy (Agrawal et al. (2001), Gidaspow (1994)) is:

$$\frac{3}{2} \left[\frac{\partial}{\partial t} (\rho_s \phi_s \Theta) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \Theta) \right] = -\boldsymbol{\sigma}_s : \nabla \mathbf{v}_s + \nabla \cdot (\kappa_s \nabla \Theta) + \Gamma_{slip} - J_{coll} - J_{vis} \quad (2.5)$$

where:

$$\kappa_s = \frac{\lambda^*}{g_0} \left[\left(1 + \frac{12}{5} \eta \phi_s g_0 \right) \left(1 + \frac{12}{5} \eta^2 (4\eta - 3) \phi_s g_0 \right) + \frac{64}{25\pi} (41 - 33\eta) \eta^2 \phi_s^2 g_0^2 \right] \quad (2.6)$$

$$\Gamma_{slip} = \frac{81 \phi_s \mu_g^2 |\mathbf{v}_g - \mathbf{v}_s|^2}{g_0 d_p^3 \rho_s (\pi \Theta)^{\frac{1}{2}}} \quad (2.7)$$

$$J_{coll} = \frac{48}{\pi^{\frac{1}{2}}} \eta (1 - \eta) \frac{\rho_s \phi_s^2}{d_p} g_0 \Theta^{\frac{3}{2}} \quad (2.8)$$

$$J_{visc} = 3\beta\Theta \quad (2.9)$$

$$\lambda^* = \frac{\lambda}{1 + \frac{6\beta\lambda}{5(\rho_s \phi_s)^2 g_0 \Theta}} \quad \lambda = \frac{75 \rho_s d_p (\pi \Theta)^{\frac{1}{2}}}{48 \eta (41 - 33\eta)} \quad \eta = \frac{1 + e}{2} \quad (2.10)$$

The first and third terms on the right hand side of Equation 2.5 denote respectively the rates of production of pseudo-thermal energy by shear and gas-particle slip. The second term represents the diffusive transport of pseudo-thermal energy. The fourth and the fifth terms represent, respectively, the rates of dissipation of pseudo-thermal energy through inelastic collisions and viscous damping. The radial distribution function (a parameter applied to a continuum phase that is related to the distribution of distances among particles on the actual particulate flow) is given by:

$$g_0 = \frac{1}{1 - \left(\frac{\phi_s}{\phi_{s,max}} \right)^{\frac{1}{3}}} \quad \phi_{s,max} = 0.65 \quad (2.11)$$

The deviatoric stresses of the phases are given by:

$$\boldsymbol{\sigma}_l = \left[P_l - \left(\lambda_l + \frac{2}{3} \mu_l \right) (\nabla \cdot \mathbf{v}_l) \right] \mathbf{I} - 2\mu_s \mathbf{s}_l \quad l = g, s \quad (2.12)$$

$$\mathbf{s}_l = \frac{1}{2} [\nabla \mathbf{v}_l + (\nabla \mathbf{v}_l)^T] - \frac{1}{3} (\nabla \cdot \mathbf{v}_l) \mathbf{I} \quad l = g, s \quad (2.13)$$

$$\mu_g = \text{constant} \quad \lambda_g = 0 \quad (2.14)$$

where:

$$\mu_s = \frac{(2 + \alpha)}{3} \left\{ \frac{\xi^*}{g_0 \eta (2 - \eta)} \left(1 + \frac{8}{5} \phi_s \eta g_0 \right) \left(1 + \frac{8}{5} \eta (3\eta - 2) \phi_s g_0 \right) + \frac{6}{5} \eta \mu_b \right\} \quad (2.15)$$

$$\lambda_s = \eta\mu_b - \frac{2}{3}\mu_s \quad (2.16)$$

$$\mu_b = \frac{256\xi\phi_s^2g_0}{5\pi} \quad \xi^* = \frac{\xi}{1 + \frac{2\beta\xi}{(\rho_s\phi_s)^2g_0\Theta}} \quad \xi = \frac{5\rho_sd_p(\pi\Theta)^{\frac{1}{2}}}{96} \quad \alpha = 1.6 \quad (2.17)$$

The solid phase pressure is given by:

$$P_s = \rho_s\phi_s(1 + 4\eta\phi_sg_0)\Theta \quad (2.18)$$

2.1.2 Drag microscopic closures

The term $\mathbf{M}_I$ stands for the interface interaction forces between the gas and solid phases. Some of the forces that contribute to the momentum exchange between the phases are: stationary drag, transverse force (i.e. lift), added mass force, history force (basset force). In the case of fluidized beds with a small gas-to-particle density ratio, all the forces are neglected except for the stationary drag force, which represents the main force inducing the motion of the solid particles. The drag force of the gas over the solid phase is defined as (GIDASPOW, 1994):

$$\mathbf{M}_I = \beta (\mathbf{v}_g - \mathbf{v}_s) \quad (2.19)$$

The drag coefficient follows the model developed by Wen and Yu (1966), Gidaspow et al. (1983):

$$\beta = \frac{3}{4}C_D \frac{\rho_g\phi_s\phi_g|\mathbf{v}_g - \mathbf{v}_s|}{(d_p\epsilon_p)} (\phi_g)^{-2.65} \quad (2.20)$$

The Wen-Yu drag model was developed for liquid-solid fluidized flows. Such flows are always homogeneous by nature. In their model, the authors added a correction term $(\phi_g)^{-4.7}$, to accurately describe the drag force acting on an individual particle immersed in an homogeneous multiparticle system. While this correction suits homogeneous systems, it does not suit an heterogeneous situation such as that in riser flows. This correction does not account for the effects of cluster formation and evolution over the drag. The presence of clusters decreases the value of the drag coefficient. It has been shown that the drag coefficient for heterogeneous flows is smaller than that of homogeneous ones. This discrepancy is due to the formation of coherent solid structures in heterogeneous flows that decrease the area of contact between the two phases, allowing an easier bypass of the gas, leading to a significant decrease in the magnitude of the drag force. The Wen-Yu correction term was then modified by Gidaspow et al. (1983) to $(\phi_g)^{-2.65}$ which better suits typical gas-solid riser flows (but does not account for clusters and other flow heterogeneities). The single particle drag coefficient for $Re_p < 1000$ (ROWE, 1961) is given by:

$$C_D = \frac{24}{Re_p} \left(1 + 0.15Re_p^{0.687}\right) \quad (2.21)$$

For $Re_p \geq 1000$ (ROWE, 1961), it is given by:

$$C_D = 0.44 \quad (2.22)$$

The Reynolds number based on particle size is:

$$Re_p = \frac{|\mathbf{v}_g - \mathbf{v}_s| d_p \rho_g \phi_g}{\mu_g} \quad (2.23)$$

Finally, the volumetric continuity requires that:

$$\phi_g + \phi_s = 1 \quad (2.24)$$

2.2 Filtered Two-Fluid Model

The two-fluid microscopic equations can be transformed into filtered equations by spatial averaging over a certain length scale (filter size). In the filtered equations, the microscopic effects appear as filtered and residual terms which require additional constitutive relations to close the formulation. The terms that require closure are the filtered and residual stresses of both phases and the interphase interaction forces.

In this work, volume average filtering is performed following Anderson and Jackson (1967). The filtered or resolved variables are defined by the filtering operation:

$$\bar{f}(\mathbf{x}, t) = \int_{V_\infty} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}, t) d\mathbf{y} \quad (2.25)$$

where $\mathbf{x}$ represents the position of the center of the filter, $\mathbf{y}$ the integrating variable representing the position of the cell that is being integrated, V_∞ is the region over which the filtering is performed and $G(\mathbf{x}, \mathbf{y})$ is a sub-grid space cut that limits the size of the smaller scales to be resolved. It should satisfy $\int_{V_\infty} G(\mathbf{x}, \mathbf{y}) d\mathbf{y} = 1$. The sub-grid filter is usually made to match with the numerical grid volume V , so $G(\mathbf{x}, \mathbf{y}) = 1/V$. Therefore:

$$\bar{f}(\mathbf{x}, t) = \frac{1}{V} \int_V f(\mathbf{x}, t) dV \quad (2.26)$$

Each variable can then be written as a sum of a filtered (resolved) part and a sub-grid fluctuation (unresolved part):

$$f(\mathbf{x}, t) = \bar{f}(\mathbf{x}, t) + f'(\mathbf{x}, t) \quad (2.27)$$

Filtered phase variables are obtained by applying the Favre or mass weighted averaging. For a specific phase, ℓ , we write:

$$\tilde{f}_\ell(\mathbf{x}, t) = \frac{\int_V \phi_\ell(\mathbf{x}, t) f_\ell(\mathbf{x}, t) dV}{\int_V \phi_\ell(\mathbf{x}, t) dV} \quad \ell = g, s \quad (2.28)$$

Consequently, the phase weighted fluctuations are given by:

$$f''(\mathbf{x}, t) = f(\mathbf{x}, t) - \tilde{f}(\mathbf{x}, t) \quad (2.29)$$

In what follows, overbars denote volume-averaged filtered variables, while overtilde represents phase fraction weighted filtered variables. Note that, the corresponding fluctuations are not equal $f' \neq f''$. A prime denotes a fluctuation based on a volume average, whereas a double prime denotes a fluctuation based on a mass-weighted average.

Following these definitions, applying the averaging procedure to the microscopic two fluid model presented in the previous section, the resulting filtered two-fluid model is given by:

$$\frac{\partial}{\partial t} (\rho_g \bar{\phi}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g) = 0 \quad (2.30)$$

$$\frac{\partial}{\partial t} (\rho_s \bar{\phi}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s) = 0 \quad (2.31)$$

$$\frac{\partial}{\partial t} (\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g \tilde{\mathbf{v}}_g) = -\bar{\phi}_g \nabla \tilde{\boldsymbol{\sigma}}_g - \nabla \cdot \boldsymbol{\tau}'_g - (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_g \bar{\phi}_g \mathbf{g} \quad (2.32)$$

$$\frac{\partial}{\partial t} (\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s \tilde{\mathbf{v}}_s) = -\nabla \cdot \bar{\boldsymbol{\sigma}}_s - \nabla \cdot \boldsymbol{\tau}'_s - \bar{\phi}_s \nabla \cdot \tilde{\boldsymbol{\sigma}}_g + (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_s \bar{\phi}_s \mathbf{g} \quad (2.33)$$

where $\bar{\mathbf{M}}_I$ is the filtered drag force of the gas over the solid phase, given by:

$$\bar{\mathbf{M}}_I = \overline{\beta (\mathbf{v}_g - \mathbf{v}_s)} \quad (2.34)$$

$\mathbf{B}'_{gs}$ is the fluctuation of the buoyancy force of the gas over the solid phase, given by:

$$\mathbf{B}'_{gs} = - \left[\overline{\phi_s \nabla \cdot \boldsymbol{\sigma}_g} - \bar{\phi}_s \nabla \cdot \bar{\boldsymbol{\sigma}}_g \right] \approx - \left[\overline{\phi_s \nabla P_g} - \bar{\phi}_s \nabla \bar{P}_g \right] \quad (2.35)$$

A generalized effective interface interaction force between the two phases may be written as the product of an effective drag coefficient and the favre average slip velocity:

$$\beta_{\text{eff}} (\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s) = \mathbf{B}'_{gs} + \bar{\mathbf{M}}_I \quad (2.36)$$

β_{eff} is called the effective drag coefficient (owing to the predominance of drag as compared to the buoyancy fluctuation term), which results:

$$\beta_{\text{eff}} = \frac{\overline{\beta (\mathbf{v}_g - \mathbf{v}_s)}}{(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s)} - \frac{\left[\overline{\phi_s \nabla P_g} - \bar{\phi}_s \nabla \bar{P}_g \right]}{(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s)} \quad (2.37)$$

Also, a drag coefficient correction may be defined by relating the effective drag coefficient to the filtered micro-scale drag coefficient, i.e.:

$$H = 1 - \frac{\beta_{\text{eff}}}{\beta} \quad (2.38)$$

Thus, we have:

$$\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I = (1 - H) \bar{\beta} (\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s) \quad (2.39)$$

The filtered deviatoric stress tensor for the gas phase is given by:

$$\tilde{\boldsymbol{\sigma}}_g = P_{fil,g} \mathbf{I} - 2\mu_{fil,g} \tilde{\mathbf{S}}_g \quad (2.40)$$

where the filtered gas pressure and filtered gas viscosities are:

$$P_{fil,g} = \tilde{P}_g - \left(\lambda_g + \frac{2}{3} \mu_g \right) (\nabla \cdot \tilde{\mathbf{v}}_g) \quad (2.41)$$

$$\mu_{fil,g} = \mu_g \quad (2.42)$$

$$\lambda_g = 0 \quad (2.43)$$

The filtered deviatoric stress tensor for the solid phase is given by:

$$\bar{\boldsymbol{\sigma}}_s = P_{fil,s} \mathbf{I} - 2\mu_{fil,s} \tilde{\mathbf{S}}_s \quad (2.44)$$

The filtered solid pressure and filtered solid dynamic viscosity are given by:

$$P_{fil,s} = \bar{P}_s - \overline{\left(\lambda_s + \frac{2}{3} \mu_s \right) (\nabla \cdot \mathbf{v}_s)} \quad (2.45)$$

$$\mu_{fil,s} = \bar{\mu}_s \quad (2.46)$$

The filtered strain rate tensor (for $\ell = g, s$) is given by:

$$\tilde{\mathbf{S}}_\ell = \frac{1}{2} \left[\nabla \tilde{\mathbf{v}}_\ell + (\nabla \tilde{\mathbf{v}}_\ell)^T \right] - \frac{1}{3} (\nabla \cdot \tilde{\mathbf{v}}_\ell) \mathbf{I} \quad (2.47)$$

The residual stresses (for $\ell = g, s$) are defined by:

$$\boldsymbol{\tau}'_\ell = \rho_\ell \bar{\phi}_\ell (\widetilde{\mathbf{v}}_\ell \widetilde{\mathbf{v}}_\ell) - \rho_\ell \bar{\phi}_\ell \widetilde{\mathbf{v}}_\ell \widetilde{\mathbf{v}}_\ell \quad (2.48)$$

In analogy with the viscous stresses, the residual stresses may also be expressed in terms of residual parameters for pressures and viscosities (just like the usual analogy in turbulence regarding viscous and Reynolds stresses, hypothesis of Boussinesq):

$$\boldsymbol{\tau}'_\ell = P_{res,\ell} \mathbf{I} - 2\mu_{res,\ell} \tilde{\mathbf{S}}_\ell \quad (2.49)$$

Assuming isotropy, the normal components of the residual stresses define the residual pressure as:

$$P_{res,\ell} = \frac{1}{3} \text{tr}(\boldsymbol{\tau}'_\ell) \quad (2.50)$$

The shear components of the residual stresses define the residual viscosity as:

$$\boldsymbol{\tau}'_{shear,\ell} = 2\mu_{res,\ell} \tilde{\mathbf{S}}_{shear,\ell} \quad (2.51)$$

Figure 6: Snapshot of the solid volume fraction in a large periodic domain

Source: [Igci et al. \(2008\)](#)

where the shear components of the filtered strain rate tensor (for $\ell = g, s$) are given by:

$$\tilde{\mathbf{s}}_{shear,\ell} = \frac{1}{2} \left(\nabla \tilde{\mathbf{v}}_\ell + (\nabla \tilde{\mathbf{v}}_\ell)^T \right) \quad (2.52)$$

The residual viscosity results:

$$\mu_{res,\ell} = \frac{|\boldsymbol{\tau}'_{shear,\ell}|}{2|\tilde{\mathbf{s}}_{shear,\ell}|} \quad (2.53)$$

The filtered kinetic energy of the phases is given by:

$$k_\ell = \frac{1}{2} \widetilde{\mathbf{v}''_{\ell,i} \mathbf{v}''_{\ell,i}} \approx \frac{1}{2} \frac{tr(\boldsymbol{\tau}'_\ell)}{\rho_\ell \bar{\phi}_\ell} \quad (2.54)$$

where:

$$\mathbf{v}''_\ell = \mathbf{v}_\ell - \tilde{\mathbf{v}}_\ell \quad (2.55)$$

Figure 7: Difference between grid, filter and domain size

Source: elaborated by the author

2.3 Filtering process

Figure 6 represents a snapshot of the solid volume fraction in a large periodic domain illustrating different filter sizes (IGCI et al., 2008). Figure 7 shows the difference between the domain, filter and grid size. The grid size is of the order of 10 particle diameters. The domain size is the size of the whole computational domain. The filter size may vary from the grid size, which is equivalent to no filtering at all, to the domain size, which is equivalent to filtering over the whole domain as in Agrawal et al. (2001). A filter length is chosen to determine a region, then averaging is performed for a desired quantity (ex : filtered drag coefficient) over the cells present in this region. Different regions under the same filter size are statistically equivalent, meaning that they have the same probability of occurrence all over the domain. Figure 8 illustrates the filtering process. The filter size is a square 4x4, which means it takes into account four grids in both the horizontal and vertical directions. So 16 grid cells are included in the calculation of the filtered quantities for this filter. The volume of each cell, V_i , equals the grid size squared (for a 2D simulation). The volume average of the gas volume fraction is simply calculated as:

$$\bar{\phi}_g = \frac{\phi_{g,1}V_1 + \phi_{g,2}V_2 + \dots + \phi_{g,i}V_i + \dots}{V_1 + V_2 + \dots + V_i + \dots} = \frac{\sum \phi_{g,i}V_i}{\sum V_i} \quad (2.56)$$

Figure 8: Post MFIX filtering procedure

Source: Elaborated by the author

The Favre or mass weighted average of a quantity, say the gas velocity in the vertical direction $\tilde{v}_g$ is expressed as:

$$\tilde{v}_g = \frac{\overline{\phi_g v_g}}{\overline{\phi_g}} \quad (2.57)$$

where $\overline{\phi_g v_g}$ is calculated in the same way as $\overline{\phi_g}$:

$$\overline{\phi_g v_g} = \frac{\phi_{g,1} v_{g,1} V_1 + \phi_{g,2} v_{g,2} V_2 + \dots + \phi_{g,i} v_{g,i} V_i + \dots}{V_1 + V_g + \dots + V_i + \dots} = \frac{\sum \phi_{g,i} v_{g,i} V_i}{\sum V_i} \quad (2.58)$$

All filtered quantities are calculated in the same manner. When all the required quantities are computed, the filter is moved to another region of 16 grids. When the filter have already passed over all the regions in a particular snapshot, a next snapshot is considered and so on. All the snapshots are taken inside the statistical steady state flow regime. Averaged data are obtained through filtering in space and time: since all the snapshots are taken inside the statistical steady state regime, they are considered statistically equivalent. A

Figure 9: One marker binning procedure

Source: Elaborated by the author

Figure 10: Two markers binning procedure

Source: Elaborated by the author

suitable number of snapshots must be considered, so that robust averaging statistics are obtained.

2.3.1 Binning

The gathered filtered data are classified by ranges of relevant independent variables (markers) and stored while statistically averaged inside suitable bins. This method was first introduced by [Igci et al. \(2008\)](#), where filtered properties like slip velocity, solid volume fraction, and drag force were merged together while statistically averaged inside bins defined by narrow ranges of filtered solid volume fraction. This is called the one marker analysis, which is illustrated in [Figure 9](#).

Later on, the two-marker analysis was developed, which is presented in [Figure 10](#). It was first introduced by [Milioli et al. \(2013\)](#). In addition to the first marker, the filtered solid volume fraction, a second marker, the favre averaged slip velocity, was introduced into the analysis. In this procedure, the filtered values are grouped in a double entry table, where the entries are the first and the second markers. Thus, the obtained average of the filtered values becomes a function of the two parameters. While this procedure allows for more refined correlations, it is actually unknown whether a two-marker analysis is accurate enough. In this study, a new parameter, the filtered solid kinetic energy is investigated as

Figure 11: Three markers binning procedure

Source: Elaborated by the author

a third marker in addition to the filtered solid volume fraction and filtered slip velocity. Schneiderbauer and Pirker (2014) found this parameter (actually the filtered kinetic energy of space velocity fluctuations of the solid phase, here named filtered solid kinetic energy for shorter) to be a representative marker in sub-grid modeling of gas-solid fluidized flows. Therefore, the two-marker binning procedure is then extended to a three-marker binning procedure. Figure 11 illustrates this situation. For conditions similar to those currently applied, previous studies showed that a filtered solid volume fraction range $0 < \bar{\phi}_s < 0.645$ and a filtered slip velocity range $0 < \tilde{v}_{slip,y}/v_t < 5.2$, cover all possible occurrences in the flow field (see Milioli et al. (2013), Sarkar et al. (2016), Mouallem et al. (2018a), Mouallem et al. (2018b)). For the first and second markers, respectively, 64 and 80 bins provided good enough resolutions for any filtered parameter analysis. As for the third marker, the filtered solid kinetic energy, tests were performed showing that a range of $0 < k_s/v_t^2 < 5.24$ covers all possible occurrences in the flow field for all the different conditions practiced in the current simulations. 80 bins of the third marker were found adequate for good enough resolution for any filtered parameter analysis.

3 TURBULENCE AND THE FORCING FUNCTION METHOD

Taking inspiration from applications of the forcing function method to numerical direct simulation of mono-phase turbulent flows, Milioli (2016) extended the procedure to deal with gas-solid fluidized flows. However, contrary to the intent of providing for controlled turbulent fields usual in turbulence studies, the author disturbed both the phases in order to externally control the filtered scalar shear rate of the solid phase (which was under consideration as a marker for filtered stresses and the drag coefficient correction). Forcing was introduced over the drag force term in the momentum conservation equations of the microscopic two-fluid model equations for both the phases. Differently from the proposition of Milioli (2016), the forcing function is now applied over the gas phase alone in order to artificially generate a gas turbulent field, whose effects over the solid phase is to be evaluated. The basics regarding the forcing function method is described next, which is followed by the set up for the application of current concern.

3.1 Generation of Homogeneous Isotropic Turbulence

Statistically, stationary Homogeneous Isotropic Turbulence (HIT) allows us to study different features of turbulent flows. HIT does not exist in nature, and can not be obtained through laboratory experiments; however, it can be easily established artificially through numerical simulations. Homogeneous isotropic turbulence decays due to the dissipation process through viscosity. However, it can be maintained and sustained, in numerical simulations, by artificially injecting energy into the flow through the so called forcing functions. This procedure consists of performing DNS, adding an "artificial" energy production term in the NS equations which will compensate the dissipative terms so that a statistical stationary steady state is obtained. Orszag and Patterson (1972) and Rogallo (1981) first introduced the pseudo-spectral method to perform DNS of homogeneous turbulence. Eswaran and Pope (1988) first developed the forcing function method at low wavenumbers. The physical space is transformed into spectral space using Fourier transforms. The method consists of injecting energy in the low wavenumber band, at each wavenumber independently. This translates to constantly feeding the large scale structures in the flow, which feed the smaller structures following the Kolmogorov cascade. The energy injected follows the Ornstein-Uhlenbeck random stochastic model.

Lately, another method is being extensively used in the physical space. It is called the linear forcing method. Lundgren (2003) developed a procedure to obtain HIT by adding a term which is directly proportional to the velocity vector itself in the physical space. Thus, energy is injected, contrary to the previous method, for all wavenumber modes.

Figure 12: Flow regime for different Stokes numbers

Source: Sinclair (2011)

3.2 Stokes number

Stokes number depicts the effects of gas turbulence on the motion of single particles. It is defined as the ratio of the particle response time to the fluid response time, given respectively by:

$$\begin{aligned}\tau_p &= \frac{d_p^2 \rho_s}{18\mu_f} \\ \tau_f &= \frac{L_f}{v_f}\end{aligned}\tag{3.1}$$

where d_p represents the particle diameter, ρ_s the particle density, μ_f the fluid viscosity, L_f the characteristic length of the fluid phase, v_f the characteristic velocity of the fluid phase. The Stokes number becomes:

$$St = \frac{\tau_p}{\tau_f} = \frac{\rho_s d_p \langle v_{g,y} \rangle}{18\mu_f}\tag{3.2}$$

where $\langle v_{g,y} \rangle$ represents the domain averaged gas phase velocity in the axial (vertical) direction.

Figure 12 illustrates the effects of Stokes number over the particle motion. Low Stokes number corresponds to the viscous flow regime. In this regime, when a particle meets a gas vortex, it follows the fluid streamlines as a tracer. When multiple particles are present in the flow, their trajectories are tangent to the streamlines of the fluid phase, resulting in a low particle collision rate. In contrast, high Stokes number corresponds to the inertia flow regime, characteristic of heavy particles which are not affected by turbulent eddies of the fluid phase. The particles break through the streamlines of the carrier phase, resulting in a high particle collision rate when multiple particles are present on the flow.

3.3 Brownian motion and Ornstein-Uhlenbeck process

'Brownian motion' is now considered as a means of introducing the randomic treatment to be enforced over a gas in order to artificially generate turbulence. In 1827, the

botanist Robert Brown noticed, through his microscope, the random movement of pollen particles of size 10^{-3}cm in water (BROWN, 1828). He was not able to find a physical explanation for that observation and thought that the particles were alive because they were able to move. Later on, Einstein (1905) explained in details how the individual molecules of water caused the movement of the pollen particles. That discovery also served as a strong evidence of existence of atoms and molecules. In short, pollen particles were bombarded by random water molecules ¹ in random directions and intensities in a very brief period of time which lead to a random resulting force that caused the random-like movement of the pollen particles. The random motion of solid particles in a suspended fluid resulting from their collision with the moving fluid particles was called 'Brownian motion'.

Considering $\vec{X}$ as the position of a particle of mass m in space, its equation of motion following Newton's second law is:

$$m\ddot{\vec{X}} = \Sigma\vec{F} \quad (3.3)$$

where $\ddot{\vec{X}}$ is the acceleration term, and $\Sigma\vec{F}$ the sum of forces acting on the particle which are:

- Field force $\vec{F}(\vec{X})$. It could be electric/magnetic/gravitational force(s) for instance.
- Friction force $\gamma\dot{\vec{X}}$, where γ represents a friction coefficient. This force resists to the movement of the particle in the fluid. The coefficient γ can be determined from Stoke's law (assuming that it holds on this scale) which describes the drag force acting on a spherical particle in a fluid.
- Random force $\alpha\overline{\xi(t)}$, where α is a constant and $\overline{\xi(t)}$ is the white noise function. This force represents the random collisions of fluid molecules with the particle. It has zero average value $\langle\xi(t)\rangle = 0$ and $\langle\xi(t_2)\xi(t_1)\rangle = \delta(t_2 - t_1)$ which means that impacts are uncorrelated over time.

Putting all terms together and dividing by the particle mass, it comes that:

$$\ddot{\vec{X}} = \frac{1}{m}\vec{F}(\vec{X}) - \frac{\gamma}{m}\dot{\vec{X}} + \frac{\alpha}{m}\overline{\xi(t)} \quad (3.4)$$

This is the Langevin equation of motion for the Brownian particle. The first and second terms on the right hand side of Equation 3.4 are deterministic forces and can be grouped in one term $A(\dot{\vec{X}}(t), t)$. The white noise coefficient could also be written in a generic form $B(\dot{\vec{X}}(t), t)$. When the white noise coefficient is constant, the white noise function is called additive noise. Otherwise, it is called multiplicative noise. For the sake of simplicity

¹ 10^{12} collisions per second for a liquid under normal conditions

$B(\dot{X}(t), t)$ is taken as a constant. Assuming one dimensional analysis for simplicity, the previous equation can be written as:

$$\ddot{X}(t) = A(\dot{X}(t), t) + B\xi(t) \quad (3.5)$$

or

$$d\dot{X}(t) = A(\dot{X}(t), t)dt + B\xi(t)dt \quad (3.6)$$

Integrating between t and $t + \delta t$, then considering an average value for the deterministic term², when $\delta t \rightarrow dt$, we get:

$$d\dot{X}(t) = A(\dot{X}(t))dt + BdW(t) \quad (3.7)$$

The integral of the white noise $dW(t)$ is called the Wiener stochastic process. The Wiener process is a Markovian process³. The Wiener process has zero mean and a Gaussian distribution with a standard deviation $\sigma = \sqrt{dt}$, where dt is a characteristic time related to the particle movement. Moreover, it can be written as $dW(t) = \sqrt{dt}R_G$, where R_G represents a random number taken from a normal distribution, $\langle R_G \rangle = 0$ and $\langle R_G^2 \rangle = 1$. The previous equation becomes:

$$d\dot{X}(t) = A(\dot{X}(t))dt + B\sigma R_G \quad (3.8)$$

This equation is similar to the Ornstein-Uhlenbeck stochastic process. It is used in physics, engineering, biology, medicine, economics, and its terms are modeled in each case to describe the particular application. The Ornstein-Uhlenbeck process is a mathematical diffusion model that can describe the velocity of a particle undergoing a Brownian motion. In our case, we will use this model as a scheme to describe the random stochastic forcing function f_t at time t :

$$f_{t+\Delta t} = Af_t + B\sigma R_G \quad (3.9)$$

where the first term on the right hand side represents the deterministic part of the forcing function, and the second term represents the randomic part. Some properties of the (OU) process are:

- $\langle f_t \rangle = 0$
- $\langle f_t^2 \rangle = \sigma^2$
- $\langle f_t f_{t+\Delta t} \rangle = \sigma^2 \exp\left(-\frac{\Delta t}{\tau^*}\right)$

² The variation of the deterministic term $A(\dot{X}(t), t)$ is negligible in the time interval δt , which is of the order of the molecular timescale. δt is macroscopically very small even though hundreds of billions of collisions occur during it.

³ A Markovian model is a particular type of stochastic model where only the present value of the variable is relevant to predict the future. Everything in the past is irrelevant.

Here, Δt is a time step, σ^2 is the variance of a flow relevant parameter with Gaussian distribution (a parameter sensitive to turbulence, such as velocity), and τ^* is a characteristic time scale associated to the dominant frequency in the temporal series of this concerning parameter. Two mathematical forms of the forcing function were tested in the present work:

- Algebraic form $f_{t+\Delta t} = \left(1 - \frac{\Delta t}{\tau^*}\right) f_t + \sqrt{\frac{2\Delta t}{\tau^*}} \sigma R_G$
- Exponential form $f_{t+\Delta t} = \exp\left(\frac{-\Delta t}{\tau^*}\right) f_t + \sqrt{1 - \left(\exp\left(\frac{-\Delta t}{\tau^*}\right)\right)^2} \sigma R_G$

Various expressions of the forcing function exist in the literature, each of them is employed according to the conditions of the case of interest. The algebraic form comes from [Pope \(2000\)](#), while the exponential form was taken from [Andrews et al. \(2005\)](#). After performing different tests to evaluate these forms, the two expressions yielded similar results. For the sake of simplicity, the algebraic form was taken in what follows.

3.4 Random number generation

The randomness of the forcing function is due to the term R_G which should be taken from a Gaussian distribution. Various random number generators exist in the literature. The random number generator algorithm⁴ developed by [Park and Miller \(1988\)](#) is used to determine the term R_G . [Figure 13](#) shows more than 1000 different random numbers generated by this algorithm. Park-Miller algorithm can generate more than billion random numbers without repetition. These numbers have zero mean, standard deviation of one, and a Gaussian distribution as shown in [Figure 14](#).

Figure 13: Random values generated by Park-Miller algorithm

Source: Elaborated by the author

Figure 14: Probability density function of the random numbers generated by the Park-Miller algorithm

Source: Elaborated by the author

⁴ FORTRAN code available in [Appendix A](#)

Figure 15: f values for $\sigma = 6.61\text{cm/s}$ and $\tau^* = 0.1621\text{s}$. Δt varied in the interval $10^{-4} < \Delta t < 10^{-3}$ (see [section 4.1](#))

Source: Elaborated by the author

3.5 Forcing function implementation in the two-fluid model

The forcing function is introduced in [Equation 2.3](#), the momentum equation of the gas phase, through the gravity force as follow:

$$\frac{\partial}{\partial t}(\rho_g \phi_g \mathbf{v}_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g \mathbf{v}_g) = -\phi_g \nabla \cdot \boldsymbol{\sigma}_g - \mathbf{M}_I + (1 + cf)\rho_g \phi_g \mathbf{g} \quad (3.10)$$

Where f represents the forcing function and c represents a constant multiplier introduced in order to calibrate the turbulence intensity of the imposed fluctuations. [Figure 15](#) presents the values of f obtained using the algebraic form of forcing and the Park-Miller algorithm to generate the term R_G .

[Figure 16](#) illustrates the body force term $VBF = (1 + cf)\rho_g \phi_g \mathbf{g}$ for different values of the constant forcing multiplier $c = 0$, $c = 0.001$, $c = 0.005$ and $c = 0.01$ (for one of the simulations presented in [section 4.2](#)). The figure shows VBF at a particular grid cell in the numerical domain. The black line stands for VBF for $c = 0$, which corresponds to applying no forcing at all. As expected, no matter the value of c , the average value of the body force remains constant throughout the process. As seen in the figure, an increase in the value of c corresponds to an increase of the fluctuation magnitude of VBF . Owing to momentum conservation, this also imposes higher velocity fluctuations and consequent higher turbulence intensity. This method will be used later, when a solid phase is present in the flow together with the gas phase, and where the gas phase will be perturbed by the forcing function method. This will allow to asses the response of the solid phase to gas sub-grid turbulence.

Figure 16: Body force as a function of the constant multiplier c

Source: Elaborated by the author

4 NUMERICAL SIMULATIONS

2D simulations were performed in this study. 3D simulations were not carried out because of their high computational cost. It has been reported, previously, that results from 2D and 3D simulations were found to be qualitatively similar, yet quantitatively different. When higher quantitative accuracy is to be pursued, 3D simulations will be required, and this is a future objective. For the present analysis, however, as a qualitative behavior is of main concern, the 2D simulations suffice.

Simulations were performed using the open source code MFIx 2014 (Multiphase Flow with Interface eXchange, release 2014). One of the advantages of MFIx is that it is an open source code, so that any modifications and implementations are allowed. It is also widely used for simulations of two-phase flows under two-fluid formulations. MFIx (SYAMLAL et al., 1993) is a numerical code specific for gas-solid flow simulations, which includes Euler-Euler two-fluid based formulations, developed and made available by NETL (National Energy Technology Laboratory, DOE-USA). MFIx is a FORTRAN written parallelized code.

The governing equations in MFIx's two-fluid model are discretized through the finite volume method. The resulting numerical model is solved through a point by point numerical technique. Diffusive terms are discretized following the second order central differencing scheme. For advection terms there are various alternative discretizing methods, ranging from the first order upwind method up to higher order TVD procedures (e.g. van Leer, Minmod, Muscl, Superbee). Superbee was applied following previous studies. The pressure-velocity coupling is solved through the SIMPLE algorithm. The numerical code of MFIx is fully described in Syamlal et al. (1993).

4.1 Turbulence set-up

In order to close the forcing function procedure set-up, the values of σ , τ^* and c must be set. The data values for the first two parameters are taken from Fede and Simonin (2006), who developed a DNS simulation under gas physical conditions very close to the one in this study. Through their procedure (a rigorous application of forcing in the spectral space) energy-containing eddies of $12.8mm$ are continuously fed, which is quite suitable to the current analysis since numerical grids of one order of magnitude smaller than that length scale are applied. The turbulent flow field generated by Fede and Simonin (2006) delivers a root mean square velocity fluctuation of $6.61cm/s$, a lagrangian timescale of $0.1621s$, and an average turbulent kinetic energy of the turbulent gas field $TKE = 43.7cm^2/s^2$ for a 2D condition. As an approximation in the current forcing implementation, $\sigma = 6.61cm/s$ and $\tau^* = 0.1621s$ are taken, in the physical space, over

Figure 17: Evolution of gas velocity magnitude for $c = 0.05, 0.065$ and 0.08 in a particular snapshot in time

Source: Elaborated by the author

the gravitational term in the gas momentum equation. Owing to those assumptions, the resulting gas turbulent field comes out distorted, so that a calibration procedure is required, which is performed through the multiplier constant c (it is set so that the correct average turbulent kinetic energy of the turbulent field, i.e. $43.7 \text{ cm}^2/\text{s}^2$ is recovered).

The set-up of c was done through 2D simulations on the gas phase alone using MFIX. Gas physical properties are shown in Table 1. The computational domain was $16 \text{ cm} \times 16 \text{ cm}$ square with periodic boundary conditions in all directions. The computational mesh was 128×128 (this is the same domain and grid applied in the gas-solid simulations described in section 4.2). Gas was at rest at $t = 0 \text{ s}$ ($u = v = 0$). Pressure gradient in the vertical direction was imposed to compensate the gravity force:

$$\frac{\Delta P_y}{L} = \rho_g \langle \phi_g \rangle g \quad (4.1)$$

The application of $\Delta P_y/L$ rendered a downward flow in the vertical direction, as the domain average gas velocity $\langle v_{g,y} \rangle$ became negative (possibly owing to numerical instabilities). A correction factor was applied to $\Delta P_y/L$ to slightly increase its magnitude (it was increased by 0.005% which made $\langle v_{g,y} \rangle$ oscillate around 0, thereby, eliminating the downward gas flow). Figure 17 shows a flow snapshot of the development of the turbulent gas field for different c values, $c = 0.05, 0.065$, and 0.08 . It can be seen that an increase in c gives rise to bigger gas structures, therefore changing the turbulent gas flow pattern. Figure 18 shows the out-coming time variation of the domain average turbulent kinetic energy (TKE) of the gas for the three values of c . A spectral analysis¹ was pursued to compute the TKE analyzed here. As expected, an increase in c yields an increase in the turbulent kinetic

¹ Details of the spectral analysis and post-processing code are shown in details in Appendix B

Figure 18: Time variation of the turbulent kinetic energy (TKE) for different c coefficients

Source: Elaborated by the author

energy. The desired value of the gas turbulent kinetic energy ($TKE = 0.00437m^2/s^2$) corresponds to a value of c that lies in the interval $0.05 < c < 0.065$ as seen in Figure 18. An appropriate choice of c , based on this graph is $c \approx 0.06$. The constant forcing multiplier is, then, set to $c = 0.06$ in all the following simulations where sub-grid gas turbulence is required, as described in section 4.2. We notice that the order of magnitude of the time step Δt varied a lot between all different cases (shown in Table 2). To obtain a consistent forcing intensity in all the simulations, we fixed $\Delta t = 5.10^{-3}$ for gas-solid flow simulations.

4.2 Numerical set-up

Figure 19: Computational domain $\langle \phi_g \rangle = 0.15$ at $t = 0$

Source: Elaborated by the author

Figure 19 shows the numerical computational domain. We consider a 2D square of 16 cm x 16 cm under periodic boundary conditions in all directions. According to Agrawal et al. (2001), a grid size between 1 and 2 mm can capture all the meso-scale structures for the current particulate and provides results independent of the grid size. The grid size is 1.25 mm which results in a 128x128 mesh. Figure 19 shows the initial conditions for a run with domain average solid volume fraction $\langle \phi_s \rangle = 0.15$. The chess board configuration, which stands for imposing alternating areas of lower and higher solid volume fractions (14% and 16% as shown in the figure) provided a fast transition into the statistical steady state regime. Gas and solid velocities in the horizontal and vertical directions at $t = 0$ are set to zero. Figure 20 illustrates the predicted domain average vertical gas velocity $\langle v_{g,y} \rangle$ as function of time for a case with domain average solid volume fraction $\langle \phi_s \rangle = 0.15$. As seen, the gas velocity starts from zero as imposed by the initial conditions, passes by a transient regime represented by the blue curve, then enters the statistical steady state regime represented by the red curve. In the statistical steady state regime (red curve) the average of a certain variable in time and space are statistically equivalent, and all space averages vary in time around a well established value. The filtering process is done only while the simulation is in the statistical steady state regime.

Table 1 presents the physical properties for the gas and solid phases. The domain

Figure 20: Domain average gas phase axial (vertical) velocity for the suspension case simulation under $\langle\phi_g\rangle = 0.15$

Source: Elaborated by the author

Table 1: Physical properties of gas and particles

Symbol	Property	Value
d_p	particle diameter	7.5×10^{-5} m
ρ_s	particle density	1500 kg/m ³
ρ_g	gas density	1.3 kg/m ³
μ_g	gas viscosity	1.8×10^{-5} kg/m.s
e_p	coefficient of restitution	0.9
g	gravitational acceleration	9.80665 m/s ²
v_t	terminal settling velocity	0.2184 m/s
v_t^2/g	characteristic length	0.00486 m
v_t/g	characteristic time	0.0223s
$\rho_s v_t^2$	characteristic stress	71.55 kg/m.s ²

Source: Elaborated by the author

average gas Reynolds number, fixed in each simulation, is given by:

$$\langle Re_g \rangle = \frac{d_p \rho_g \langle \phi_g \rangle \langle v_{g,y} \rangle}{\mu_g} \quad (4.2)$$

where $\langle v_{g,y} \rangle$ represents the domain averaged gas phase velocity in the axial (vertical) direction. The domain average solid volume fraction $\langle \phi_s \rangle$ was also set constant in the various simulations, at the values of 0.05, 0.15 and 0.25. For each domain averaged solid volume fraction, the domain average gas Reynolds number was first calculated for the respective suspension case. A suspension simulation consists of applying a pressure gradient

Table 2: Simulations set-up

		$\langle \phi_s \rangle$					
		0.05		0.15		0.25	
		Forcing coefficient c					
		0	0.06	0	0.06	0	0.06
$\langle Re_g \rangle / \langle Re_g \rangle_{susp}$	1.00	Sim1	Sim5	Sim9	Sim13	Sim17	Sim21
	8.15	Sim2	Sim6	Sim10	Sim14	Sim18	Sim22
	16.30	Sim3	Sim7	Sim11	Sim15	Sim19	Sim23
	24.45	Sim4	Sim8	Sim12	Sim16	Sim20	Sim24

Source: Elaborated by the author

Table 3: Stokes number for each simulation case

		$\langle\phi_s\rangle$		
		0.05	0.15	0.25
		Stokes number St		
$\langle Re_g\rangle/\langle Re_g\rangle_{susp}$	1.00	297.92	170.14	81.94
	8.15	2428.02	1386.63	667.85
	16.30	4856.04	2773.26	1335.69
	24.45	7284.06	4159.90	2003.4

Source: Elaborated by the author

in the vertical direction to exactly balance the weight of the gas and solid mixture existing in the domain:

$$\frac{\Delta P_y}{L} = \rho_s \langle\phi_s\rangle g + \rho_g \langle\phi_g\rangle g \quad (4.3)$$

After calculating the suspension case domain average gas Reynolds number $\langle Re_g \rangle_{susp}$, the actual $\langle Re_g \rangle$ is set fixed in each simulation by composing a ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1.00, 8.15, 16.30$ and 24.45 for each considered domain average solid volume fraction $\langle\phi_s\rangle$. The ranges of $\langle\phi_s\rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ that were enforced cover usual riser flow conditions from suspension up to pneumatic transport. Each simulation is run for two forcing coefficient values $c = 0$ (no forcing is applied) and $c = 0.06$.

Table 2 shows the summary of the simulations set-up. The simulations were performed up to 32 seconds of real flow time. For all the considered cases, the statistical steady state regimes were established between $t = 0s$ and $t = 2s$, the latest, so that for all the cases the statistical steady state results were taken in the interval $2s < t < 32s$, as illustrated in figure 20. The filtering and binning procedures, described in section 2.3 and subsection 2.3.1, were performed inside the statistical steady state regime. This interval was found more than enough to provide robust statistics.

Table 3 shows the corresponding Stokes numbers for all the simulations of Table 2. Notice that applying the forcing function method did not have any effect on the domain

average vertical gas velocity $\langle v_{g,y} \rangle$. For instance, let's consider the case of Sim9 and Sim13, the domain average solid volume fraction and gas Reynolds number are $\langle \phi_s \rangle = 0.15$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$. The only difference between these two simulations lies in the forcing coefficient c , where $c = 0$ for Sim9 and $c = 0.06$ for Sim13. Both, Sim9 and Sim13, yielded same values of domain average vertical gas velocity ($\langle v_{g,y} \rangle = 0.49 m/s$). Since, Stokes number does not depend on the forcing coefficient c , Sim9 and Sim13 present same values of Stokes number. That applies for all pairs of simulations where the only difference is in the value of the forcing coefficient c . As can be seen in [Table 3](#), the Stokes number in all cases is very high, meaning that all the simulated flows fall in the inertia flow regime category as presented in [Figure 12](#).

5 RESULTS AND DISCUSSION

This chapter presents two kinds of analyses. The first concerns the inclusion of a third marker, the filtered solid kinetic energy, in the filtered parameters correlation. The second discusses the effects of gas sub-grid turbulence, generated by the forcing function procedure, over filtered parameters of interest. The results were obtained for the set of simulations presented in [Table 2](#) for the gas and particle properties presented in [Table 1](#). All the graphs are given for a unique filter size $\Delta_f/(v_t^2/g) = 4.112$, which corresponds to a square window of 2 *cm* x 2 *cm* (16 x 16 grid cells). The effects of the filter size over the filtered parameters are not discussed here, and can be found elsewhere (see [Igci et al. \(2008\)](#), [Igci and Sundaresan \(2011\)](#), [Milioli et al. \(2013\)](#), [Agrawal et al. \(2013\)](#), [Sarkar et al. \(2016\)](#)). The filtered parameters are presented as functions of the filtered solid volume fraction $\bar{\phi}_s$ (first marker), the dimensionless filtered Favre average slip velocity $\tilde{v}_{slip,y}/v_t$ (second marker) and the dimensionless filtered solid kinetic energy k_s/v_t^2 (third marker).

[Figure 21](#) shows snapshots of the performed simulations for the domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 (columns), and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1, 8.15, 16.30, 24.45$ (rows). The results are for the cases without enforced gas sub-grid turbulence (plots including gas turbulence are similar and not shown here). As discussed in [Mouallem et al. \(2018a\)](#) and [Mouallem et al. \(2018b\)](#), the two macro-scale parameters affect the flow topology and filtered parameters significantly. By increasing the domain average solid volume fraction $\langle\phi_s\rangle$ from 0.05 to 0.25, the solid structures become denser and heavier. On the other hand, while increasing the gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$ from 1 up to 24.45, the solid becomes more uniformly distributed throughout the domain and the flow tends to be more homogeneous. An autocorrelation analysis was performed regarding the flows length scales and solid structures densities, which is presented in [Appendix E](#).

Among the various filtered parameters of interest, the current analysis concentrates on the drag coefficient correction H ([Equation 2.38](#)), the solid residual pressure and viscosity $P_{res,s}$, and $\mu_{res,s}$ ([Equation 2.50](#) and [Equation 2.53](#)), and the filtered gas turbulent kinetic energy k_g ([Equation 2.54](#)). While H , $P_{res,s}$, and $\mu_{res,s}$ are highly relevant meso-scale filtered parameters, k_g is of high relevance in the current analysis where effects of sub-grid gas turbulence are of main concern. The kinetic energy, residual pressure and viscosity are made dimensionless by v_t^2 , $\rho_s v_t^2$ and $\rho_s v_t^3/g$.

Results for the effects of the flow macro-scale over meso-scale filtered parameters can be found in [Appendix F](#) and [Appendix G](#). The Results for $\langle Re_g\rangle/\langle Re_g\rangle_{susp}=1$ and 8.15 are shown in the two following sections, while those for $\langle Re_g\rangle/\langle Re_g\rangle_{susp}=16.30$ and 24.45 are presented in [Appendix C](#) and [Appendix D](#).

Figure 21: Grayscale plots of solid volume fraction in the domain inside the statistical steady state regime, for simulations with domain average solid fractions $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 (columns), and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1, 8.15, 16.30, 24.45$ (rows), and $c = 0$

Source: Elaborated by the author

5.1 Third marker analysis

In this section, filtered results are presented as a function of the filtered solid volume fraction $\bar{\phi}_s$ (first marker), for three different dimensionless filtered slip velocities (second marker) $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red), and 4.85 (blue) for different dimensionless filtered solid kinetic energies k_s/v_t^2 (third marker). The selected values of the second marker are of high occurrence in the flow field (see Mouallem et al. (2018a) and Mouallem et al. (2018b)), and values for the third marker are chosen for better exposing its influence over the filtered parameters of concern. To improve the clarity of the results even further, the choice of k_s/v_t^2 may be different for each case. The chosen values of k_s/v_t^2 are the ones that correspond to the less fluctuating curves (which also mean higher occurrence in the flow field).

Figure 22 shows the variation of the drag coefficient correction, H , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 22a, 22c, 22e stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$, for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Figures 22b, 22d, 22f stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 8.15$ for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively.

The variation of H with the filtered slip velocity and filtered solid volume fraction is well known from previous works (e.g. Milioli et al. (2013)). Higher values of filtered slip velocities and filtered solid volume fractions relate to higher values of H . Looking at a unique filtered slip velocity, say 2.03 (blue curves), it is seen that H increases when k_s/v_t^2 decreases for all the cases. However, this trend is less pronounced for the higher gas Reynolds ratio as shown in figures 22b, 22d and 22f, and seems to disappear for the lower filtered solid volume fraction. It should be noted that this behavior is inverted for higher gas Reynolds ratios, as shown in figure 32 of Appendix C. H increases as k_s/v_t^2 increases for low slip velocities (0.85 and 2.03) as shown in Figures 32a, 32b, 32c, 32d and 32f. Notice also that an opposite behavior is seen in Figure 32e, similarly to that of lower gas Reynolds ratios. Results of H for lower and higher number of Reynolds ratios seem to be in contradiction regarding the effect of the third marker k_s/v_t^2 . A possible cause for this disagreement may be related to the suitability of the markers as true independent variables, which is an issue requiring further investigation. Possible regime transitions may also account for the observed contradiction, and this is a matter for further investigation.

Figure 23 shows the variation of the dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 23a, 23c, 23e stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$, for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Figures 23b, 23d, 23f stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 8.15$ for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively.

In all the cases, the dimensionless residual solid pressure results are independent of the filtered slip velocity. For all the three filtered slip velocities (0.85, 2.03 and 4.85), the curves

of the residual solid pressure superpose each other for all the cases. It means that the filtered slip velocity is not a marker for the residual solid pressure. This result is consistent with previous findings of Milioli et al. (2013), who also performed 2D simulations; it should be noticed, however, that in 3D simulations of Sarkar et al. (2016), some correlation was found between the residual stresses and filtered slip velocity. On the other hand, the residual solid pressure increases as k_s/v_t^2 increases, for all the cases. That was quite expected since both parameters are linearly proportional to the trace of the Reynolds-like stresses, as seen in Equation 2.50 and Equation 2.54. A feature to note is that $P_{res,s}/(\rho_s v_t^2)$ spreads through a larger range of $\bar{\phi}_s$ for lower $\tilde{v}_{slip,y}/v_t$, irrespective of k_s/v_t^2 . In other words, there are no occurrences of $P_{res,s}/(\rho_s v_t^2)$ at larger $\bar{\phi}_s$ under high $\tilde{v}_{slip,y}/v_t$. Figure 23 also shows that both the macro-scale parameters, $\langle \phi_s \rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ have little effect over $P_{res,s}/(\rho_s v_t^2)$ for all $\tilde{v}_{slip,y}/v_t$ and k_s/v_t^2 . The results for higher $\langle \phi_s \rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ presented in figure 33 of Appendix C behave the same way as those for lower ratios of figure 23.

Figure 24 shows the variation of the dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 24a, 24c, 24e stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$, for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Figures 24b, 24d, 24f stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 8.15$ for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively.

Just like the residual solid pressure, the residual solid viscosity is not significantly affected by the filtered slip velocity. The curves present some fluctuations, unlike those of the residual pressure. However, the behavior of $\mu_{res,s}/(\rho_s v_t^3/g)$ is the same as that of $P_{res,s}/(\rho_s v_t^2)$ regarding the markers as well as the macro-scale parameters, with some minor differences. For higher filtered solid volume fraction, the residual viscosity tends to increase slightly with the slip velocity, as shown in figures 24a, 24b and 24c for the lowest value of k_s/v_t^2 , and in figure 24f for the highest value of k_s/v_t^2 . Also, the increasing of the residual solid viscosity as k_s/v_t^2 increases shows that the shear components of the Reynolds-like stresses are more sensitive to k_s/v_t^2 than the shear components of the strain rate tensor. The results for higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ shown in figure 34 of Appendix C behave in the same way as those of lower ratios of figure 24.

Figure 25 shows the variation of the dimensionless gas kinetic energy, k_g/v_t^2 , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 25a, 25c, 25e stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$, for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Figures 25b, 25d, 25f stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 8.15$ for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively.

As seen, the gas kinetic energy increases as the filtered slip velocity and the filtered solid kinetic energy both increase for all $\langle \phi_s \rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$. It is clear that higher $\tilde{v}_{slip,y}/v_t$ and higher k_s/v_t^2 are both associated to higher velocity fluctuations in the gas phase, no matter the domain average solid volume fraction and gas Reynolds number. The filtered

solid volume fraction has little effect on the gas kinetic energy for low slip velocities. The gas kinetic energy tends to be constant as the filtered solid volume fraction increases for low slip velocity (0.85) for figures 25a and 25b. In contrast, it slightly decreases for the other cases as shown in figures 25c, 25d, 25e and 25f. For higher slip velocities (2.03 and 4.85), the gas kinetic energy increases as the filtered solid volume fraction increases. It is seen that the curves slopes are higher for the higher filtered slip velocity (4.85) than they are for the intermediate one (2.03). By comparing figures 25a and 25b, 25c and 25d, 25e and 25f, it is seen that all the values of the gas kinetic energy decrease as the gas Reynolds ratio increases for all the domain average solid volume fractions. This result was expected since by increasing the gas domain average Reynolds number ratio, the flow becomes more homogeneous, with consequent decreasing velocity fluctuations in all phases. Again, the results for higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ shown in figure 35 of Appendix C present the same behavior as those for lower ratios of figure 25.

Figure 22: Drag coefficient correction, H , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 8.15 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red), and 4.85 (blue) and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 23: Dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 8.15 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red), and 4.85 (blue) and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 24: Dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 8.15 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red), and 4.85 (blue) and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 25: Dimensionless gas kinetic energy, k_g/v_t^2 , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 8.15 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red) and 4.85 (blue), and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

5.2 Forcing function analysis

In this section, results are shown for one particular dimensionless filtered slip velocity $\tilde{v}_{slip,y}/v_t = 0.85$, for different dimensionless filtered solid kinetic energies k_s/v_t^2 . Just like in the previous section, values of k_s/v_t^2 are chosen that correspond to less fluctuating curves in order to improve the clarity of the results. The dimensionless filter size is also the same as before $\Delta_f/(v_t^2/g) = 4.112$. The results are shown for two values of the turbulence constant multiplier $c = 0$ (full lines) and $c = 0.06$ (dashed lines).

In what follows, the curves that correspond to $c = 0.06$ are called 'forcing curves', and the ones relative to $c = 0$ are called 'non-forcing curves'.

Figures 26 to 29 show the concerning results. Figure 26 shows results of the drag coefficient correction, H . Figure 27 shows results of the dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$. Figure 28 shows results of the dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$. Figure 29 shows results of the dimensionless gas kinetic energy, k_g/v_t^2 . All the figures show the variation of the concerning parameters with the filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures a, c, and e stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$, for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Figures b, d and f stand for gas Reynolds ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 8.15$ for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , respectively. Further results, figures 36 to 39, are presented in Appendix D for higher gas Reynolds number ratios (results were also produced for other values of $\tilde{v}_{slip,y}/v_t$ and not shown here).

Without any exception, for all the conditions experimented, no significant effects of gas sub-grid turbulence were observed on any of the concerning filtered parameters. For all the filtered parameters (H , $P_{res,s}/(\rho_s v_t^2)$, $\mu_{res,s}/(\rho_s v_t^3/g)$, k_g/v_t^2), there are no significant differences between non-forcing curves (full lines) and forcing curves (dashed lines). Results for other filtered parameters were also produced ($P_{fil,s}/(\rho_s v_t^2)$, $\mu_{fil,s}/(\rho_s v_t^3/g)$, $P_{res,g}/(\rho_s v_t^2)$, $\mu_{res,g}/(\rho_s v_t^3/g)$) which show the same insensitivity to gas sub-grid turbulence. Even some variation on Froude number were experimented, for smaller particle sizes (down to $20 \mu m$), still showing no significant effect of gas sub-grid turbulence. In addition, a preliminary two-marker based analysis was also performed (with the filtered solid volume fraction as first marker, and the filtered slip velocity as second marker), which showed no significant effects of gas sub-grid turbulence as well. Results for other referred filtered parameters, Froude numbers, and from two-marker analyses were not included in this work since no additional information could be extracted from them.

The current results indicate that gas sub-grid turbulence has no effect whatsoever over the meso-scale hydrodynamics of gas-solid riser flows for high Stokes numbers particulates. The results also make it clear that the presence of the solid phase modulates the turbulence on the gas phase the same way, irrespective of imposition or not of sub-grid turbulence (since k_g/v_t^2 is not affected by gas sub-grid turbulence).

Figure 26: Drag coefficient correction, H , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 8.15 . The results stand for two turbulence constant multipliers $c = 0$ (full lines) and $c = 0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 27: Dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 8.15 . The results stand for two turbulence constant multipliers $c=0$ (full lines) and $c=0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 28: Dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 8.15 . The results stand for two turbulence constant multipliers $c = 0$ (full lines) and $c = 0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 29: Dimensionless gas kinetic energy, k_g/v_t^2 , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 8.15 . The results stand for two turbulence constant multipliers $c = 0$ (full lines) and $c = 0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

6 CONCLUSION

The ultimate goal of this research is to contribute to the improvement of the sub-grid models used in Large Scale Simulations (LSS) of gas-solid fluidized riser flows. LSS is performed for industrial size risers. Due to computational limitations, LSS imposes coarse grids, which do not resolve all the flow structures. It is well known, however, that meso-scale structures that are filtered in LSS, considerably affect the overall hydrodynamics of fluidized beds. Hence, recovering meso-scale effects is a must. This can be done by including sub-grid models in LSS. Sub-grid models may be derived by filtering over results of meso-scale highly resolved simulations under two-fluid formulations. Sub-grid models for flow parameters, like those of the drag coefficient correction, residual solid pressure and viscosity, are usually correlated to appropriate filtered flow variables like filtered solid volume fraction and filtered slip velocity (named markers). To improve those models, it is necessary to establish which filtered flow variables truly affect the filtered parameters. In this study, the filtered solid kinetic energy is advanced as an additional marker, and gas sub-grid turbulence is considered as a possible trend affecting filtered data. The gas sub-grid turbulence is artificially imposed by the forcing function method. In addition, different macro-scale flow conditions were enforced by varying the domain average solid volume fraction and domain average gas Reynolds number. The analysis was performed for dilute gas-solid flows typical of Fluid Catalytic Cracking risers.

A two fluid model under microscopic formulation was used. Closure equations for solid pressure and viscosity were taken from the kinetic theory of granular flows. An additional equation, the pseudo-thermal energy conservation equation was resolved in order to provide a granular temperature that is required. All the simulations were performed in 2D periodic domains, for unique particle size, Froude and Stokes numbers, using the MFIX code. Highly resolved simulation results were collected for a time interval of 30s inside the statistical steady state regime. Four filtered parameters were taken into consideration: the drag coefficient correction, filtered solid pressure and viscosity, and filtered gas kinetic energy. Filtered results were classified, for a unique filter size, following a three markers binning procedure, where the filtered solid volume fraction was considered as the first marker, the filtered slip velocity as the second marker, and the filtered solid kinetic energy as the third marker. For the macro-scale variables taken into account, i.e. the domain average solid volume fraction and domain average gas Reynolds number ratio, three values of the former (0.05, 0.15, 0.25) and four of latter (1, 8.15, 16.30, 24.45) were considered. The forcing function scheme followed the Ornstein-Uhlenbeck stochastic process. An algebraic mathematical form of the forcing function was chosen. The forcing function random number was generated by the Park-Miller algorithm. A constant forcing multiplier

was set in order to provide a gas turbulent field as described by [Fede and Simonin \(2006\)](#).

Results have shown that all filtered parameters, namely the drag coefficient correction and solid residual pressure and viscosity were significantly affected by the filtered solid kinetic energy as a marker. On the other hand, the residual parameters showed no relevant dependency on the filtered slip velocity, which is an important marker for the drag coefficient correction as discussed in the literature. Otherwise, there was significant dependence of the solid residual pressure and viscosity on the filtered solid kinetic energy. Both of these parameters increase as k_s increases. The residual solid pressure is proportional to k_s as both of them are related to the trace of the Reynolds-like stresses. The dependence of the filtered solid viscosity on k_s give some insights about the correlations between the mean velocity space derivatives and shear components of the Reynolds-like stress tensor, since the ratio between these two values represents the residual solid viscosity. It is shown that this ratio increases as k_s increases. Therefore, the shear values of velocity fluctuation become more dominant than the mean velocity space derivatives. The drag coefficient correction, H , increases when k_s decreases for low gas Reynolds number ratios, while an opposite behavior was noticed for higher Reynolds ratios. The dependency of H on k_s is less pronounced for high gas Reynolds number ratios and disappears for low filtered solid volume fractions and high filtered slip velocities.

Gas sub-grid turbulence was shown to have no significant effects on the filtered parameters. First, simulations of the gas phase alone were performed including the forcing function. Different values of the constant turbulence multiplier were considered, and one value that generates a gas turbulent field similar to that of [Fede and Simonin \(2006\)](#) was chosen. Later, simulations where the solid phase was introduced in the turbulent gas field were performed. The performed simulations with forcing function required considerable computational time compared to their counterparts with no forcing at all.

The present results lead to the conclusion that, not only a high Stokes number particulate is not affected by the carrier fluid turbulence (as largely evidenced in literature), but also structures of such solid particles (clusters) are not affected either. There was an expectation that gas sub-grid turbulence could possibly affect cluster formation/dissipation mechanisms, thereby affecting the heterogeneous pattern of the flow, ultimately leading to changes on meso-scale filtered parameters. That expectation did not prevail, at least at the light of current simulations. Of course, the accuracy of the method of investigation must be considered as a possible cause for mispredictions, and this issue is taken now regarding the markers that were assumed in the analyses of the filtered parameters. Certainly, more fundamental issues related to the microscopic two-fluid modeling itself (such as the adequacy of the assumed micro-scale model for drag, or the accuracy of the kinetic theory based treatment for dispersed particles treated as a continuum) can not be discussed at the light of the current results. In the current studies, filtered data were classified

by narrow ranges of filtered solid volume fraction, filtered slip velocity and filtered solid kinetic energy, which were assumed as independent variables relevant to the meso-scale flow filtered parameters (named markers). It is just possible that those markers are either unsuitable or insufficient, as they may be hiding hydrodynamics effects dissipated by the statistical averaging procedures that are performed in the current binning process. Clearly, the gas sub-grid turbulence issue must be reconsidered having in view other markers or combinations of markers, as the currently considered ones were not proved (nor disproved) as adequate independent variables.

To elaborate more on the results of this study, several issues must be addressed in the future. These issues include:

- The Stokes number, St

It has been shown in the literature that gas turbulence have no significant effect over the motion of high Stokes particles. This study showed that gas turbulence does not have any considerable effect over the meso-scale structures of high Stokes particles as well. The analysis should be extended to low Stokes numbers to examine how gas turbulence affects the meso-scale structures of such low Stokes particles.

- The constant turbulence multiplier, c

A unique constant turbulence multiplier value was considered in this study. Further analysis should include a wide interval of multiplier values which correspond to different gas turbulence intensities.

- Adequacy of markers (independent variables)

This is an open issue requiring a more in-depth evaluation.

Besides, research is also needed in more fundamental issues, such as:

- Newtonian rheology is usually assumed for both phases, the gas as well as the solid phase that accounts for the particulate treated as a continuum. While the Newtonian assumption sounds correct for the gas phase, there is no evidence that it is equally adequate for the solid phase. This is an issue for further research.
- Most highly resolved simulations analyses on literature concentrate on monodisperse particulates. As real gas-solid flows are usually characterized by wide granulometry distributions, polydisperse analyses are needed.
- Hydrodynamic scaling is quite a challenge in gas-solid fluidized flows. In order to exploit that matter, much extensive computational experimentation is needed for various Froude number particulates and macro-scale flow conditions. That would be a start for addressing hydrodynamic scaling in the field.

- The most practiced microscopic closure for drag comes from a well accepted correlation by [Wen and Yu \(1966\)](#), which nevertheless was originally derived for gas-liquid uniformly fluidized flows. This situation does not suit the very heterogeneous gas-solid fluidized flows, and new approaches are needed. A possibility would be to derive new micro-scale correlations from predictions with discrete element methods, for instance.
- Besides drag, other interface effects among phases may become relevant in gas-solid fluidized flows. Effects such as friction, electrostatic and moisture could be assessed in future highly resolved simulation analyses.
- The kinetic theory of granular flows, which is used to derive closure properties for solid phases treated as continua, is still to be validated. This is a challenge waiting for new fresh ideas.

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Appendixes

APPENDIX A – PARK-MILLER ALGORITHM

The FORTRAN code of the Park-Miller algorithm is given by the two functions `random_uniform(guess_0)` and `random_normal(guess_0)`. `guess_0` is a random negative value chosen arbitrarily. In the current study, `guess_0=-2` was assumed.

```
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
DOUBLE PRECISION FUNCTION random_uniform(guess_0)

INTEGER guess_0
INTEGER uni_ia, uni_im, uni_iq, uni_ir, uni_ntab, uni_ndiv
INTEGER uni_j, uni_k, uni_iv(32), uni_iy
DOUBLE PRECISION uni_am, uni_eps, uni_rnmx
PARAMETER (uni_ia=16807, uni_im=2147483647, uni_am=1.0/uni_im,
            uni_iq=127773, uni_ir=2836)
PARAMETER (uni_ntab=32)
PARAMETER (uni_ndiv=1+(uni_im-1)/32, uni_eps=1.2e-7, uni_rnmx=1.0-uni_eps)

save uni_iv, uni_iy
data uni_iv /uni_ntab*0/, uni_iy /0/

if (guess_0.LE.0 .OR. uni_iy.EQ.0) then
guess_0=max(-guess_0,1)

DO uni_j=uni_ntab+8,1,-1
uni_k=guess_0/uni_iq
guess_0=uni_ia*(guess_0-uni_k*uni_iq)-uni_ir*uni_k

if (guess_0.LT.0) guess_0=guess_0+uni_im
if (uni_j.LE.uni_ntab) uni_iv(uni_j)=guess_0

end do

ni_iy=uni_iv(1)
end if

uni_k=guess_0/uni_iq
guess_0=uni_ia*(guess_0-uni_k*uni_iq)-uni_ir*uni_k
```

[illegible]

APPENDIX B – SPECTRAL ANALYSIS

Spectral analysis usually used in turbulence studies may also be useful in gas-solid fluidized flow analysis. In this appendix, this issue is briefly considered aiming for future application as a tool in gas-solid fluidized flow studies. The theory in this section is taken from Pope (2000), chapter 6. The Fourier transform of a velocity vector $\mathbf{u}$ in physical space at position $\mathbf{x}$ and time t is

$$\hat{\mathbf{u}}(\boldsymbol{\kappa}, t) = \mathcal{F}(\mathbf{u}(\mathbf{x}, t)) \quad (\text{B.1})$$

where $\boldsymbol{\kappa}$ represents a wavenumber vector in the spectral space. The complex conjugate of the Fourier transform of $\mathbf{u}$ is given by

$$\hat{\mathbf{u}}^*(\boldsymbol{\kappa}, t) = \hat{\mathbf{u}}(-\boldsymbol{\kappa}, t) \quad (\text{B.2})$$

The Covariance in spectral space is defined as

$$\widehat{\mathcal{R}}_{ij}(\boldsymbol{\kappa}, t) = \langle \hat{u}_i^*(\boldsymbol{\kappa}, t) \hat{u}_j(\boldsymbol{\kappa}, t) \rangle \quad (\text{B.3})$$

where $\langle \cdot \rangle$ represents an average. Also, the velocity spectrum is defined as

$$\Phi_{ij}(\bar{\boldsymbol{\kappa}}, t) = \sum_{\boldsymbol{\kappa}} \delta(\bar{\boldsymbol{\kappa}} - \boldsymbol{\kappa}) \widehat{\mathcal{R}}_{ij}(\boldsymbol{\kappa}, t) \quad (\text{B.4})$$

The kinetic energy of the Fourier mode is defined by

$$\hat{E}(\boldsymbol{\kappa}, t) = \frac{1}{2} \langle \hat{u}_i^*(\boldsymbol{\kappa}, t) \hat{u}_i(\boldsymbol{\kappa}, t) \rangle = \frac{1}{2} \widehat{\mathcal{R}}_{ii}(\boldsymbol{\kappa}, t) \quad (\text{B.5})$$

The turbulent kinetic energy is

$$TKE(t) = \frac{1}{2} \langle u_i u_i \rangle = \sum_{\boldsymbol{\kappa}} \frac{1}{2} \widehat{\mathcal{R}}_{ii}(\boldsymbol{\kappa}, t) = \sum_{\boldsymbol{\kappa}} \hat{E}(\boldsymbol{\kappa}, t) = \int_{-\infty}^{+\infty} E(|\boldsymbol{\kappa}|) d\boldsymbol{\kappa} = \iiint_{-\infty}^{+\infty} \frac{1}{2} \Phi_{ii}(\bar{\boldsymbol{\kappa}}, t) d\bar{\boldsymbol{\kappa}} \quad (\text{B.6})$$

For simplicity, the energy-spectrum function $E(k)$ is introduced. Figure 31 shows the energy spectrum $E(k)$ as a function of the wavenumbers k . The values of the energy spectrum were averaged in time from $t = 5s$ to $t = 15s$. The blue and the red curves represent the Kolmogorov and the computed slopes, respectively. Even though the grid size is coarse for such analysis compared to the traditional DNS, the obtained results seems to be reasonable. The energy-spectrum function is a scalar function of a scalar k . As defined before, the velocity correlation function $\Phi_{ij}(\boldsymbol{\kappa}, t)$ is a tensor. The directional information in this tensor are disregarded¹ by only taking in consideration its trace $\Phi_{ii}(\boldsymbol{\kappa}, t)$. The

¹ Since we are usually interested in the magnitude of a scale, not in its direction properties

Figure 30: Illustration of the two dimensional shell integration

trace is calculated as $\Phi_{ii}(\boldsymbol{\kappa}, t) = \Phi_{11}(\boldsymbol{\kappa}, t) + \Phi_{22}(\boldsymbol{\kappa}, t)$. The same procedure is followed for the wavenumber vector $\boldsymbol{\kappa}$ by integrating the wavenumbers of the same magnitude $|\boldsymbol{\kappa}| = k$ in all directions². The magnitude of the wave number vector is calculated following $k = |\boldsymbol{\kappa}| = \sqrt{\kappa_1^2 + \kappa_2^2}$. Figure 30 illustrates the shell integration process. In 2D, this leads to an integration over a circle $S(k)$ with radius k centered at the origin. Henceforth, the energy spectrum function will be

$$E(k, t) = \oint\!\!\!\oint E(\boldsymbol{\kappa}, t) dS(k) = \oint\!\!\!\oint \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}, t) dS(k) \quad (\text{B.7})$$

Note that $E(\boldsymbol{\kappa}, t) = \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}, t)$. For homogeneous isotropic turbulence, integrating in 2D space, the surface integral becomes an integral over a circle, and results:

$$E(k, t) = \int_0^{+\infty} 2\pi k E(|\boldsymbol{\kappa}|, t) dk \quad (\text{B.8})$$

Substituting (B.7) in (B.6), the turbulent kinetic energy TKE is then calculated by:

$$TKE(t) = \iiint_{-\infty}^{+\infty} \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}, t) d\boldsymbol{\kappa} = \int_0^{+\infty} \oint\!\!\!\oint \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}, t) dS(k) dk = \int_0^{+\infty} E(k, t) dk \quad (\text{B.9})$$

² Note that $\boldsymbol{\kappa}$ is a vector while k is a scalar

Figure 31: Mean energy spectrum

Source: Elaborated by the author

The MATLAB code that calculates the turbulent kinetic energy from the velocity field in the physical space, based on the information in this section, results:

```
close all
clc
% Time interval in seconds
t1=5;
t2=15;

deltat=0.02; % timestep
dim=128;     % number of points in one dimension
Lx=0.16;     % domain size in meters in the x-dir
Ly=Lx;       % domain size in meters in the y-dir
dx=Lx/dim;   % grid spacing in x-dir
dy=dx;       % grid spacing in y-dir

array_dim=dim*dim;
counter=0;
timesteps=(t2-t1)/deltat+1; % number of timesteps
kin_E=zeros(timesteps,1);
```

```

for t=t1:deltat:t2
    % U_g and V_g are unidimensional vectors of velocity values
    % load U_g and V_g
    U_g1=U_g((counter*array_dim+1):(counter+1)*array_dim);
    V_g1=V_g((counter*array_dim+1):(counter+1)*array_dim);
    counter=counter+1;
    uvel=U_g1*0.01; % convert from centimeters to meters
    vvel=V_g1*0.01;
    dim=128;      % number of points in one dimension
    u=reshape(uvel,dim,dim); % reshape arrays to have them in 2D
    v=reshape(vvel,dim,dim);
    %% Compute FFT (Fast Fourier Transform)
    scaling = (2*pi)^2*dim^2;
    extension = 0;
    NFFT = 2.^(nextpow2(size(u))+extension);
    u_fft=fft2(u,NFFT(1),NFFT(2))./scaling; % --> definition of FFT
    %
    NFFT = 2.^(nextpow2(size(v))+extension);
    v_fft=fft2(v,NFFT(1),NFFT(2))./scaling;
    %
    Rij_x=(u_fft.*conj(u_fft));
    Rij_y=(v_fft.*conj(v_fft));

    %% Compute velocity tensor phi
    phi = (Rij_x+Rij_y);

    %% Compute  $\kappa$  vector
    dim = size(phi,1)/2+1;
    E=zeros(dim,1);
    kappa=zeros(dim,2);
    for j=1:2*(dim-1)
        for i=1:2*(dim-1)
            kx = i*pi/Lx;
            ii = i;
            if (i > dim);
                kx=(2*(dim)-i)*pi/Lx;
                ii=(2*(dim)-i);
            end
            ky = j*pi/Ly;

```

```

        jj = j;
        if (j > dim);
            ky=(2*(dim)-j)*pi/Ly;
            jj=(2*(dim)-j);
        end
        kappa_pos = round(sqrt(ii^2+jj^2)+0.5)-1;
        if kappa_pos > dim
            kappa_pos = dim;
        end

        kappa(kappa_pos,1) = kappa(kappa_pos,1) + sqrt(kx^2+ky^2);
        kappa(kappa_pos,2) = kappa(kappa_pos,2) + 1;

        E(kappa_pos) = E(kappa_pos) + 0.5*phi(i,j);
    end
end

%kappa(:,1) is the sum of magnitudes for a specified value of k
%kappa(:,2) is the number of points of on the same radius k
kappa(:,1) = kappa(:,1)./kappa(:,2); % average magnitude per point
E1=E*2*pi./kappa(:,2).*(kappa(:,1));
% we need to divide E per kappa(:,2) to get the average value of E
% for each point on the same radius k

kin_E(counter,1)=trapz(kappa(:,1),E1);

end
plot(t1:0.02:t2,kin_E(:,1),'k')
xlabel('Time(s)')
ylabel('TKE (m^2/s^2)')
legend('TKE')
```


APPENDIX C – THIRD MARKER ANALYSIS - RESULTS FOR HIGH REYNOLDS NUMBER RATIOS

Figure 32 shows the variation of the drag coefficient correction, H , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 32a, 32c, 32e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 32b, 32d, 32f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 33 shows the variation of the dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 33a, 33c, 33e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 33b, 33d, 33f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 34 shows the variation of the dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 34a, 34c, 34e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 34b, 34d, 34f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 35 shows the variation of the dimensionless gas kinetic energy, k_g/v_t^2 , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 35a, 35c, 35e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 35b, 35d, 35f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 32: Drag coefficient correction, H , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$ and 24.45 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red) and 4.85 (blue), and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 33: Dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$ and 24.45 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red) and 4.85 (blue), and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 34: Dimensionless residual solid pressure, $\mu_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 16.30$ and 24.45 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red) and 4.85 (blue), and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

Figure 35: Dimensionless residual solid pressure, k_g/v_t^2 , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 16.30$ and 24.45 . The results stand for dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ (black), 2.03 (red) and 4.85 (blue), and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy. All graphs for $c = 0$.

Source: Elaborated by the author

APPENDIX D – FORCING FUNCTION ANALYSIS - RESULTS FOR HIGH REYNOLDS NUMBER RATIOS

Figure 36 shows the variation of the drag coefficient correction, H , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 36a, 36c, 36e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 36b, 36d, 36f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 37 shows the variation of the dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 37a, 37c, 37e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 37b, 37d, 37f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 38 shows the variation of the dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^3/g)$, with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 38a, 38c, 38e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 38b, 38d, 38f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 39 shows the variation of the dimensionless gas kinetic energy, k_g/v_t^2 , with filtered solid volume fraction, gas Reynolds number ratios and filtered solid kinetic energy. Figures 39a, 39c, 39e stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$, for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Figures 39b, 39d, 39f stand for gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 24.45$ for $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively.

Figure 36: Drag coefficient correction, H , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$ and 24.45 . The results stand for two turbulence constant multipliers $c=0$ (full lines) and $c=0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 37: Dimensionless residual solid pressure, $P_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 16.30$ and 24.45 . The results stand for two turbulence constant multipliers $c=0$ (full lines) and $c=0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t=0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 38: Dimensionless residual solid viscosity, $\mu_{res,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 16.30$ and 24.45 . The results stand for two turbulence constant multipliers $c = 0$ (full lines) and $c = 0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

Figure 39: Dimensionless gas kinetic energy, k_g/v_t^2 , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for different solid kinetic energies, domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 , and gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 16.30$ and 24.45 . The results stand for two turbulence constant multipliers $c=0$ (full lines) and $c=0.06$ (dashed lines), dimensionless filtered axial slip velocities $\tilde{v}_{slip,y}/v_t = 0.85$ and dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$. Thicker curves represent higher filtered solid kinetic energy.

Source: Elaborated by the author

APPENDIX E – AUTOCORRELATION ANALYSIS

An autocorrelation analysis was performed over the current gas-solid flow simulation data in order to evaluate its potential as a tool for future analysis of sub-grid filtered parameters as well as hydrodynamic scaling. This appendix describes the concerning development.

E.1 Methodology

The spatial two-dimensional autocorrelation function reports how a relevant field variable taken at a given point correlates to itself taken at another point, as a function of the distance between the points and direction. The mathematical expression of the spatial autocorrelation function is given by

$$ACF(a, b) = g(x, y) \circledast g(x, y) \quad (\text{E.1})$$

Where ACF represents the autocorrelation function, $g(x, y)$ the distribution function of the variable of interest, x and y the Cartesian coordinates, a and b the displacement or distance away from x and y respectively. When applied on a field of real scalar values the operator $\circledast$ can be either a correlation or convolution. Equation E.1, in its discrete form for a $M \times N$ domain, can be written as

$$ACF(ii, jj) = \sum_{i=1}^{i=M} \sum_{j=1}^{j=N} g(i, j) g(i + ii, j + jj) \quad (\text{E.2})$$

The two equations presented above are not practical to use because of their high computational cost. An alternative and more efficient way of calculating the autocorrelation function is from the Fourier transform of the power spectrum of the given data field. Convolution in physical space is transformed to a simple multiplication in the spectral space, which is computationally cheaper. The power spectrum is calculated by multiplying the Fourier transform of the function by its complex conjugate. In other words, we compute the power spectrum of $g(x, y)$ following:

$$P(w) = [\mathfrak{F}(g(x, y))] * [\mathfrak{F}^*(g(x, y))] \quad (\text{E.3})$$

Then by applying the inverse Fourier transform, we get the autocorrelation function in the physical space

$$ACF(a, b) = \mathfrak{F}^{-1}(P(w)) \quad (\text{E.4})$$

E.2 Numerical processing

In the current work, an autocorrelation code was written in Matlab. A numerical domain is taken that comprises by 128x128 grids. All the following examples and cases

Figure 40: ACF of a Gaussian noise

Source: Elaborated by the author

were computed in less than one second of processing on an ordinary computer. In what follows, at first a series of standard examples are presented for validation and to get an in-depth understanding of the data generated by the autocorrelation function. Later on, the autocorrelation function is applied on simulations snapshots of solid volume fraction for gas-solid flows under different conditions practiced in the current work. The simulations are just the ones presented in Table 2, performed using the open source code MFIX under the two-fluid model formulation.

E.2.1 Validation tests

Three validation tests are presented in this section: Gaussian noise, circle, and random ellipses. Figure 40 shows a two-dimensional field of random values with a normal distribution and its respective autocorrelation. Figure 40a illustrates a 3D view of a 2D field whose values at each grid cell were taken from a normal distribution whose mean

Figure 41: ACF of circle

Source: Elaborated by the author

and standard deviation equal respectively 0 and 1. Figure 40b represents an $x - y$ view of Figure 40a. The 3D autocorrelation function of Figure 40a is shown in Figure 40c. Its $x - y$ view is shown in Figure 40d. Figure 41 and Figure 42 present, respectively, the same data for a circle and random ellipses elongated in the vertical direction.

The values at each grid cell in the case of the Gaussian noise (Figure 40) are random. The value itself at a certain grid is not important; what is important is the spatial distribution of these random values. This spatial randomness follows the Gaussian noise distribution. This results in an even power spectrum, in other words, there is no dominant frequency. In theory, the normalized autocorrelation function of an even power spectrum is, by definition, the Dirac delta function, where an impulse exists at the origin and a null value everywhere else. This is exactly what the four plots in Figure 40 show.

Figure 41 illustrates the autocorrelation function of a circle. An analysis of this case will not be done here and can be found in Heilbronner (1992).

Figure 42: ACF of random ellipses

Source: Elaborated by the author

Figure 42 illustrates the autocorrelation function of random elongated ellipses. Figure 42a represents the three dimensional field where random ellipses of the same size elongated in the y -direction are present. The values of the cell grids delimited by each ellipse are constant, and these values are randomly attributed for each ellipse. Figure 42b represent a $x - y$ view of Figure 42a. The three dimensional autocorrelation function of these random ellipses is shown in Figure 42c. Its $x - y$ view is shown in Figure 42d.

As shown in figures 40, 41 and 42, all the ACF are symmetric, so it is enough to show and analyze half of them. It is of interest to evaluate the longitudinal and transversal correlations defined as a cut of the ACF from the origin along the positive directions of y - and x - directions respectively.

Figure 43 shows different longitudinal and transversal correlations of the three cases. Figure 43a shows the longitudinal correlation of the Gaussian noise. The transversal correlation is not shown here because it has the same shape. The profile presents a

Figure 43: Longitudinal and transversal correlations for different test cases: (a) noise, (b) circle, (c) and (d) ellipses

Source: Elaborated by the author

sharp decrease from 1 to 0, which means that, for a small displacement the field values become highly uncorrelated. That was expected since the random values were taken from a Gaussian noise. Figure 43b shows the longitudinal correlation of the circle case. The transversal correlation presents the same slope and it is not presented here. This curve is in accord with the results presented in Heilbronner (1992). The fact that the longitudinal and transversal correlations are identical means that there is no preference between the x - and y - directions. Figures 43c and 43d show respectively the longitudinal and transversal correlations of the random ellipses case. The longitudinal correlation remains higher than its transversal counterpart, as it moves away from the origin, meaning that the values are more correlated in the y - direction than in the x - direction. This can be interpreted as if the structures present in the original figure are orientated in the y - direction, which indeed is the case.

Figure 44: ACF of a domain snapshot of solid volume fraction fluctuations for a simulation with $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$.

Source: Elaborated by the author

E.2.2 Application to gas-solid flows

Having validated the autocorrelation code and analyzed the output of the autocorrelation function data, the code is now used on different solid volume fraction snapshots related to different simulation conditions.

In what follows, the domain average solid volume fraction value is subtracted from all the solid volume fraction values in each grid cell of the numerical domain. Therefore, the variable in consideration is the solid volume fraction fluctuation.

Figure 44 illustrates the autocorrelation function of a solid volume fraction snapshot for domain average solid volume fraction $\langle\phi_s\rangle=0.15$ and domain average gas Reynolds number ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$. Figure 44a represents a 3D view of the 2D snapshot, where the z -axis represents the values of solid volume fraction fluctuations. Figure 44b

Figure 45: ACF of a domain snapshot of solid volume fraction fluctuations for a simulation with $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 24.45$.

Source: Elaborated by the author

represents a $x - y$ view of Figure 44a. Figure 44c represents the correspondent 3D auto-correlation function. Figure 44d shows an $x - y$ view of the 3D autocorrelation function. Similar to the Gaussian noise and circle cases presented respectively in figures 40 and 41, the ACF of the solid volume fraction fluctuation snapshot decreases in a similar way in all directions. It means that the structures are equally correlated in all directions, with no preference to any direction over another.

Figure 45 illustrates the data set for domain average solid volume fraction $\langle\phi_s\rangle=0.15$ and domain average gas Reynolds number ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 24.45$. The corresponding ACF presents a similar shape to that of the case of random ellipses shown in Figure 42. The ACF is elongated in the y - direction, meaning that the correlation in the y - direction remains higher than that of the x - direction, resulting in coherent solid structures oriented in the y - direction.

Figure 46: Longitudinal and transversal correlations for simulations with $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ (a) and 24.45 (b).

Source: Elaborated by the author

Figure 46a represents the longitudinal and transversal autocorrelation functions for domain average solid volume fraction $\langle\phi_s\rangle=0.15$ and domain average gas Reynolds number ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$, while Figure 46b represents the data for domain average solid volume fraction $\langle\phi_s\rangle=0.15$ and domain average gas Reynolds number ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 24.45$.

As noted above, the ACF of the snapshot for the domain average gas Reynolds number ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ presents non preferred direction. This is shown also in Figure 46a, where the longitudinal and transversal autocorrelations are plotted together. The curves present an identical decreasing slope from 1 to 0, making clear the non preferred direction conclusion. Additionally, this case lies down between two extreme scenarios: the Gaussian noise and the circle cases. For the first, a sharp decrease from 1 to 0 is obtained meaning that the values are highly uncorrelated; for the second a moderate decrease in ACF means that a high correlation exists. The ACF of the gas-solid snapshot is an intermediate case between the two extreme cases, implying that there is a certain degree of correlation. This point is an issue for further investigation.

On the other hand, the ACF of snapshot of the domain average gas Reynolds ratio $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 24.45$ presented a preferred vertical direction. Figure 46b makes that finding very clear. As seen, the longitudinal correlation remains higher than its transversal counterpart, similar to the ellipses case of Figure 42. The solid structures are therefore oriented in the y - direction. This fact was observed in Mouallem et al. (2018a) by means of solid fraction gray scale plots, and is now quantified in the current autocorrelation analysis.

Figure 47: Integral length scales as a function of time following the three methods of integration for the longitudinal and transversal autocorrelation curves of a domain snapshot of solid volume fraction fluctuations for a simulation with $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp}=1$ and 24.45

Source: Elaborated by the author

E.3 Length scales determination

In theory, integral length scales in turbulence are defined from the autocorrelation function of the velocity field as:

$$L_{int} = \int_0^\infty ACF(r, t) dr \quad (E.5)$$

which stands for integrating the area under the autocorrelation curve. In practice, when the ACF curve is obtained either by experiments or numerical simulations, the domain in which it is calculated is finite, hence, the application of Equation E.5 is not straightforward. There are uncertainties on how to define the numerical domain over which the integration should be performed (see Dias et al. (2004), Tritton (1988), Yaglom (1987), Katul and

Parlange (1995)). Inspired on methods used in turbulence, three traditional approaches are considered to define an integral or dominant scale for solid structures. Notice that turbulence and gas-solid flows are not alike, since they present totally different dominant mechanisms (viscous for turbulence, collisional for gas-particle flows). The three approaches investigated here are:

- Integration over the entire domain
- Integration up to the first 'zero-crossing'
- Integration up to the value where $ACF = 1/e$

where e is the Euler irrational number ($e = 2.7182 \dots$). Snapshots in the statistical steady state were taken up to 20s. ACF was calculated for each snapshot. Then, the three methods presented above were applied for all the obtained autocorrelation curves.

Figure 47 shows the integral length scales as a function of time for each snapshot following the three methods of integration for the longitudinal and transversal autocorrelation curves, of a domain snapshot of solid volume fraction fluctuations, for a simulation with $\langle \phi_s \rangle = 0.15$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 24.45. The integration over all the domain, up to the first zero crossing, and up to $ACF = 1/e$ are represented, respectively, by the red, blue and black curves.

As seen by the figure, the method $ACF = 1/e$ presents the least fluctuations among the three methods and looks the most promising. As expected, longitudinal and transversal integral lengths oscillate around the same mean value for $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ as shown in figures 47a and 47b. By increasing the domain average gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ from 1 up to 24.45, we notice that both, the longitudinal and transversal integral lengths considerably increase as illustrated by figures 47c and 47d. The longitudinal integral length, however, grows higher than the transversal counterpart.

Time average values of the various length scales were computed through a high number of snapshots in the statistical steady state regime, which are present in Table 4. The study was extended to different values of domain average solid volume fractions $\langle \phi_s \rangle = 0.05, 0.15$, and 0.25 . Notice that the length in Table 4 are given in number of grids. In the current case, each computational grid is a square of $1.25 \text{ mm} \times 1.25 \text{ mm}$, so an integral length scale of 2 grids corresponds to 2.5 mm . All the three methods present the same behavior:

- By increasing the domain average gas Reynolds number ratio, the longitudinal and transversal integral lengths increase. The increase of the longitudinal integral length is higher than that for the transversal one. The structures become wider in the

Table 4: Longitudinal and transversal integral length scales (in number of grids) for different simulation conditions with $\langle\phi_s\rangle=0.05, 0.15$, and 0.25 , and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 24.45 .

			$\langle\phi_s\rangle$		
			0.05	0.15	0.25
$\langle Re_g\rangle/\langle Re_g\rangle_{susp}=1$	Longitudinal	All domain	4.508	5.113	5.346
		First zero	4.907	5.788	6.393
		1/e	2.628	3.438	4.056
	Transversal	All domain	3.255	4.497	5.078
		First zero	3.919	5.382	6.370
		1/e	2.440	3.331	4.041
$\langle Re_g\rangle/\langle Re_g\rangle_{susp}=24.45$	Longitudinal	All domain	19.76	14.596	12.639
		First zero	20.33	17.023	14.632
		1/e	14.96	14.217	11.601
	Transversal	All domain	2.387	5.828	6.303
		First zero	5.424	9.390	9.486
		1/e	3.724	7.403	7.495

Source: Elaborated by the author

Figure 48: Longitudinal and transversal correlations for simulations with $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ (a) and 24.45 (b).

Source: Elaborated by the author

transversal direction and even wider in the longitudinal direction, no matter the domain average solid volume fraction.

- By increasing the domain average solid volume fraction, the longitudinal and transversal integral lengths increase for all the cases, except for the longitudinal integral length for the higher Reynolds.

Table 5: ACF peak for different simulation conditions with $\langle\phi_s\rangle=0.05, 0.15$, and 0.25 and $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and 24.45

			$\langle\phi_s\rangle$		
			0.05	0.15	0.25
$\langle Re_g\rangle/\langle Re_g\rangle_{susp}$	1	$ACF(0,0)$	122.09	511.87	777.12
	24.45		52.254	72.287	62.02

Source: Elaborated by the author

E.4 Structures uniformity

In the previous section, a normalized ACF was considered for all the analyses that were performed. However, in order to study heterogeneity related issues, the dimensional autocorrelation must be considered. The magnitude of the peak value of the ACF (obtained at zero displacement in space) is directly related to uniformity. Equation E.2, at the origin, gives:

$$ACF(0,0) = \sum_{i=1}^{i=M} \sum_{j=1}^{j=N} g(i,j)g(i,j) \quad (E.6)$$

Where $g(x,y)$ is the solid volume fraction fluctuation, it comes that:

$$ACF(0,0) = \sum_{i=1}^{i=M} \sum_{j=1}^{j=N} \phi'_s(i,j)\phi'_s(i,j) \quad (E.7)$$

which is nothing but the variance of the solid volume fraction. Figure 48 shows the curves of the longitudinal and transversal ACF of Figure 46 in their dimensional form. Figure 48a shows the curves for $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp}=1$, while Figure 48b stands for $\langle\phi_s\rangle=0.15$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp}=24.45$. The peak value $ACF(0,0)$ is close to 500 for the first and around 20 for the second. Therefore, for low Reynolds a relatively high variance of solid volume fraction fluctuation is present compared to that of high Reynolds. As a higher variance is related to a higher non-uniformity, the low domain average gas Reynolds number ratio gives rise to a more heterogeneous flow field. Table 5 shows the different ACF peaks for different simulation conditions.

As can be seen, for the low gas Reynolds number ratio, the peak value increases as the domain average solid volume fraction $\langle\phi_s\rangle$ increases, i.e. the variance increases when more solid is present. Moreover, the peak value decreases as shown earlier in Figure 48 as domain average gas Reynolds number ratio increases. Imposing higher gas Reynolds decreases fluctuations resulting in a more homogeneous flow.

E.5 Conclusion

The autocorrelation function analysis provides integral length scales which may be related to size and orientation of solid structures in gas solid-flows. By comparing longitudinal and transversal integral lengths, conclusions may be drawn on preferred orientation and size of solid structures. By imposing higher gas Reynolds number, solid structures become longer and wider (by size). The same is found as the domain average solid volume fraction is increased. Also, the dimensional peak value of the ACF shows that the solid structures become less uniform at higher gas Reynolds number ratios and lower domain average solid volume fractions.

As demonstrated, the integral lengths from the current autocorrelation analysis are quite sensitive to macro-scale conditions, and may be thought of as possible promising markers to account for macro-scale effects in meso-scale filtered parameters correlation. Those integral lengths may also prove relevant for hydrodynamic scaling of gas-solid fluidized flows. Both marker and scaling related issues are matters for future research.

APPENDIX F – ON THE EFFECTS OF THE FLOW MACRO-SCALE OVER MESO-SCALE FILTERED PARAMETERS IN GAS-SOLID RISER FLOWS

On the effects of the flow macro-scale over meso-scale filtered parameters in gas-solid riser flows

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HIGHLIGHTS

- Sub-grid closures are required in filtered formulations of gas–solid fluidized flows.
- Filtering over meso-scale predictions does provide data for sub-grid correlation.
- Owing to a lack of scale separation, correlation to the macro-scale is also required.
- It is showed that the flow macro-scale considerably affects sub-grid parameters.

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ABSTRACT

Filtered two-fluid formulations of gas–solid fluidized flows require closure models to deal with sub-grid filtered parameters, which have been derived from filtering over results of meso-scale highly resolved simulations with two-fluid modeling. Trusting on scale separation, the correlation of filtered parameters has been performed to meso-scale filtered data only, disregarding any macro-scale effects. In this work, the correctness of such practice is tested, and it fails. Two macro-scale parameters associated to flow topology, namely the average solid volume fraction and the average gas Reynolds number, are both considered as for their effects over relevant filtered parameters. This is done by filtering over results of highly resolved simulations, where the concerning macro-scale parameters are held constant at various levels. The current interest is directed towards dilute conditions typical of riser flows. Results show that both the concerning macro-scale parameters should be accounted for in sub-grid correlation if higher accuracy is pursued.

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1. Introduction

Sub-grid filtered models intended for macro-scale simulations of gas-solid fluidized flows have been developed departing from results of meso-scale highly resolved simulations with two-fluid modeling under available micro-scale closing, frequently referred to as microscopic two-fluid modeling (Agrawal et al., 2001, 2013; Andrews IV et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011; Parmentier et al., 2012; Özel et al., 2013;

Milioli et al., 2013; Schneiderbauer and Pirker, 2014; Sarkar et al., 2016). Here, micro-scale refers to all length scales smaller than the smallest particulate coherent structure in the flow; macro-scale refers to all length scales captured in large scale simulations; and meso-scale refers to intermediate length scales, which are captured in highly resolved simulations. The meso-scale simulations are supposed to catch all the length scales of the solid phase in the flows since enough refined numerical grids are practiced. In most of the literature reported cases periodic boundaries are applied over reduced domains under enforced suspension like conditions, which are provided through the imposition of an axial gas pressure gradient chosen to exactly match the

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Nomenclature

B'	fluctuation of gas-solid buoyancy force (N m^{-3})	ρ	density (kg m^{-3})
C_D	single particle drag coefficient (nd)	σ	deviatoric stress tensor (N m^{-2})
d_p	particle diameter (m)	τ'	residual stress tensor (N m^{-2})
E	symmetric tensor	ϕ	volume fraction (nd)
g, g	acceleration of gravity (ms^{-2})	Subscripts	
H	drag coefficient correction (nd)	eff	effective, or meso-scale related
I	unit tensor (nd)	fil	filtered
M	drag force (N m^{-3})	g	gas phase
P	pressure (N m^{-2})	i, j	coordinate directions
Re_p	particle size based Reynolds number (nd)	l	interface
s	strain rate tensor due to viscous plus pressure effects (s^{-1})	ℓ	a generic phase, either s or g
t	time (s)	res	residual
v	velocity vector (ms^{-1})	s	solid phase
y	vertical (axial) Cartesian coordinate (m)	x, y	horizontal and vertical (axial) directions
Greek letters		Other symbols	
β	micro-scale gas-solid drag coefficient ($\text{kg m}^{-3} \text{s}^{-1}$)	—	filtered volume average
Δ_f	filter size (m)	$\langle \rangle$	domain volume average
λ	bulk viscosity (N s m^{-2})	$\sim$	filtered Favre or mass weighed average, $\tilde{f} = \frac{\phi f}{\phi}$
μ	dynamic viscosity (N s m^{-2})		

gravity acting on the gas-solid mixture. This procedure gives rise to flow patterns that are supposed to correctly stand for the meso-scale of any possible macro-scale fluidized flow. In other words, scale separation is assumed to prevail, and the macro-scale is assumed not to affect the meso-scale of the flow. In order to derive filtered parameters, the meso-scale flow fields that are generated are filtered by space and time averaging over a number of snapshots inside the statistical steady state regime. Filtering windows are defined and made to sweep all over the domains while collecting statistics of filtered parameters classified according to relevant filtered independent variables. The usual meso-scale simulations are held for particular values of domain average solid volume fraction, and filtered results gathered for various domain average solid volume fractions are then combined together in the same statistics. This practice is consistent with the supposed independence of the meso-scale in relation to the macro-scale, as the sub-grid filtered data become statistically averaged among those for various different flow conditions surrounding the filtering region. The assumption that the flow topology that develops around a filtering region has negligible effect over filtered data finds some support on instability studies of granular flows (Goldhirsch et al., 1993; Tan and Goldhirsch, 1997).

Following such usual approach, Agrawal et al. (2001) and Andrews IV et al. (2005) advanced highly resolved simulations aiming for filtered models for the gas-solid drag coefficient as well as for filtered and residual pressures and viscosities. Further extending those works, Igci et al. (2008) developed highly resolved simulations over enlarged domains which allowed filtering over regions of various different sizes, thereby making the sub-grid filtered results adaptable to different grid sizes in the macro-scale simulations. Just like the previous works, they also merged together in the same statistics filtered data of different simulations set for a range of domain average solid volume fractions from very dilute to very dense. The filtering procedure was carried out over a very large number of snapshots, providing for a very robust statistics inside the statistical steady state regime. For a particular snapshot a window (filter) was defined and displaced throughout the whole domain while collecting inside averages (the filtered data). These data were classified by ranges of filtered solid volume fraction and stored into related bins. This was done for all the concern-

ing snapshots, and averages were stored for each individual bin. The procedure was repeated for all the simulations under various domain average solid volume fractions, and statistical averaging was performed altogether for each individual bin. Igci et al. (2008) showed that the resulting filtered data significantly vary with both filter size and solid volume fraction. In a complementary work by the same authors (Igci and Sundaresan, 2011) sub-grid models were advanced for filtered drag coefficient and for filtered and residual pressure and viscosity of the solid phase.

In the works cited so far (Agrawal et al., 2001; Andrews IV et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011) filtered parameters have been related to filtered solid volume fraction and filter size. It so happens that different flow patterns, ranging from very homogeneous to very heterogeneous, may occur for any particular values of filter size and filtered solid volume fraction. In order to account for such heterogeneity extent of the flow, Milioli et al. (2013) introduced an additional independent variable in their filtered parameter correlation (named 2nd marker, while the solid volume fraction was named 1st marker). Schneiderbauer and Pirker (2014), Agrawal et al. (2013) and Sarkar et al. (2016) developed analyses similar to those of Milioli et al. (2013).

The above cited works look for correlating relevant filtered parameters to inside-filter variables taking no account of any macro-scale related effects. The well known lack of scale separation in gas-solid fluidized flows (van der Hoef et al., 2006) is, therefore, ignored. There has been, however, a number of works pointing towards the necessity of accounting for macro-scale effects. Milioli and Milioli (2011) performed transient highly resolved simulations under varying average gas flow velocities. They applied axial gas pressure gradients in excess to that required to match the gravity acting on the gas-solid mixture, thereby giving rise to accelerated flows running through a wide range of domain average gas velocities. Their filtered results, gathered over the whole domain, showed noticeable effects of the domain average gas velocity over the size and shape of the solid coherent structures that were formed, also considerably affecting filtered stresses. The authors suggested that the flow topology may have a role on sub-grid modeling that need to be further investigated. Another assessment related to macro-scale accounting in filtered sub-grid correlation was advanced by Parmentier et al. (2012). They per-

formed highly resolved simulations with microscopic two-fluid modeling over a small 2D bubbling bed, which provided a bubbling bed topology as opposed to suspension like conditions. Sub-grid correlations were then derived from filtering, including a macro-scale length in the filter size dependence. [Parmentier et al. \(2012\)](#) also argued towards the need for a coarse grid dynamical adjustment analogous to that practiced in large eddy simulation of turbulent flows. [Özel et al. \(2013\)](#) extended the work of [Parmentier et al. \(2012\)](#) by incorporating vertical periodic boundaries over 3D bubbling bed conditions, and also by extending the development to include stresses analyses as done in previous works. Even though a correlation to a macro-scale length has been removed, the requirement for dynamical adjustment was still very much emphasized in [Özel et al. \(2013\)](#). The propositions of [Parmentier et al. \(2012\)](#) and [Özel et al. \(2013\)](#) are consistent with those of previous works while providing, in addition, an accountancy of macro-scale effects. There has also been a number of studies making it clear the necessity of accounting for macro-scale effects in sub-grid modeling of gas-solid flows which are based on the energy minimization multi-scale approach of [Li and Kwauk \(1994\)](#). Following this line, the analyses of [Wang and Li \(2007\)](#) and [Qi et al. \(2007\)](#) unveiled significant impacts of macro-scale quantities such as gas flow rate, solids flux and solids inventory over the sub-grid structure of dilute and dense flows. The concept of energy minimization was also implemented by [Wang et al. \(2011\)](#) for developing a cluster structure dependent drag model accounting for the local gas pressure gradient, gas fraction and phase velocities, which have been related to macro-scale conditions.

The current work intends to contribute to the discussion on the significance of macro-scale related parameters regarding their effects over relevant filtered parameters. Instead of following the procedure of post-correcting sub-grid correlations by means of dynamical adjustment while simulating at the large scale, as in some literature proposals, an approach is followed aiming for a prior insertion of relevant macro-scale effects straight into the correlations. The current work takes a first step in that direction by discussing effects of flow macro-scale trends over relevant meso-scale filtered parameters. In order to do so, the frequently assumed topology independency of filtered sub-grid parameters is questioned on the basis of new highly resolved simulations with microscopic two-fluid modeling. Different domain average solid volume fractions and gas flow Reynolds numbers are imposed over the whole domains so as to simulate different macro-scale flow conditions (while filtering is performed over smaller windows defined over those domains). The current analysis focus on the effects of those macro-scale features so as to investigate a possible correlation of relevant filtered parameters to the flow topology manifested from outside the filtered region. Alongside with the usual periodic boundaries, various average solid volume fractions and axial gas flow rates were enforced, and statistical steady state conditions were thereby provided at various different flow conditions. The current interest is limited to dilute flow conditions which are typical of riser flows. The results show that the filtered parameters of concern, namely the drag coefficient correction, and the filtered and residual pressures and viscosities of the phases, all considerably change with both the average solid volume fraction and gas Reynolds number. It is pointed out that a more rigorous sub-grid modeling do require macro-scale effects to be included, the average solid volume fraction and the average gas Reynolds number standing as relevant parameters to be accounted for.

2. Microscopic and filtered two-fluid models

In this work sub-grid filtered data are derived from results of highly resolved simulations with hydrodynamic two-fluid modeling

under micro-scale closing. This usually called microscopic two-fluid modeling is described next, and so it is the filtered two-fluid formulation, since the sub-grid filtered data of concern are defined from filtering over the two-fluid model equations. The hydrodynamic two-fluid model comprises a set of continuity and momentum conservative equations, together with closures for stresses, viscosities, pressures and interface interaction effects. The two-fluid model that is used in this work is based on the developments of [Anderson and Jackson \(1967\)](#), and the microscopic closures that are assumed are as described by [Agrawal et al. \(2001\)](#), all of them included in the open source code MFIX ([Syamlal et al., 1993](#)), which is used in the present work. [Table 1](#) brings the formulation of the concerning filtered two-fluid model, while the microscopic formulation is fully described in [Agrawal et al. \(2001\)](#). In the microscopic formulation, microscopic closures are required to deal with dispersed particulates treated as a continuum solid phase. Those usually come from the kinetic theory of granular flows, which includes an equation for granular energy conservation and correlations for solid phase properties as a function of a granular temperature ([Jenkins and Savage, 1983](#); [Lun et al., 1984](#); [Gidaspow, 1994](#); [Garzó and Dufty, 1999](#)). Microscopic closures are also required to deal with interface momentum exchanges. Even though many different kinds of interactions may occur in gas-particle fluidized flows (see, for instance, [Ishii, 1975](#); [Enwald et al., 1996](#); [Gidaspow, 1994](#)), drag is recognized as the most relevant in usual applications. Therefore, the interface gas-solid interaction is usually described through a generalized drag effect of the gas over the solid phase. The kinetic theory developments of [Lun et al. \(1984\)](#) and the drag model of [Wen and Yu \(1966\)](#) are applied in the present work just as done in [Agrawal et al. \(2001\)](#). Also, following the usual concerning literature ([Agrawal et al., 2001, 2013](#); [Andrews IV et al., 2005](#); [Igci et al., 2008](#); [Igci and Sundaresan, 2011](#); [Parmentier et al., 2012](#); [Özel et al., 2013](#); [Milioli et al., 2013](#); [Schneiderbauer and Pirker, 2014](#); [Sarkar et al., 2016](#)), no turbulence model is included in the current microscopic two-fluid modeling approach. This is so owing to two reasons: i. regarding the solid phase, as highly resolved simulations are intended, all possible scales of solid structures are expected to be captured; and ii. regarding the gas phase, as only high Stokes number conditions are considered, no significant effect of the sub-grid gas turbulence is expected over the solid flow hydrodynamics.

Filtering operators applied over the microscopic two-fluid model conservative equations give rise to the filtered two-fluid model conservative equations (Eqs. (6)–(9) in [Table 1](#)). In filtered formulations dependent variables, $f(\mathbf{x}, t)$, are described as a composition of a filtered part added to a sub-grid fluctuation or unresolved part, that is

$$f(\mathbf{x}, t) = \bar{f}(\mathbf{x}, t) + f'(\mathbf{x}, t) \quad (1)$$

The filtered part is defined as

$$\bar{f}(\mathbf{x}, t) = \int_{\mathbf{x}} f(\mathbf{x}, t) G(\mathbf{x}) d(\mathbf{x}) \quad (2)$$

The filter function $G(\mathbf{x})$ is a sub-grid space cut that limits the size of the smaller scales to be resolved. The sub-grid filter is usually made to match with the numerical grid volume V , so that $G(\mathbf{x}) = 1/V$ for any $\mathbf{x} \in V$. Therefore

$$\bar{f}(\mathbf{x}, t) = \frac{1}{V} \int_V f(\mathbf{x}, t) dV \quad (3)$$

While filtering over the two-fluid model equations some filtered products of dependent variables with phase fractions do appear which need to be developed. This is done by applying Favre or mass weighed averaging. For a phase ℓ , either gas or solid,

$$\overline{f_{\ell}(\mathbf{x}, t) \phi_{\ell}(\mathbf{x}, t)} = \bar{f}_{\ell}(\mathbf{x}, t) \bar{\phi}_{\ell}(\mathbf{x}, t) \quad (4)$$

and

$$\tilde{f}_\ell(\mathbf{x}, t) = \frac{\int_V \phi_\ell(\mathbf{x}, t) f_\ell(\mathbf{x}, t) dV}{\int_V \phi_\ell(\mathbf{x}, t) dV} \quad (5)$$

The filtering procedure gives rise to two new terms in the momentum equations, in addition to those in the unfiltered conservative differential equations (see Table 1 in Agrawal et al., 2001). One of the new terms accounts for the fluctuations on the buoyancy exerted by the gas over the solid phase. This buoyancy fluctuation is usually composed with the filtered drag thereby defining an effective interface interaction force, usually referred to as effective drag force owing to the predominance of the drag in gas-solid fluidized flows. The other new term accounts for residual stresses in both the phases.

The effective drag coefficient defined in Table 1, β_{eff} , is usually expressed in terms of a drag coefficient correction related to the filtered drag coefficient, $\bar{\beta}$, given by the microscopic model (see

Table 1 in Agrawal et al., 2001) as evaluated in terms of filtered variables (i.e. $\bar{\phi}_s$, $\bar{\phi}_g$, $\tilde{\mathbf{v}}_s$, $\tilde{\mathbf{v}}_g$). The drag coefficient correction is defined as

$$H = 1 - \frac{\beta_{\text{eff}}}{\bar{\beta}} \quad (19)$$

Therefore, the effective drag force is cast as

$$\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I = (1 - H)\bar{\beta}(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s) \quad (20)$$

The filtered and residual pressures and viscosities ($P_{\text{fil},\ell}$, $\mu_{\text{fil},\ell}$, $P_{\text{res},\ell}$, $\mu_{\text{res},\ell}$ for $\ell = g, s$), which account for filtered deviatoric and residual stresses as defined in Table 1, are given by

$$P_{\text{fil},g} = \bar{P}_g - \frac{2}{3}\mu_g(\nabla \cdot \tilde{\mathbf{v}}_g) \quad (\text{assuming } \lambda_g = 0) \quad (21)$$

$$\mu_{\text{fil},g} = \mu_g \quad (22)$$

Table 1

Filtered two-fluid model.

Filtered continuity and momentum conservation equations	
$\frac{\partial}{\partial t}(\rho_g \bar{\phi}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g) = 0$	(6)
$\frac{\partial}{\partial t}(\rho_s \bar{\phi}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s) = 0$	(7)
$\frac{\partial}{\partial t}(\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \tilde{\mathbf{v}}_g \tilde{\mathbf{v}}_g) = -\bar{\phi}_g \nabla \cdot \tilde{\boldsymbol{\sigma}}_g - \nabla \cdot \boldsymbol{\tau}'_g - (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_g \bar{\phi}_g \mathbf{g}$	(8)
$\frac{\partial}{\partial t}(\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \tilde{\mathbf{v}}_s \tilde{\mathbf{v}}_s) = -\nabla \cdot \tilde{\boldsymbol{\sigma}}_s - \nabla \cdot \boldsymbol{\tau}'_s - \bar{\phi}_s \nabla \cdot \tilde{\boldsymbol{\sigma}}_g + (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_s \bar{\phi}_s \mathbf{g}$	(9)
Filtered volumetric continuity	
$\bar{\phi}_g + \bar{\phi}_s = 1$	(10)
Closures	
Filtered deviatoric and residual stresses	
$\tilde{\boldsymbol{\sigma}}_g = [\bar{P}_g - (\lambda_g + \frac{2}{3}\mu_g)(\nabla \cdot \tilde{\mathbf{v}}_g)]\mathbf{I} - 2\mu_g \tilde{\mathbf{s}}_g = P_{\text{fil},g}\mathbf{I} - 2\mu_{\text{fil},g}\tilde{\mathbf{s}}_g$	(11)
$\tilde{\boldsymbol{\sigma}}_s = [\bar{P}_s - (\lambda_s + \frac{2}{3}\mu_s)(\nabla \cdot \tilde{\mathbf{v}}_s)]\mathbf{I} - 2\mu_s \tilde{\mathbf{s}}_s = P_{\text{fil},s}\mathbf{I} - 2\mu_{\text{fil},s}\tilde{\mathbf{s}}_s$	(12)
$\boldsymbol{\tau}'_\ell = \rho_\ell \bar{\phi}_\ell \tilde{\mathbf{v}}_\ell \tilde{\mathbf{v}}_\ell - \rho_\ell \bar{\phi}_\ell \tilde{\mathbf{v}}_\ell \tilde{\mathbf{v}}_\ell \sim P_{\text{res},\ell}\mathbf{I} - 2\mu_{\text{res},\ell}\tilde{\mathbf{s}}_\ell \text{ for } \ell = g, s$	(13)
$\tilde{\mathbf{s}}_\ell = \frac{1}{2}[\nabla \tilde{\mathbf{v}}_\ell + (\nabla \tilde{\mathbf{v}}_\ell)^T] - \frac{1}{3}(\nabla \cdot \tilde{\mathbf{v}}_\ell)\mathbf{I} \text{ for } \ell = g, s$	(14)
Filtered drag force	
$\bar{\mathbf{M}}_I = \overline{\beta(\mathbf{v}_g - \mathbf{v}_s)}$	(15)
Buoyancy fluctuation force (viscous terms are usually disregarded as lower order)	
$\mathbf{B}'_{gs} = -[\bar{\phi}_s \nabla \cdot \tilde{\boldsymbol{\sigma}}_g - \bar{\phi}_s \nabla \cdot \tilde{\boldsymbol{\sigma}}_g] \approx -[\bar{\phi}_s \nabla \bar{P}_g - \bar{\phi}_s \nabla \bar{P}_g]$	(16)
Effective drag force	
$\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I = \beta_{\text{eff}}(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s)$	(17)
$\beta_{\text{eff}} = \frac{\overline{\beta(\mathbf{v}_g - \mathbf{v}_s)}}{(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s)} - \frac{[\bar{\phi}_s \nabla \bar{P}_g - \bar{\phi}_s \nabla \bar{P}_g]}{(\tilde{\mathbf{v}}_g - \tilde{\mathbf{v}}_s)}$	(18)

$$P_{\text{fil},s} = \bar{P}_s - (\lambda_s + \frac{2}{3}\mu_s)(\nabla \cdot \mathbf{v}_s) \quad (23)$$

$$\mu_{\text{fil},s} = \bar{\mu}_s \quad (24)$$

$$P_{\text{res},\ell} = \frac{1}{3} \text{tr}(\boldsymbol{\tau}'_\ell) \quad (25)$$

$$\mu_{\text{res},\ell} = \frac{|\boldsymbol{\tau}'_{\text{shear},\ell}|}{2|\mathbf{s}_{\text{shear},\ell}|} \quad (26)$$

The evaluation of residual viscosities through Eq. (26) considers only the shear components of the tensors as the normal components are much larger and hinder the shear effects. In all the previous equations, where applicable, for any symmetric tensor $\mathbf{E}$

$$|\mathbf{E}| = \sqrt{\frac{1}{2} \mathbf{E} : \mathbf{E}^T} = \sqrt{\frac{1}{2} \sum (E_{ij} E_{ij})} \quad (27)$$

$$|\mathbf{E}_{\text{shear}}| = \sqrt{\frac{1}{2} \sum_{i \neq j} (E_{ij} E_{ij})} \quad (28)$$

The effective drag coefficient, given by Eq. (18) (which may also be cast in terms of the drag coefficient correction of Eq. (19)), and the filtered and residual pressures and viscosities, given by Eqs. (21)–(26), are the closures that are required by the filtered two-fluid model. Those are also the parameters that are derived from filtering over results of highly resolved simulations which are presented in this work.

3. Simulation and filtering procedure

Following previous works (Agrawal et al., 2001, 2013; Andrews IV et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011; Milioli et al., 2013; Sarkar et al., 2016), all the simulations in the present work have been performed using MFIX, an open source code developed and made available by NETL (National Energy Technology Laboratory, DOE-USA). MFIX is widely used for gas-solid flow simulations and has been verified extensively (Syamlal et al., 1993). Its is a FORTRAN written parallelized code. The governing equations in MFIX's two-fluid model are discretized through the finite volume method. The resulting numerical model is solved through a point by point numerical technique. Diffusive terms are discretized following the second order central differencing scheme. For advection terms there are various alternative discretizing methods, ranging from the first order upwind method up to higher order TVD procedures (following previous works, the second order Superbee procedure is used in the present work). The pressure-velocity coupling is solved through the SIMPLE algorithm. The numerical code of MFIX relevant to two-fluid modeling is fully described in Syamlal (1998).

The present highly resolved simulations were carried out for a typical fluid catalytic cracking particulate, the same as in previous works (Igci et al., 2008; Igci and Sundaresan, 2011; Milioli et al.,

2013; Agrawal et al., 2013). Table 2 brings the gas and solid properties of concern. A unique particle Froude number was considered.

A two-dimensional square domain of 16 cm x 16 cm was considered under periodic boundaries in all directions. A numerical mesh of 128 x 128 grids was applied, resulting a grid size of 1.25 mm x 1.25 mm (according to Agrawal et al. (2001), grid sizes between 1 and 2 mm do provide grid size reasonably independent filtered results for conditions as those in Table 2).

Alongside with periodic boundaries, various average axial gas flow rates were enforced over the domain, thereby allowing for statistical steady state conditions to be attained at various domain average gas Reynolds numbers. Different domain average solid volume fractions $\langle \phi_s \rangle$ were imposed, of 0.05, 0.15 and 0.25, covering a range relevant to rapid riser flows. A domain average gas Reynolds number $\langle \text{Re}_g \rangle$, taking the particle size as the relevant length scale, is defined as

$$\langle \text{Re}_g \rangle = \frac{\rho_g \langle \phi_g \rangle \langle v_{g,y} \rangle d_p}{\mu_g} \quad (29)$$

In the simulations for different $\langle \phi_s \rangle$, the ratio $\langle \text{Re}_g \rangle / \langle \text{Re}_g \rangle_{\text{susp}}$ was set unchanged, at values of 1.0, 4.08, 8.15, 12.23, 16.30, 20.34 and 24.45. This range was found suitable for producing streams closing towards pneumatic transport for the different $\langle \phi_s \rangle$ that were enforced. $\langle \text{Re}_g \rangle$ stands for the domain average gas Reynolds number, while $\langle \text{Re}_g \rangle_{\text{susp}}$ stands for its value under suspension like conditions, which results from imposing a gas pressure gradient in the axial direction of the domain that exactly matches the gravity acting on the gas-solid mixtures, i.e.

$$\frac{\Delta P_g}{Y_{\text{length}}} = \rho_s \langle \phi_s \rangle g + \rho_g \langle \phi_g \rangle g \quad (30)$$

where Y_{length} is the length of the domain in the axial direction. For conditions other than suspension like, $\langle \text{Re}_g \rangle$ is enforced over the whole domain through a MFX boundary condition that imposes the domain average gas flux as a constant in simulations over periodic domains.

The simulations give rise to fields of dependent variables over the grid mesh, and a filtering procedure is carried out providing for filtered data. The storage of filtered data is done over 64 x 80 bins, meaning 64 gaps of filtered solid volume fraction and 80 gaps of filtered slip velocity (this binning resolution was found adequate in previous works Sarkar et al., 2016). The procedure for filtering and binning is fully described in both Igci et al. (2008) and van der Hoef et al. (2006). In general terms, one must consider a suitable number of snapshots of the flow field in the statistical steady state regime, so that good averaging statistics are collected (a snapshot shows the flow field over the whole domain for a particular fixed time). Then a window (or filter) must be defined over the domain comprising a number of numerical cells. Averaging over this region provides averaged or filtered data. The window is made to move in space all over the domain and in time through the various snapshots, and the collected averaged data are classified by ranges of suitable independent variables (markers) and stored in bins. Two markers are defined following Milioli et al. (2013), with the filtered solid volume fraction as the 1st marker and the filtered slip velocity as the 2nd marker. Different window sizes provide filtered results for different filter sizes. Considering the assumed domain size, filter sizes up to 4 cm x 4 cm may be considered as previous works show that filter sizes up to 1/4 of the domain size do provide filtered data independent of domain size (Igci et al., 2008).

The data collecting procedure provides filtered data stored as a function of the 1st and 2nd markers, filter size, $\langle \text{Re}_g \rangle / \langle \text{Re}_g \rangle_{\text{susp}}$ and $\langle \phi_s \rangle$. In previous works (Igci et al., 2008; Igci and Sundaresan, 2011; Milioli et al., 2013; Agrawal et al., 2013; Sarkar et al., 2016) filtered

Table 2
Physical properties of gas and solid.

d_p	Particle diameter	7.5×10^{-5} m
e_p	Particle sphericity	1
ρ_s	Particle density	1500 kg/m ³
ρ_g	Gas density	1.3 kg/m ³
μ_g	Gas viscosity	1.8×10^{-5} kg/(m s)
e	Coefficient of restitution	0.9
v_t	Terminal settling velocity	0.2184 m/s
$Fr_p = v_t^2 / (gd_p)$	Particle Froude Number	64.85

statistics of different simulations for a range of $\langle\phi_s\rangle$, as low as 0.01 and as high as 0.58, have all been merged together. In this procedure, a window with any particular average solid volume fraction and average slip velocity is assumed to statistically provide about the same filtered results irrespective of the average solid volume fraction on the neighborhood. As the current intent is to evaluate the effects of the flow topology, filtered data are gathered for each particular $\langle\phi_s\rangle$, and no merging for different $\langle\phi_s\rangle$ is performed.

4. Results and discussion

In the analyses that follow parameters have been cast dimensionless following previous works (Agrawal et al., 2001; Andrews IV et al., 2005; Igci et al., 2008). Particle density (ρ_s), terminal settling velocity of a particle (v_t) and gravity acceleration (g) have been taken as characteristic density, velocity and gravity, respectively. It follows that the characteristic time and length become v_t/g and v_t^2/g , respectively. Therefore, drag coefficients, viscosities and pressures (and stresses) are made dimensionless by $\rho_s g/v_t$, $\rho_s v_t^3/g$, and $\rho_s v_t^2$, respectively. Filtered results were bin averaged through time intervals inside the statistical steady state flow condition for each $\langle Re_g \rangle$ and $\langle\phi_s\rangle$ that were enforced in the various simulations. Table 3 shows the complete simulation schedule, which was defined having as a reference the $\langle Re_g \rangle_{susp}$ for each different $\langle\phi_s\rangle$. Noticeable in this table is the fact that, for any particular gas Reynolds number ratio kept as a constant, $\langle Re_g \rangle$ results lower for higher $\langle\phi_s\rangle$. This is just a consequence of a more intense damping on the gas by drag in domains containing more particles.

Before starting the analyses of the filtered results, the various fluidized conditions that were considered are briefly evaluated on the basis of domain averaged as well as instantaneous results (given in Figs. 1 and 2, respectively). Fig. 1 shows time evolution profiles of domain average axial phase velocities, axial slip velocity and axial gas pressure gradient, for all the practiced $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$, for the cases with $\langle\phi_s\rangle = 0.15$. The profiles for $\langle\phi_s\rangle = 0.05$ and 0.25 are similar (not showed). For all the cases, including those not showed, statistical steady state conditions were already attained at about 45 dimensionless time (~ 1 s). A dimensionless time interval from 45 to 450 was found adequate for gathering good statistics from all the simulations. Fig. 1a and b show that the fluctuations on the domain average velocity profiles result very small at higher gas Reynolds numbers, and quite considerable at the suspension like conditions, while Fig. 1c and d show that both the domain average axial slip velocity and the domain average axial gas pressure gradient keep fluctuating around the same well defined time averages for all the gas Reynolds numbers, as expected. An issue may be raised on whether the high fluctuating velocity profiles observed at suspension conditions (and not observed at higher gas Reynolds numbers) could be just a consequence of an imposed gas pressure gradient instead of an imposed gas flow rate (as done for the higher gas Reynolds number cases). In order to clarify that issue, an additional simulation was

performed, where a suspension condition was alternatively generated by enforcing an axial gas flow rate (exactly matching the domain average value found under the pressure gradient imposed situation). The graphs in Fig. 1 also include results from that additional simulation. As seen, the alternative simulation provides a much less fluctuating profile for the domain average axial gas velocity (Fig. 1a), but produces equally high fluctuating profiles for both the domain average axial solid velocity and the domain average axial slip velocity (Fig. 1b and c). Under the alternative simulation procedure, it is now the domain average axial gas pressure gradient that keeps fluctuating, as expected (Fig. 1d). It is concluded that a higher inherent flow instability, and not the particular boundary condition type, is the factor that actually imposes high fluctuations under suspension like conditions. Also, despite the observed differences, both the procedures for suspension simulation do provide the same flow topology and filtered results (not showed). Anyway, all the filtered results for the suspension like conditions to be showed ahead have been derived from simulations under prescribed axial gas pressure gradient.

Fig. 2 shows grayscale plots of solid volume fraction over the whole domain for snapshots inside the statistical steady state regime. The pictures stand for simulations with domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 (columns), and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1, 8.15, 16.30$ and 24.45 (lines). The figures show a considerable effect of both parameters over the flow topology. An increase on gas Reynolds number ratio for a given domain average solid volume fraction causes the regions with higher solid concentration (clusters) to stretch in the axial direction, and the flow field to grow increasingly homogeneous. Otherwise, an increase on domain average solid volume fraction for a given gas Reynolds number ratio gives rise to denser and thicker structures. Effects similar to those were reported by Milioli and Milioli (2011) for a much coarser particulate ($Fr_p = 1235.4$), even though the current particulate Froude number is about 19 times smaller. This similitude of behavior is suggestive having in view future scaling concerns.

The changes in topology that are observed in Fig. 2, as $\langle\phi_s\rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ are varied, point towards effects of those variables over sub-grid filtered parameters, of which the significance is addressed next. Results are presented here for the drag coefficient correction (Fig. 3), filtered and residual pressures and viscosities (Figs. 5–8), as a function of the 1st and 2nd markers, i.e. the filtered solid volume fraction, $\bar{\phi}_s$, and the dimensionless filtered axial slip velocity $\bar{v}_{slip,y}/v_t$, respectively. The filtered axial slip velocity is defined as $\bar{v}_{slip,y} = \bar{v}_{g,y} - \bar{v}_{s,y}$. The figures stand for domain average gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1.0, 4.08, 8.15, 12.23, 16.30, 20.34$ and 24.45 , and domain average solid volume fractions $\langle\phi_s\rangle = 0.05, 0.15$, and 0.25 . The effects over filtered parameters of the filter size, 1st and 2nd markers, have already been well discussed in previous works (Igci et al., 2008; Igci and Sundaresan, 2011; Milioli et al., 2013; Agrawal et al., 2013; Sarkar et al., 2016). Owing to that, and considering that the main concern is currently turned to analyzing the effects of $\langle\phi_s\rangle$ and $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$, results are presented here for a unique filter size, $\Delta_f/(v_t^2/g) = 4.112$ (i.e. a $2\text{ cm} \times 2\text{ cm}$ filter size), and no further discussion is advanced regarding the 1st and 2nd markers. It is though remarked that results standing for other filter sizes have similar behavior to those currently analyzed, and can be found elsewhere (Chavez-Cussy, 2017; Chavez-Cussy et al., Unpublished results). It is also pointed that one marker analyses (with binning on filtered solid volume fraction alone) were not pursued. For any filtered parameter, the averaging together of data without accounting for a second marker (in addition to the filtered solid volume fraction as 1st marker) does provide less accurate or even distorted results, and the one marker procedure was therefore dismissed.

Table 3
 $\langle Re_g \rangle$ in the various simulations. A pair $\langle Re_g \rangle / \langle Re_g \rangle_{susp}, \langle\phi_s\rangle$ defines a particular simulation.

$\langle Re_g \rangle / \langle Re_g \rangle_{susp}$	$\langle\phi_s\rangle$		
	0.05	0.15	0.25
1.00	4.42	2.26	0.96
4.08	18.03	9.21	3.92
8.15	36.02	18.42	7.83
12.23	54.06	27.63	11.75
16.30	72.05	36.83	15.67
20.34	89.90	46.04	19.54
24.45	108.07	55.25	23.50

Fig. 1. Time evolution of the dimensionless domain average axial gas velocity $\langle v_{g,y} \rangle / v_t$ (a), axial solid velocity $\langle v_{s,y} \rangle / v_t$ (b), axial slip velocity $\langle v_{g,y} - v_{s,y} \rangle / v_t$ (c), and axial gas pressure gradient $-(\partial P_g / \partial y) / (\rho_s g)$ (d), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 1$ ($\bullet$), 4.08 ($\triangleright$), 8.15 (∇), 12.23 ($\diamond$), 16.30 ($\triangleleft$), 20.34 ($\square$) and 24.45 ($\triangle$); alternative results provided for $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 1$ enforcing an axial gas flow rate ($\circ$). The profiles stand for the domain average solid volume fraction $\langle \phi_s \rangle = 0.15$.

Fig. 3 shows the variation of the drag coefficient correction, H , with the filtered solid volume fraction and filtered slip velocity, for the various simulations under different settings of domain average solid volume fraction and domain average gas Reynolds number, for the dimensionless filter size $\Delta_f / (v_t^2 / g) = 4.112$. It is opportune to notice that H stands for a correction over the filtered Wen and Yu's drag coefficient (Wen and Yu, 1966), which is suitable to homogeneous flows, in order to provide for an effective drag coefficient suitable to heterogeneous flows. Therefore, the smaller H is the more homogeneous is the flow. Irrespective of the domain average solid volume fraction, the current results show that a higher domain average gas Reynolds number causes H to decrease, an effect that becomes more prominent at lower filtered solid volume fractions and lower filtered slip velocities. This behavior comes from the flow becoming more homogeneous at higher gas Reynolds numbers and lower solid volume fractions, which is supported by the solid volume fraction grayscale plots of Fig. 2. In regions of lower slip velocities H is lower and, as the gas Reynolds number increases, the spread among the profiles become larger and grow through a larger range of solid volume fractions. At very low slip velocities the comparison among the profiles becomes difficult due to the occurrence of the profiles in ranges of solid volume fractions that hardly overlap (not showed in the graphs). At very high slip velocities the effect of the domain average gas Reynolds number becomes not significant. In general, gas Reynolds number ratios up to 8.15 have no significant effects on H , no matter the slip velocity. Another feature showed in Fig. 3a is that the H profiles approach each other at both very high and very low filtered solid volume fractions (as compared to the domain average), suggesting an inside-filter topology that becomes independent of the domain average gas Reynolds number. Fig. 3a shows results for $\langle \phi_s \rangle = 0.15$ only; results for $\langle \phi_s \rangle = 0.05$ and 0.25 are alike, and can be found elsewhere (Chavez-Cussy, 2017).

Fig. 3b shows a considerable effect of the domain average solid volume fraction over H , for $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 12.23$, even though not systematic. In general, Fig. 3 shows that H is considerably affected by both the domain average gas Reynolds number and the domain average solid volume fraction, noticeably for $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}}$ above 8.15. Therefore, the currently available sub-grid models for H (e.g. Milioli et al., 2013; Sarkar et al., 2016) do require enhancement in order to account for the effects of those macro-scale parameters.

Fig. 3 shows significant effects of both $\langle \phi_s \rangle$ and $\langle Re_g \rangle$ over the drag coefficient correction mostly at dimensionless filtered slip velocities typically below 2.03. One may argue on how dominant are those conditions over the whole flow field, since a low predominance would dismiss the necessity for correlating H to $\langle \phi_s \rangle$ and $\langle Re_g \rangle$. In order to enlighten that issue, the probability density function (pdf) of the dimensionless filtered slip velocity has been plotted for the various cases, which are presented in Fig. 4. Fig. 4a, b and c show the concerning pdf profiles for the various $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}}$, for a particular filter size ($\Delta_f / (v_t^2 / g) = 4.112$), for $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25, respectively. Each graph stands for the filtered solid volume fraction of higher occurrence in each case, which just matches $\langle \phi_s \rangle$ owing to the relatively large filter size that was considered. For all the cases in Fig. 4, it is seen that the occurrence of dimensionless filtered slip velocities below 2.03 is actually very dominant. This result shows that, indeed, H does require correlation to both $\langle \phi_s \rangle$ and $\langle Re_g \rangle$.

The analyses that follow next are related to the effects of $\langle \phi_s \rangle$ and $\langle Re_g \rangle$ over filtered and residual stresses of both gas and solid phases. Owing to the predominance of relatively low filtered slip velocities in the flow field, it is found enough to present the oncoming discussion for a unique low filtered slip velocity of high occurrence ($\tilde{v}_{\text{slip},y} / v_t = 0.85$). Figs. 5 and 6 show results of the

Fig. 2. Grayscale plots of solid volume fraction in the domain for snapshots inside the statistical steady state regime, for simulations with domain average solid volume fractions $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 (columns), and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1, 8.15, 16.30$ and 24.45 (lines).

dimensionless filtered pressure and viscosity of the solid phase, respectively. For all the practiced domain average solid volume fractions (0.05, 0.15 and 0.25), there are very significant effects of the domain average gas Reynolds number, with both $P_{fil,s}$ and

$\mu_{fil,s}$ decreasing by up to one order of magnitude as $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ is increased from 1 to 24.45. Figs. 5a and 6a present the concerning results for $\langle \phi_s \rangle = 0.15$; results for $\langle \phi_s \rangle = 0.05$ and 0.25 can be found in Chavez-Cussy (2017). The dropping of $P_{fil,s}$ and $\mu_{fil,s}$ with increasing $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ comes as a consequence of the filtered granular temperature considerably dropping as the domain average gas Reynolds number grows high, which is actually quite coherent, since at the more homogeneous conditions provided by the higher domain average gas Reynolds numbers, all field fluctuations become smaller, including the solid velocity fluctuations that define the granular temperature (Chavez-Cussy et al., Unpublished results). Figs. 5b and 6b show results of $P_{fil,s}$ and $\mu_{fil,s}$, respectively, for $\langle \phi_s \rangle = 0.15$ and 0.25 , under $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1, 12.23$, and 20.34 . As seen, there is no significant effect of $\langle \phi_s \rangle$ over those parameters, except for some slight impact at the higher $\bar{\phi}_s$.

Figs. 7 and 8 show results of the dimensionless residual pressure and viscosity of the solid phase, respectively. Except for the well known difference in order of magnitude (Agrawal et al., 2001), the profiles are similar to those of Figs. 5 and 6, for the dimensionless filtered pressure and viscosity of the solid phase. Both $P_{res,s}$ and $\mu_{res,s}$ are very significantly affected by the domain average gas Reynolds number, for all practiced domain average solid volume fractions (0.05, 0.15 and 0.25). Figs. 7a and 8a present the concerning results for $\langle \phi_s \rangle = 0.15$; results for $\langle \phi_s \rangle = 0.05$ and 0.25 can be found in Chavez-Cussy (2017). Just as seen for $P_{fil,s}$ and $\mu_{fil,s}$, $P_{res,s}$ and $\mu_{res,s}$ also decrease by up to one order of magnitude as $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ is increased from 1 to 24.45. Figs. 7 and 8 also show results of the dimensionless residual pressure and viscosity of the gas phase, respectively. Regarding the effects of the domain average solid volume fraction and gas Reynolds number, the behaviors of $P_{res,g}$ and $\mu_{res,g}$ are quite similar to those of $P_{res,s}$ and $\mu_{res,s}$, respectively. The dropping of the residual stress parameters of both phases with increasing gas Reynolds numbers is due to the lower velocity fluctuations associated to the more homogeneous conditions that prevail at those higher gas Reynolds numbers. This gives rise to lower granular temperatures, as already pointed, and also causes lower residual stresses in both the phases (related results are presented in Chavez-Cussy et al., Unpublished results). Figs. 7b and 8b show results for the residual parameters ($P_{res,s}$, $P_{res,g}$, $\mu_{res,s}$ and $\mu_{res,g}$), for $\langle \phi_s \rangle = 0.15$ and 0.25 , under $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1, 12.23$, and 20.34 . For $\langle \phi_s \rangle = 0.15$ and 0.25 no significant impacts are seen at any $\bar{\phi}_s$, except for the higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ ($= 20.34$), which show some slightly discrepant

Fig. 3. Drag coefficient correction, H , as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for: (a) gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 ($\circ$), 8.15 ($\triangleleft$), 12.23 ($\diamond$), 16.30 ($\triangleright$), 20.34 ($\square$) and 24.45 (∇), under a domain average solid volume fraction $\langle \phi_s \rangle = 0.15$; (b) domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (full lines), 0.15 (gray symbols) and 0.25 (white symbols), under a gas Reynolds number ratio $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 12.23$. The results stand for the dimensionless filtered axial slip velocities $\tilde{v}_{slip,y} / v_t = 0.85, 2.03$ and 4.85 , and the dimensionless filter size $\Delta_f / (v_t^2 / g) = 4.112$.

Fig. 4. Probability density function (pdf) of the dimensionless filtered axial slip velocity, $\tilde{v}_{slip,y}/v_t$, for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 ($\circ$), 8.15 ($\triangleleft$), 12.23 ($\diamond$), 16.30 ($\triangleright$), 20.34 ($\square$) and 24.45 (∇), for the domain average solid volume fractions $\langle\phi_s\rangle = 0.05$ and filtered solid volume fraction $\bar{\phi}_s = 0.05$ (a), $\langle\phi_s\rangle = 0.15$ and $\bar{\phi}_s = 0.15$ (b), and $\langle\phi_s\rangle = 0.25$ and $\bar{\phi}_s = 0.25$ (c). The results stand for the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

Fig. 5. Dimensionless filtered solid pressure, $P_{fl,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for: (a) gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 ($\circ$), 8.15 ($\triangleleft$), 12.23 ($\diamond$), 16.30 ($\triangleright$), 20.34 ($\square$) and 24.45 (∇), under a domain average solid volume fraction $\langle\phi_s\rangle = 0.15$; (b) domain average solid volume fractions $\langle\phi_s\rangle = 0.15$ (gray symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ ($\circ$), 12.23 ($\diamond$) and 20.34 ($\square$). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.85$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

values of the residual parameters at lower $\bar{\phi}_s$. Figs. 7b and 8b also include profiles of the concerning parameters for $\langle\phi_s\rangle = 0.05$, under $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 20.34$. In these cases, especially for $P_{res,s}$ and $P_{res,g}$, a very significant disagreement between profiles do appear as $\langle\phi_s\rangle$ changes from 0.15 or 0.25 to 0.05. Such behavior may be associated to homogeneity changes as the flow becomes more dilute under high gas Reynolds number conditions.

As the flow field grows homogeneous when the average gas Reynolds number increases (as seen in Fig. 2), the space fluctuations on both the phases diminish and, as a consequence, the

related pressures and viscosities systematically drop (as seen in Figs. 7 through 8). It is noticeable that this behavior is opposed to that of mono-phase turbulent flows, where higher Reynolds numbers do provide for higher fluctuations, giving rise to higher residual pressures and viscosities. This is a very relevant trend to account for regarding any analogy attempt between gas-solid flows and mono-phase turbulent flows.

Most of the figures, for all of the effective, filtered and residual parameters related to drag and stresses of current concern, do show some nonsystematic behavior, especially for gas Reynolds

Fig. 6. Dimensionless filtered solid dynamic viscosity, $\mu_{fil,s}/(\rho_s v_t^2/g)$, as a function of the filtered solid volume fraction, ϕ_s , for: (a) gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (□), 20.34 (□) and 24.45 (▽), under a domain average solid volume fraction $\langle \phi_s \rangle = 0.15$; (b) domain average solid volume fractions $\langle \phi_s \rangle = 0.15$ (gray symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (○), 12.23 (◇) and 20.34 (□). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.85$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

Fig. 7. Dimensionless residual solid and gas pressures, $P_{res,\ell}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, ϕ_s , for: (a) gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (□), 20.34 (□) and 24.45 (▽), under a domain average solid volume fraction $\langle \phi_s \rangle = 0.15$; (b) domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (lines), 0.15 (gray symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (○), 12.23 (◇) and 20.34 (□). The lines stand for $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 20.34$ (full lines for the solid phase; dashed lines for the gas phase). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.85$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

Fig. 8. Dimensionless residual solid and gas dynamic viscosities, $\mu_{res,\ell}/(\rho_s v_t^2/g)$, as a function of the filtered solid volume fraction, ϕ_s , for: (a) gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (—), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (□), 20.34 (□) and 24.45 (▽), under a domain average solid volume fraction $\langle \phi_s \rangle = 0.15$; (b) domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (lines), 0.15 (gray symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (○), 12.23 (◇) and 20.34 (□). The lines stand for $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 20.34$ (full lines for the solid phase; dashed lines for the gas phase). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.85$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

number ratios above 20.34. A possible cause for that behavior could be a major change in flow topology, which turns from a clustered pattern into a growingly homogeneous flow as gas

Reynolds number increases. Otherwise, the nonsystematic behavior may also suggest that the primary markers that have been taken for classifying filtered data (i.e. filtered solid volume fraction

and filtered slip velocity) may not be quite suitable or insufficient, especially for high Reynolds flow conditions.

5. Summary and conclusions

Meso-scale highly resolved simulations with two-fluid modeling have been used to provide sub-grid closure models applicable to filtered two-fluid formulations intended for macro-scale simulations of gas-solid fluidized flows. In the usual procedure, sub-grid models are derived from filtering over results of highly resolved simulations, and relevant filtered parameters such as effective drag coefficients and residual stresses related parameters are correlated to suitable filtered dependent variables. It comes out that the provided correlations do not take any account of macro-scale conditions, namely the flow topology, which is consistent with the usual scale separation assumption. This article is intended to verify whether such a macro-scale dependence is required to be accounted for, and to what extent. In order to do so, two macro-scale parameters usually associated to flow topology are considered as for their effects over relevant filtered parameters. Those are the macro-scale average solid volume fraction and the macro-scale average gas flow Reynolds number. The developments were carried out for dilute flow conditions typical of riser flows.

The current highly resolved simulations were performed using the well established microscopic two-fluid model of the MFI code, where microscopic closures for fluid properties and stresses of the solid phase are brought from Lun's kinetic theory of granular flows (Lun et al., 1984), and the microscopic closure for drag is provided by Wen and Yu's drag model (Wen and Yu, 1966). All the simulations were carried out for a unique particulate typical of fluid catalytic cracking widely studied in previous works. As a unique Froude number was considered, scaling was not treated at any extent. The simulations were performed over 2D periodical domains keeping the domain average axial gas flow rate and solid volume fraction as constants at various different dilute conditions typical of riser flows. Results were collected over statistical steady state conditions and through a time interval large enough to provide for robust statistics. Averaged filtered results were then gathered for particular filter sizes sweeping over the domain in space and time, and stored as a function of relevant filtered independent variables (filtered solid volume fraction and filtered slip velocity), for each pair of macro-scale conditions imposed in the simulations (domain average solid volume fraction and domain average gas Reynolds number).

Grayscale plots of solid volume fraction taken from snapshots inside the statistical steady state regime showed marked effects of both macro-scale imposed conditions. An increased average gas Reynolds number caused solid structures to stretch in the axial direction and increasing flow homogeneity, while an increased average solid volume fraction gave rise to denser and thicker structures. These topology impacts affected relevant filtered parameters at different extents under different conditions. Results were presented for the drag coefficient correction, and for filtered and residual pressures and viscosities of the phases. The drag coefficient correction was significantly affected by the average gas Reynolds number noticeably at lower filtered solid volume fractions and lower filtered slip velocities, no matter the average solid volume fraction. Otherwise, the effect of the average solid volume fraction over the drag coefficient correction was significant only at higher gas Reynolds numbers. Regarding the filtered and residual pressures and viscosities of the phases, very significant effects of both the macro-scale parameters were observed, of up to one order of magnitude at some conditions. In general, there were significant quantitative variations of all the relevant filtered parameters, which were even more intense at high average gas Reynolds num-

bers and, it was showed that the conditions on which the macro-scale parameters considerably affect relevant filtered parameters are quite dominant in the concerning flow fields. In addition, at the higher average gas Reynolds numbers some marked changes of behavior also occurred, which were associated to topology evolution towards a more homogeneous condition. It was observed that residual pressures and viscosities drop at higher gas Reynolds number flow conditions, which is an effect opposite to what happens in mono-phase turbulence. The present results allow to ultimately conclude that a more rigorous sub-grid modeling of dilute gas-solid flows must also embrace macro-scale effects, the average solid volume fraction and the average gas Reynolds number standing as relevant parameters to be accounted for.

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APPENDIX G – MACRO-SCALE EFFECTS OVER FILTERED AND RESIDUAL STRESSES IN GAS-SOLID RISERFLOWS

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Macro-scale effects over filtered and residual stresses in gas-solid riser flows

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HIGHLIGHTS

- Macro-scale considerably affects filtered and residual stresses in gas-solid riser flows.
- Variations of up to two orders of magnitude on filtered and residual pressures and viscosities.
- Opposite to monophasic turbulence, higher gas flow rates cause lower stresses.
- Some observed non-systematic behavior suggests reassessment of independent variables.

GRAPHICAL ABSTRACT

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ABSTRACT

Sub-grid models for filtered and residual stresses are required as closures in filtered two-fluid modeling of gas-solid fluidized flows. An approach for deriving such models consists of filtering over results from highly resolved simulations with microscopic two-fluid modeling, which are mostly performed under suspension like conditions as separation of scales is assumed. This means that no macro-scale effects are accounted for. In this work effects of flow macro-scale are evaluated by practicing conditions from suspensions up to pneumatic transport, under solid concentrations typical of risers, applying highly resolved simulations with microscopic two-fluid modeling in periodic domains. Results show that the domain average gas Reynolds number and the domain average solid volume fraction both considerably affect filtered and residual stresses of both phases. It becomes evident that accurate sub-grid models require macro-scale effects to be accounted for.

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1. Introduction

The multi-scale nature of gas-solid fluidized flows has prompted modeling approaches for lower scales aiming to provide closure models for larger scales. In the so called microscopic two-fluid modeling approach meso-scale solutions are provided, which have been used to derive sub-grid closure models for macro-scale

simulations with filtered formulations. In hydrodynamic modeling, those sub-grid models stand for filtered interphase interactions, and filtered and residual stresses in the phases. Besides being the driving force in gas-solid fluidization, interphase interactions deeply affect any aspect of the flow topology. Stresses on each phase also play a significant role, considerably affecting length and time scales associated to coherent structures in the flow. There is an extensive literature largely attesting those facts, including Jenkins and Savage (1983), Lun et al. (1984), Gidaspow (1994), Johnson and Jackson (1987), Li and Kwauk (1994), Enwald et al.

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Nomenclature

B'	fluctuation of gas-solid buoyancy force (N m^{-3})	ε_p	particle sphericity (nd)
C_D	single particle drag coefficient (nd)	Θ	granular temperature ($\text{m}^2 \text{s}^{-2}$)
d_p	particle diameter (m)	κ_s	granular thermal conductivity ($\text{kg m}^{-1} \text{s}^{-1}$)
e	restitution coefficient for particle-particle collisions (nd)	λ	bulk viscosity (N s m^{-2})
$\mathbf{E}$	symmetric tensor	μ	dynamic viscosity (N s m^{-2})
$\mathbf{g}$, g	acceleration of gravity (m s^{-2})	ρ	density (kg m^{-3})
g_0	radial distribution function (nd)	$\boldsymbol{\sigma}$	deviatoric stress tensor (N m^{-2})
$\mathbf{I}$	unit tensor (nd)	$\boldsymbol{\tau}'$	residual stress tensor (N m^{-2})
J_{coll}	rate of dissipation of granular energy by collisional damping ($\text{J m}^{-3} \text{s}^{-1}$)	ϕ	volume fraction (nd)
J_{vis}	rate of dissipation of granular energy by viscous damping ($\text{J m}^{-3} \text{s}^{-1}$)	Subscripts	
$\mathbf{M}$	drag force (N m^{-3})	fil	filtered
P	pressure (N m^{-2})	g	gas phase
Re_p	particle size based Reynolds number (nd)	i, j	coordinate directions
$\mathbf{s}$	strain rate tensor due to viscous plus pressure effects (s^{-1})	l	interface
t	time (s)	ℓ	a generic phase, either s or g
$\mathbf{v}$	velocity vector (m s^{-1})	max	maximum
y	vertical (axial) Cartesian coordinate (m)	res	residual
Greek letters		s	solid phase
β	micro-scale gas-solid drag coefficient ($\text{kg m}^{-3} \text{s}^{-1}$)	x, y	horizontal and vertical (axial) directions
Γ_{slip}	rate of production of granular energy by gas-particle slip ($\text{J m}^{-3} \text{s}^{-1}$)	Other symbols	
Δ_f	filter size (m)	–	filtered by volume averaging
		$\langle \rangle$	domain volume average
		$\sim$	filtered by Favre or mass weighed averaging, $\tilde{f} = \frac{\phi f}{\phi}$

(1996), Sinclair (1997), Jackson (2000), Sundaresan (2000), van der Hoef et al. (2006), among many others. So much so that in the field of research aiming for sub-grid closures for filtered two-fluid modeling not only filtered interphase interactions are investigated, but also filtered and residual stresses (e.g. Agrawal et al., 2001; Igci et al., 2008; Parmentier et al., 2012; Özel et al., 2013; Milioli et al., 2013; Schneiderbauer and Pirker, 2014; Sarkar et al., 2016). The present work is concerned with the behavior of filtered and residual stresses in dilute gas-solid fluidized flows, specially regarding effects of macro-scale flow conditions, and is intended as a contribution to future correlation developments for those sub-grid closures.

Filtered and residual stresses are definitions relevant to filtered two-fluid formulations under the fundamental assumption of continuum for all the phases. Models for those parameters can be derived by filtering over meso-scale flow fields, which are usually provided by highly resolved simulations with microscopic two-fluid formulations (Agrawal et al., 2001; Andrews IV et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011a,b; Parmentier et al., 2012; Özel et al., 2013; Milioli et al., 2013; Agrawal et al., 2013; Schneiderbauer and Pirker, 2014; Sarkar et al., 2016). In microscopic two-fluid modeling closures for stresses are straightforward for the gas phase, while the kinetic theory of granular flows is advanced in order to define continuum properties for the particulate treated as a solid phase (Jenkins and Savage, 1983; Lun et al., 1984; Gidaspow, 1994; Garzó and Dufty, 1999). The concerning highly resolved simulations are mostly performed over periodic domains under suspension like conditions. The usual filtering procedure is well described in literature (e.g. Igci et al., 2008; van der Hoef et al., 2006).

From their highly resolved simulation predictions Agrawal et al. (2001), Andrews IV et al. (2005), Igci et al. (2008), and Igci and Sundaresan (2011a,b) derived filtered and residual stresses (pressures and viscosities). Agrawal et al. (2001) performed simulations

for domain sizes compatible with grid sizes practiced in macro-scale simulations, under enforced ranges of domain average solid volume fraction and vertical macro-scale shear rate. Their results, collected under statistical steady state flow conditions, were filtered over the whole domain, allowing for filtered parameters to be determined. The analysis that was carried out showed that both, domain average solid volume fraction and vertical macro-scale shear rate, considerably affect filtered and residual pressures and viscosities. In addition, their results also confirmed literature claims of occurrence of solid coherent structures with characteristic sizes ranging 10–100 particle sizes, and showed that grid resolutions of about 10 particle sizes provide filtered predictions that are nearly independent of grid size (as pointed out by van der Hoef et al., 2006). Agrawal et al. (2001) also showed that vertical boundaries under either periodic, partial-slip or free-slip conditions give rise all to similar heterogeneous flow patterns. Following the work of Agrawal et al. (2001), and under the same approaches and procedures, Andrews IV et al. (2005) proposed correlations for the residual pressure and viscosity of the solid phase, the first as a function of the domain average solid volume fraction alone, and the second as a function of both the domain average solid volume fraction and the vertical macro-scale shear rate. Igci et al. (2008) further extended the works of Agrawal et al. (2001) and Andrews IV et al. (2005) by performing highly resolved simulations over larger domains and gathering filtered results for a range of filter sizes. They showed that the filtered and residual pressures and viscosities of the solid phase are functions of the filtered solid volume fraction, and considerably change with filter size. In following works, the authors actually advanced sub-grid models for those parameters (Igci and Sundaresan, 2011a,b). Milioli et al. (2013) argued that a description on the basis of filter size and filtered solid volume fraction alone is insufficient, since the flow heterogeneity is not captured. They introduced the filtered slip velocity as an assumed additional independent variable, as a means of

Table 1

Microscopic two-fluid model (following Agrawal et al., 2001).

Continuity and momentum conservation equations	
$\frac{\partial}{\partial t}(\rho_g \phi_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g) = 0$	(1)
$\frac{\partial}{\partial t}(\rho_s \phi_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s) = 0$	(2)
$\frac{\partial}{\partial t}(\rho_g \phi_g \mathbf{v}_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g \mathbf{v}_g) = -\phi_g \nabla \cdot \boldsymbol{\sigma}_g - \mathbf{M}_I + \rho_g \phi_g \mathbf{g}$	(3)
$\frac{\partial}{\partial t}(\rho_s \phi_s \mathbf{v}_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \mathbf{v}_s) = -\nabla \cdot \boldsymbol{\sigma}_s - \phi_s \nabla \cdot \boldsymbol{\sigma}_g + \mathbf{M}_I + \rho_s \phi_s \mathbf{g}$	(4)
Volumetric continuity	
$\phi_g + \phi_s = 1$	(5)
Granular energy conservation equation	
$\frac{3}{2} \left[\frac{\partial}{\partial t}(\rho_s \phi_s \Theta) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \Theta) \right] = -\boldsymbol{\sigma}_s : \nabla \mathbf{v}_s + \nabla \cdot (\kappa_s \nabla \Theta) + \Gamma_{\text{slip}} - J_{\text{coll}} - J_{\text{vis}}$	(6)
Closures	
Deviatoric stresses	
$\boldsymbol{\sigma}_\ell = [P_\ell - (\lambda_\ell + \frac{2}{3}\mu_\ell)(\nabla \cdot \mathbf{v}_\ell)] \mathbf{I} - 2\mu_\ell \mathbf{s}_\ell \quad \text{for } \ell = g, s$	(7)
$\mathbf{s}_\ell = \frac{1}{2}[\nabla \mathbf{v}_\ell + (\nabla \mathbf{v}_\ell)^T] - \frac{1}{3}(\nabla \cdot \mathbf{v}_\ell) \mathbf{I} \quad \text{for } \ell = g, s$	(8)
$\mu_g = \text{constant} \quad \lambda_g = 0$	(9)
$\mu_s = \frac{(2+\eta)}{3} \left\{ \frac{\zeta^*}{g_0 \eta (1-\eta)} (1 + \frac{8}{5} \phi_s \eta g_0) (1 + \frac{8}{5} \eta (3\eta - 2) \phi_s g_0) + \frac{8}{5} \eta \mu_b \right\} \quad \lambda_s = \eta \mu_b - \frac{2}{3} \mu_s$	(10)
$\mu_b = \frac{256 \zeta^* g_0}{5\pi} \quad \zeta^* = \frac{\zeta}{1 + \frac{2\mu_s}{(\rho_s \phi_s)^2 g_0 \Theta}} \quad \zeta = \frac{5\rho_s d_p (\pi \Theta)^{1/2}}{96} \quad \alpha = 1.6$	(11)
$\eta = \frac{1+\epsilon}{2} \quad g_0 = \frac{1}{1 - \left(\frac{\phi_s}{\phi_{s,\text{max}}} \right)^{1/3}} \quad \phi_{s,\text{max}} = 0.65$	(12)
Pressure of the solid phase	
$P_s = \rho_s \phi_s (1 + 4\eta \phi_s g_0) \Theta$	(13)
Drag force	
$\mathbf{M}_I = \beta (\mathbf{v}_g - \mathbf{v}_s)$	(14)
$\beta = \frac{3}{4} C_D \frac{\rho_g \phi_g \mathbf{v}_g - \mathbf{v}_s }{(d_p \text{Re}_p)} (\phi_g)^{-2.65}$	(15)
$C_D = \begin{cases} \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687}) & \text{for } \text{Re}_p < 1000 \\ 0.44 & \text{for } \text{Re}_p \geq 1000 \end{cases}$	(16)
$\text{Re}_p = \frac{ \mathbf{v}_g - \mathbf{v}_s d_p \rho_g \phi_g}{\mu_g}$	(17)
Granular thermal conductivity	
$\kappa_s = \frac{\gamma}{g_0} \left\{ (1 + \frac{12}{5} \eta \phi_s g_0) (1 + \frac{12}{5} \eta^2 (4\eta - 3) \phi_s g_0) + \frac{64}{25\pi} (41 - 33\eta) \eta^2 \phi_s^2 g_0^2 \right\}$	(18)
$\gamma^* = \frac{\gamma}{1 + \frac{6\mu_s}{5(\rho_s \phi_s)^2 g_0 \Theta}} \quad \gamma = \frac{75\rho_s d_p (\pi \Theta)^{1/2}}{48\eta (41 - 33\eta)}$	(19)
Granular energy production rate by gas-particle slip, and dissipation rates by collisional and viscous damping	
$\Gamma_{\text{slip}} = \frac{81\phi_s \mu_s^2}{g_0 d_p^2 \rho_s (\pi \Theta)^{1/3}} \quad J_{\text{coll}} = \frac{48}{\pi^{1/2}} \eta (1 - \eta) \frac{\rho_g \phi_g^2}{d_p} \Theta^{3/2} \quad J_{\text{vis}} = 3\beta \Theta$	(20)

Table 2

Filtered two-fluid model - conservative equations and closures for filtered and residual stresses (a complete formulation can be found in Mouallem et al., 2018).

Filtered continuity and momentum conservation equations	
$\frac{\partial}{\partial t}(\rho_g \bar{\phi}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \bar{\mathbf{v}}_g) = 0$	(26)
$\frac{\partial}{\partial t}(\rho_s \bar{\phi}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \bar{\mathbf{v}}_s) = 0$	(27)
$\frac{\partial}{\partial t}(\rho_g \bar{\phi}_g \bar{\mathbf{v}}_g) + \nabla \cdot (\rho_g \bar{\phi}_g \bar{\mathbf{v}}_g \bar{\mathbf{v}}_g) = -\bar{\phi}_g \nabla \cdot \tilde{\boldsymbol{\sigma}}_g - \nabla \cdot \tilde{\boldsymbol{\tau}}'_g - (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_g \bar{\phi}_g \mathbf{g}$	(28)
$\frac{\partial}{\partial t}(\rho_s \bar{\phi}_s \bar{\mathbf{v}}_s) + \nabla \cdot (\rho_s \bar{\phi}_s \bar{\mathbf{v}}_s \bar{\mathbf{v}}_s) = -\nabla \cdot \tilde{\boldsymbol{\sigma}}_s - \nabla \cdot \tilde{\boldsymbol{\tau}}'_s - \bar{\phi}_s \nabla \cdot \tilde{\boldsymbol{\sigma}}_g + (\mathbf{B}'_{gs} + \bar{\mathbf{M}}_I) + \rho_s \bar{\phi}_s \mathbf{g}$	(29)
Closures for filtered deviatoric and residual stresses	
$\tilde{\boldsymbol{\sigma}}_g = \left[\tilde{P}_g - (\lambda_g + \frac{2}{3}\mu_g)(\nabla \cdot \bar{\mathbf{v}}_g) \right] \mathbf{I} - 2\mu_g \tilde{\mathbf{s}}_g = P_{\text{fil},g} \mathbf{I} - 2\mu_{\text{fil},g} \tilde{\mathbf{s}}_g$	(30)
$\tilde{\boldsymbol{\sigma}}_s = \left[\tilde{P}_s - (\lambda_s + \frac{2}{3}\mu_s)(\nabla \cdot \bar{\mathbf{v}}_s) \right] \mathbf{I} - 2\mu_s \tilde{\mathbf{s}}_s = P_{\text{fil},s} \mathbf{I} - 2\mu_{\text{fil},s} \tilde{\mathbf{s}}_s$	(31)
$\tilde{\boldsymbol{\tau}}'_\ell = \rho_\ell \bar{\phi}_\ell \tilde{\mathbf{v}}_\ell \tilde{\mathbf{v}}_\ell - \rho_\ell \bar{\phi}_\ell \tilde{\mathbf{v}}_\ell \tilde{\mathbf{v}}_\ell = P_{\text{res},\ell} \mathbf{I} - 2\mu_{\text{res},\ell} \tilde{\mathbf{s}}_\ell \quad \text{for } \ell = g, s$	(32)
$\tilde{\mathbf{s}}_\ell = \frac{1}{2}[\nabla \bar{\mathbf{v}}_\ell + (\nabla \bar{\mathbf{v}}_\ell)^T] - \frac{1}{3}(\nabla \cdot \bar{\mathbf{v}}_\ell) \mathbf{I} \quad \text{for } \ell = g, s$	(33)
From the above closures	
$P_{\text{fil},g} = \tilde{P}_g - \frac{2}{3}\mu_g(\nabla \cdot \bar{\mathbf{v}}_g) \quad (\text{assuming } \lambda_g = 0)$	(34)
$\mu_{\text{fil},g} = \mu_g$	(35)
$P_{\text{fil},s} = \tilde{P}_s - (\lambda_s + \frac{2}{3}\mu_s)(\nabla \cdot \bar{\mathbf{v}}_s)$	(36)
$\mu_{\text{fil},s} = \mu_s$	(37)
$P_{\text{res},\ell} = \frac{1}{3} \text{tr}(\tilde{\boldsymbol{\tau}}'_\ell)$	(38)
$\mu_{\text{res},\ell} = \frac{ \tilde{\boldsymbol{\tau}}'_{\text{shear},\ell} }{2 \tilde{\mathbf{s}}_{\text{shear},\ell} }$	(39)
where for the above symmetric tensors (accounting for shear components only since normal components are much larger and hinder shear effects),	
$ \mathbf{E}_{\text{shear}} = \sqrt{\frac{1}{2} \sum_{i,j} (E_{ij} - E_{ji})^2}$	(40)

accounting for heterogeneity extent, and proposed new sub-grid models. Agrawal et al. (2013) and Schneiderbauer and Pirker (2014) followed the same path as Milioli et al. (2013), and found similar results. Sarkar et al. (2016) proposed new sub-grid models also following the work of Milioli et al. (2013), except that based on results of 3D highly resolved simulations, while the latter practiced 2D simulations. Their correlations provide results qualitatively similar to those of Milioli et al. (2013), with some quantitative differences.

All the works cited before, aiming for sub-grid modeling, were based on highly resolved simulations performed under suspension like conditions, which were assumed relevant for any possible macro-scale flow condition. Rigorously speaking, this would be true only in a condition where scale separation prevails, which does not stand for gas-solid fluidization (van der Hoef et al., 2006). In fact, literature presents a number of works showing evidences of effects of macro-scale conditions over the flow topology as well as over filtered results. The simulations of Milioli and Milioli (2011), which were performed under accelerated gas flows and dilute conditions, showed a significant effect of the gas flow Reynolds number over both topology and filtered parameters. Parmentier et al. (2012) simulated a bubbling bed condition and proposed filtered models including a macro-scale length parameter in their filter size dependency; they also proposed a dynamical adjustment correction procedure when applying their filtered models in large-scale simulations. Özel et al. (2013) also simulated bubbling bed conditions, and derived filtered models which needed further corrections through dynamical adjustment. The need for macro-scale accountancy in sub-grid modeling is also acknowledged in various works applying energy minimization multi-scale approaches (e.g. Li and Kwauk, 1994). Wang and Li (2007) and Qi et al. (2007), for instance, identified gas flow rate, solids flux and solids inventory as relevant macro-scale parameters to be accounted for, while Wang et al. (2011) identified local parameters such as gas pressure gradients and phase velocities as capable of inserting macro-scale effects into sub-grid models.

In the present work results are presented of an investigation on the effects of macro-scale features over filtered and residual stresses. Highly resolved simulations with microscopic two-fluid modeling were performed over periodic domains. Various domain average gas flow rates were applied for conditions ranging from suspensions up to pneumatic transport, under domain average solid volume fractions typical of dilute riser flows. All the analyses were performed for flow conditions inside the statistical steady state regime. The results show that filtered and residual pressures and viscosities of both the phases are considerably affected by the imposed macro-scale conditions (i.e. domain average solid volume fraction, and domain average gas Reynolds number).

2. Microscopic and filtered two-fluid models

Conservative equations in two-fluid modeling are derived through a trivial straightforward procedure (see, for instance, Ishii, 1975; Enwald et al., 1996). In summary, integral conservative balances are performed over volumes containing both the phases separated by an interface. Thereafter, the theorems of Leibniz and Gauss are applied over the integral balances to provide local instantaneous differential equations and jump conditions. Then, averaging procedures are applied so that the continuum hypothesis holds for each phase, rendering interface interactions as field effects of one phase over the other. The so called microscopic formulation is implemented when microscopic closures are added to the set of conservative equations. In the present work a hydrodynamic microscopic two-fluid formulation is resolved providing meso-scale predictions, from which filtered and residual stresses

are derived. For the sake of completeness, both the microscopic and the filtered two-fluid approaches are briefly described next. The respective formulations are presented in Tables 1 and 2. The filtered formulation presented in Table 2 is partial, emphasizing only the parameters of current concern (a complete formulation can be found in Mouallem et al., 2018).

Table 1 presents the hydrodynamic two-fluid model as derived by Anderson and Jackson (1967) together with microscopic closures that are required, as proposed by Agrawal et al. (2001). Those closures include viscous stresses and pressure of the solid

Fig. 1. Dimensionless filtered solid pressure, $P_{fil,s}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (◁), 12.23 (◇), 16.30 (▷), 20.34 (□) and 24.45 (▽), for the domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (a), 0.15 (b), and 0.25 (c). The results stand for the dimensionless filtered axial slip velocity $\bar{v}_{slip,y}/v_t = 0.47$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

phase (a continuum that replaces the particulate) as well as inter-phase field effects. Pressure and viscosities of the solid phase are expressed as functions of a granular temperature, following the so called kinetic theory of granular flows, formulated in analogy with the kinetic theory of dense gases (Jenkins and Savage, 1983; Lun et al., 1984; Gidaspow, 1994; Garzó and Dufty, 1999). A conservation equation for the so called granular energy (or pseudo-thermal energy) provides the granular temperature (in analogy with the conventional energy conservation equation,

which provides the thermodynamic temperature). In this work the kinetic theory of granular flows as developed by Lun et al. (1984) is considered, as described in Agrawal et al. (2001). The hydrodynamic microscopic formulation also includes closures for the interphase momentum exchanges, which are mostly dominated by drag in usual applications. Here, the gas-solid interface interactions are described by a generalized drag effect of the gas over the solid, by applying the drag model of Wen and Yu (1966), just as described in Agrawal et al. (2001). The currently applied microscopic two-fluid formulation does not include any turbulence model whatsoever because: i. Concerning the solid phase, all the space and time scales are expected to be captured since highly resolved simulations are intended (Sundaresan, 2000); and ii. Concerning the gas phase, no significant sub-grid turbulence effect of the gas over the solid is expected since only high Stokes number conditions are to be practiced (e.g. Fede and Simonin, 2006).

The conservative equations of the hydrodynamic filtered two-fluid model, given in Table 2, are derived by applying space filtering operators over the counterpart equations of the microscopic formulation. In filtered formulations any dependent variable, $f(\mathbf{x}, t)$, is defined as

$$f(\mathbf{x}, t) = \bar{f}(\mathbf{x}, t) + f'(\mathbf{x}, t) \quad (21)$$

Fig. 2. Dimensionless filtered solid dynamic viscosity, $\mu_{fli,s}/(\rho_s v_t^3/g)$, as a function of the filtered solid volume fraction, ϕ_s , for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (◄), 12.23 (◇), 16.30 (◁), 20.34 (□) and 24.45 (▽), for the domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (a), 0.15 (b), and 0.25 (c). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.47$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

Fig. 3. Dimensionless filtered granular temperature, $\bar{\Theta}/v_t^2$, as a function of the filtered solid volume fraction, ϕ_s . (a) for the domain average solid volume fraction $\langle \phi_s \rangle = 0.15$, and gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (◄), 12.23 (◇), 16.30 (◁), 20.34 (□) and 24.45 (▽). (b) for $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 20.34$, and $\langle \phi_s \rangle = 0.05$ (gray symbol), 0.15 (black symbol) and 0.25 (white symbol). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.47$, and for the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

where at the right hand side, the first term accounts for the filtered variable, and the second term accounts for its sub-grid fluctuation or unresolved part. The filtered variable is given by

$$\bar{f}(\mathbf{x}, t) = \int_{\mathbf{x}} f(\mathbf{x}, t) G(\mathbf{x}) d(\mathbf{x}) \quad (22)$$

where $G(\mathbf{x})$ is a sub-grid space cut limiting the smaller scales that are resolved, which usually matches with the numerical grid volume V . In this way, $G(\mathbf{x}) = 1/V$ for any $\mathbf{x} \in V$. Following those definitions, it comes that

$$\bar{f}(\mathbf{x}, t) = \frac{1}{V} \int_V f(\mathbf{x}, t) dV \quad (23)$$

The space filtering operation applied over the two-fluid equations gives rise to some filtered products of dependent variables by phase volume fractions. In those cases Favre or mass weighed averaging is practiced, providing

$$\overline{f_{\ell}(\mathbf{x}, t) \phi_{\ell}(\mathbf{x}, t)} = \tilde{f}_{\ell}(\mathbf{x}, t) \bar{\phi}_{\ell}(\mathbf{x}, t) \quad (24)$$

where ℓ stands for the phase, either gas or solid. From this definition it comes that

$$\tilde{f}_{\ell}(\mathbf{x}, t) = \frac{\int_V \phi_{\ell}(\mathbf{x}, t) f_{\ell}(\mathbf{x}, t) dV}{\int_V \phi_{\ell}(\mathbf{x}, t) dV} \quad (25)$$

3. Simulation and filtering procedure

The simulations in the present work were performed using MFIX, an open source code developed and made available by NETL (National Energy Technology Laboratory, DOE-USA). MFIX is world widely used for gas-solid flow simulations, including highly resolved simulations with microscopic two-fluid modeling (e.g. Agrawal et al., 2001; Andrews IV et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011a,b; Milioli et al., 2013; Agrawal et al., 2013; Sarkar et al., 2016), and has been extensively verified (Syamlal et al., 1993). It is a FORTRAN written code, and its numerical solver is fully parallelized. The conservative equations in MFIX's two-fluid model are discretized by the finite volume method, and are solved through a point by point numerical technique. The discretization of diffusive terms follows the central differencing scheme; while different alternatives are available for advective terms, ranging from the first order upwind to higher order TVD schemes (the Superbee procedure is assumed here following previous works). Both first and second order precision time stepping are available (the first order Euler scheme is assumed here following previous works). The well known SIMPLE algorithm is applied for solving the gas phase pressure-velocity coupling. MFIX's numerical code is fully described in Syamlal (1998).

In the current simulations a typical fluid catalytic cracking particulate was applied, following previous works (Andrews IV et al., 2005; Agrawal et al., 2001; Igci et al., 2008; Igci and Sundaresan, 2011a,b; Milioli et al., 2013; Agrawal et al., 2013). Gas density (ρ_g) and viscosity (μ_g) were set at 1.3 kg/m^3 and

Fig. 4. Time profiles of dimensionless solid and gas axial velocities in a particular numerical cell at the center of the domain, inside the statistical steady state flow regime. (a, b) for the simulations with $\langle \phi_s \rangle = 0.15$, under various gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}}$; (c, d) for the simulations with $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 20.34$, under various $\langle \phi_s \rangle$.

$1.8 \times 10^{-5} \text{ kg/(m s)}$, respectively. Spherical particles were considered, with a diameter (d_p) of $7.5 \times 10^{-5} \text{ m}$, a density (ρ_s) of 1500 kg/m^3 , a terminal settling velocity (v_t) of 0.2184 m/s , a Froude number ($Fr_p = v_t^2/(gd_p)$) of 64.85, and a restitution coefficient (e) of 0.9. For those conditions, Agrawal et al. (2001) showed that numerical grids with sizes between 1 and 2 mm provide filtered results reasonably independent of grid size. Accounting for that, a uniform grid size of $1.25 \text{ mm} \times 1.25 \text{ mm}$ was assumed. A domain size of $16 \text{ cm} \times 16 \text{ cm}$ was adopted, which allows for filter sizes up to about $4 \text{ cm} \times 4 \text{ cm}$ to be considered (under conditions similar to the current, Igci et al. (2008) found that filter sizes up to 1/4 of the domain size provide filtered results independent of domain size). Those figures for domain and grid sizes provide a numerical mesh of 128×128 grids, which guaranties affordable computational cost.

Periodic boundaries were applied in all directions, while average axial gas flow rates and solid inventories were set constants in the various simulations. This procedure allowed for statistical steady state conditions to be attained at the different macro-scale conditions that were imposed: domain average solid volume fractions were enforced in a range typical of riser flows, i.e. $\langle \phi_s \rangle = 0.05, 0.15$ and 0.25 ; and domain average gas Reynolds numbers were enforced in a range from suspensions up to pneumatic transport, i.e. $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 1.0, 4.08, 8.15, 12.23, 16.30, 20.34$ and 24.45 . Here, $\langle Re_g \rangle$ stands for the domain average gas Reynolds number, defined as

$$\langle Re_g \rangle = \frac{\rho_g \langle \phi_g \rangle \langle v_{g,y} \rangle d_p}{\mu_g} \quad (41)$$

The domain average gas Reynolds number at suspension like conditions, $\langle Re_g \rangle_{\text{susp}}$, is attained by imposing an axial gas pressure gradient over the domain that exactly matches the gravity acting on the gas-solid mixture, which is given by

$$\frac{\Delta P_g}{Y_{\text{length}}} = \rho_s \langle \phi_s \rangle g + \rho_g \langle \phi_g \rangle g \quad (42)$$

Here, Y_{length} stands for the length of the domain in the axial direction. In the current simulations $\langle \phi_s \rangle$ was enforced through

Fig. 5. $P_{\text{res},s}/(\rho_s v_t^2)$ (a), $\mu_{\text{fil},s}/(\rho_s v_t^3/g)$ (b), as a function of the filtered solid volume fraction, ϕ_s , for the domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (gray symbols), 0.15 (black symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 1$ (○) and 20.34 (□). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{\text{slip},y}/v_t = 0.47$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

Fig. 6. Dimensionless residual solid and gas pressures, $P_{\text{res},i}/(\rho_s v_t^2)$, as a function of the filtered solid volume fraction, ϕ_s , for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{\text{susp}} = 1$ (■), 4.08 (○), 8.15 (◁), 12.23 (◇), 16.30 (▷), 20.34 (□) and 24.45 (▽), for the domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (a), 0.15 (b), and 0.25 (c). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{\text{slip},y}/v_t = 0.47$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

the initial conditions (remaining constant in the runs owing to mass conservation and periodic boundaries), while $\langle Re_g \rangle$ was enforced through a boundary condition that imposes the gas flux as a constant over the domain (except for suspension like conditions, where an axial gas pressure gradient was imposed).

From the discrete fields of dependent variables provided by the simulations, filtered data were derived and classified by gaps (narrow ranges) of filtered parameters that were assumed as independent variables, named markers (following Milioli et al. (2013)), the filtered solid volume fraction and the filtered slip velocity were taken as 1st and 2nd markers, respectively). The combinations of markers' narrow ranges defined bins on which filtered data were stored and averaged. Following Sarkar et al. (2016), 64 gaps were taken for the 1st marker and 80 gaps for the 2nd marker, defining a binning resolution that was found adequate. Filtering and binning are usual procedures that are well described, for instance, in van der Hoef et al. (2006) and Igci et al. (2008). In summary, a suitable number of successive snapshots over the whole domain are taken inside the statistical steady state flow regime so that good statistics are provided. Filtering consists of making a window (filter) to move all over the domain, in space and time, while collecting inside averages. Simultaneously to filtering, binning is also performed by statistically averaging the filtered data inside the various bins.

The procedure of data collecting and storing provided filtered data classified as a function of the 1st and 2nd markers, besides filter size. In addition, a whole collection of such results was made available for each $\langle Re_g \rangle$ and $\langle \phi_s \rangle$ that were practiced, as those macro-scale parameters were set constants in the various simulations. In previous works, since scale separation was assumed to stand, filtered results for simulations under different $\langle \phi_s \rangle$, as low as 0.01 and as high as 0.58, were statistically merged together (Igci et al., 2008; Igci and Sundaresan, 2011a,b; Milioli et al., 2013; Agrawal et al., 2013; Sarkar et al., 2016). In this way, statistically speaking, it is assumed that any particular window with given filtered solid volume fraction and filtered slip velocity provides the same filtered results for any particular parameter, irrespective of the macro-scale condition dictated by $\langle \phi_s \rangle$. In this work, however, no merging of results for different macro-scale conditions was made, since the current interest is just turned to evaluating effects of different macro-scale conditions. In other words, the scale separation hypothesis is abolished.

4. Results and discussion

Analyses including instantaneous grayscale plots of solid volume fraction, time evolution profiles of domain average velocities, and effective drag coefficient behavior, all coming out from the current simulations were already reported in Mouallem et al. (2018). Some results on filtered and residual stresses were also reported, which are now extended and more comprehensively analyzed.

For all the simulated cases, a time interval of 10 s inside the statistical steady state regime was found enough for gathering good statistics. $\langle Re_g \rangle_{susp}$ resulted 4.42, 2.26 and 0.96, for the runs with $\langle \phi_s \rangle = 0.05$, 0.15 and 0.25, respectively. Suspensions under higher solid fractions give rise to lower gas Reynolds numbers owing to a more intense damping on the gas by the solid in domains with more solid. Following previous literature (Agrawal et al., 2001; Andrews IV et al., 2005; Igci et al., 2008), particle density (ρ_s), terminal settling velocity of a particle (v_t) and gravity acceleration (g) were assumed as the characteristic scales for density, velocity and gravity, respectively. Accordingly, the characteristic time and length scales result v_t/g and v_t^2/g , respectively; and the character-

istic scales for stresses (and pressures), viscosities, strain rates and granular temperature result $\rho_s v_t^2$, $\rho_s v_t^3/g$, g/v_t and v_t^2 , respectively.

Results are presented next for filtered and residual stresses and related parameters, for the various $\langle \phi_s \rangle$ and $\langle Re_g \rangle_{susp}$ that were enforced, as functions of the 1st marker (the filtered solid volume fraction, $\bar{\phi}_s$), for a particular narrow range of the 2nd marker (the dimensionless filtered axial slip velocity, $\tilde{v}_{slip,y}/v_t = 0.47 \pm 0.04$, where $\tilde{v}_{slip,y} = \tilde{v}_{g,y} - \tilde{v}_{s,y}$), and for a particular value of the dimensionless filter size ($\Delta_f/(v_t^2/g) = 4.112$, meaning a

Fig. 7. Dimensionless residual solid and gas dynamic viscosities, $\mu_{res,\ell}/(\rho_s v_t^3/g)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for gas Reynolds number ratios $\langle Re_g \rangle/\langle Re_g \rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (☆), 20.34 (□) and 24.45 (▽), for the domain average solid volume fractions $\langle \phi_s \rangle = 0.05$ (a), 0.15 (b), and 0.25 (c). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.47$, and the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

2 cm $\times$ 2 cm filter size). The selected value of $\Delta_f/(v_t^2/g)$ matches with grid sizes usual to large scale simulations, while the selected narrow range of $\tilde{v}_{slip,y}/v_t$ is one of high predominance in all of the currently simulated cases (as showed in Mouallem et al., 2018). Effects of filter size as well as of the current 1st and 2nd markers were already extensively analyzed in previous works (Igci et al., 2008; Igci and Sundaresan, 2011a,b; Milioli et al., 2013; Agrawal et al., 2013; Sarkar et al., 2016), and will not be further considered here. Instead, the oncoming analyses concentrate on the effects of the macro-scale parameters $\langle\phi_s\rangle$ and $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$ that were imposed. It is remarked, however, that results for filter sizes and filtered slip velocities other than the presently considered show similar behavior to those currently analyzed, and can be found elsewhere (Mouallem et al., 2018; Chavez-Cussy, 2017).

Figs. 1 and 2 show effects of the domain average gas Reynolds number over the dimensionless filtered pressure and viscosity of the solid phase, $P_{fil,s}$ and $\mu_{fil,s}$, for different domain average solid volume fractions. As seen, there are very significant effects of the domain average gas Reynolds number over both the filtered parameters. As $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$ increases from 1 to 24.45, $P_{fil,s}$ decreases by up to two orders of magnitude, while $\mu_{fil,s}$ decreases by up to one order of magnitude, for $\langle\phi_s\rangle = 0.15$ and 0.25. A systematic correlation is observed, with the profiles becoming closer as the gas Reynolds number grows higher. The effect of $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$ over $P_{fil,s}$ and $\mu_{fil,s}$ becomes less clear and non-systematic for $\langle\phi_s\rangle = 0.05$. Clearly, the response of $P_{fil,s}$ and $\mu_{fil,s}$ to $\langle Re_g\rangle$ ultimately comes from the correlation of those parameters to the filtered granular temperature. At the micro-scale, the solid

pressure and viscosity derived from the kinetic theory of granular flows (as considered in the present simulations) are both strong functions of the granular temperature (Eqs. (10) and (13)). At the meso-scale, as a consequence, the counterpart filtered parameters also become strong functions of the filtered granular temperature. The observed decreasing of $P_{fil,s}$ and $\mu_{fil,s}$ as $\langle Re_g\rangle$ grows higher is, indeed, a consequence of the filtered granular temperature growing lower. Fig. 3a illustrates the dropping on granular temperature as $\langle Re_g\rangle$ increases for the simulations with $\langle\phi_s\rangle = 0.15$, under the same conditions as in Figs. 1b and 2b. The observed behavior of the filtered granular temperature is actually quite expected, owing to the more homogeneous conditions provided by the higher domain average gas Reynolds numbers (as showed and discussed in Mouallem et al., 2018). Under more homogeneous conditions all field fluctuations become smaller, including those of solid velocity fluctuations that define the granular temperature. An illustration of this fact is provided in Fig. 4a, which shows time evolution profiles of the dimensionless solid axial velocity in a particular numerical cell at the center of the domain, inside the statistical steady state flow regime, for simulations with $\langle\phi_s\rangle = 0.15$, under various gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$. It is quite clear that the solid axial velocity fluctuations become attenuated at higher domain average gas Reynolds numbers, with the related variance dropping from 13.52 to 2.07 as $\langle Re_g\rangle/\langle Re_g\rangle_{susp}$ is raised from 1 to 24.45.

The domain average solid volume fraction also affects considerably the filtered pressure and viscosity of the solid phase. This trend is showed in Fig. 5 for the cases with $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ and

Fig. 8. Solid phase dimensionless residual stresses, $|\tau'_{ij,s}|/(\rho_s v_t^2)$, and scalar shear rate, $|s_{shear,s}|/(g/v_t)$, as a function of the filtered solid volume fraction, ϕ_s , for gas Reynolds number ratios $\langle Re_g\rangle/\langle Re_g\rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (▽), 20.34 (□) and 24.45 (▽). The results stand for the domain average solid volume fractions $\langle\phi_s\rangle = 0.15$, for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.47$, and for the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

20.34, where $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 were considered. As seen, there is a significant systematic effect of $\langle\phi_s\rangle$ over both $P_{fil,s}$ and $\mu_{fil,s}$, which grows higher at higher $\bar{\phi}_s$. As $\langle\phi_s\rangle$ goes from 0.05 to 0.25 , both $P_{fil,s}$ and $\mu_{fil,s}$ come down by at least one order of magnitude, the effect being much stronger at higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$. The observed dropping on $P_{fil,s}$ and $\mu_{fil,s}$ as $\langle\phi_s\rangle$ goes higher is, again, due to lower granular temperatures caused by lower solid velocity fluctuations (the same way as it happens when $\langle Re_g \rangle$ grows higher). Fig. 3b illustrates the dropping of the filtered granular temperature at increasing $\langle\phi_s\rangle$ for $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 20.34$. This is just an effect of the resulting smaller solid velocity fluctuations as $\langle\phi_s\rangle$ grows up, which is illustrated in Fig. 4c. As seen, the solid axial velocity fluctuations (in a particular numerical cell at the center of the domain) become much smaller at higher domain average solid volume fractions, with the concerning variance dropping from 67.16 to 0.66 as $\langle\phi_s\rangle$ is increased from 0.05 to 0.25 .

All the previous observations on the behavior of $P_{fil,s}$ and $\mu_{fil,s}$, ultimately related to the response of those parameters to the solid phase velocity fluctuations, also stand for the residual pressure and viscosity of the solid phase, $P_{res,s}$ and $\mu_{res,s}$. The lower solid velocity fluctuations that prevail at higher domain average gas Reynolds numbers and higher solid volume fractions (Fig. 4a and c), which give rise to lower filtered granular temperatures (Fig. 3a and b), also cause lower residual stresses in the solid phase and, therefore, lower residual pressure and viscosity of this phase. Eqs. (38) and (39) define the concerning relationships. Figs. 6 and 7 show the effects of the domain average gas Reynolds number over $P_{res,s}$ and $\mu_{res,s}$, for different domain average solid volume fractions.

The profiles of $P_{res,s}$ and $\mu_{res,s}$ are similar to those of $P_{fil,s}$ and $\mu_{fil,s}$, despite the disparity in order of magnitude (as previously noticed by Agrawal et al., 2001). Just as seen for $P_{fil,s}$ and $\mu_{fil,s}$, an increasing of $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ from 1 to 24.45 , for both $\langle\phi_s\rangle = 0.15$ and 0.25 , causes $P_{res,s}$ to decrease by up to two orders of magnitude and $\mu_{res,s}$ to decrease by up to one order of magnitude. Again, a systematic correlation is observed, with profiles becoming closer to each other at higher gas Reynolds numbers (and again, the effect of the domain average gas Reynolds number becomes unclear and non-systematic for $\langle\phi_s\rangle = 0.05$). Fig. 8 illustrates how the normal and shear residual stresses of the solid phase are affected by the domain average gas Reynolds number for the simulations under $\langle\phi_s\rangle = 0.15$. It is quite clear the significant decrease of the solid normal and shear residual stresses as $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ increases (Fig. 8a–c). Fig. 8 also shows the behavior of the dimensionless filtered scalar shear rate of the solid phase (Fig. 8d), which also considerably decreases with increasing domain average gas Reynolds numbers. A feature to notice is that the dimensionless shear residual stress, the dimensionless filtered scalar shear rate, and also the ratio between them (i.e. the residual viscosity, given in Fig. 7) all drop with increasing $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$. This means that, even though in the same direction, the effect of the domain average gas Reynolds number is stronger on the shear residual stress than it is on the filtered scalar shear rate.

Just as seen for $P_{fil,s}$ and $\mu_{fil,s}$, $\langle\phi_s\rangle$ also considerably affects $P_{res,s}$ and $\mu_{res,s}$. Fig. 10 shows that trend for the cases with $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ and 20.34 , under $\langle\phi_s\rangle = 0.05, 0.15$ and 0.25 . The effect of $\langle\phi_s\rangle$ over both $P_{res,s}$ and $\mu_{res,s}$ grows higher at higher $\bar{\phi}_s$, just as seen

Fig. 9. Gas phase dimensionless residual stresses, $|\tau'_{ij,g}|/(\rho_s v_t^2)$, and scalar shear rate, $|s'_{shear,g}|/(g/v_t)$, as a function of the filtered solid volume fraction, $\bar{\phi}_s$, for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ (■), 4.08 (○), 8.15 (△), 12.23 (◇), 16.30 (▽), 20.34 (□) and 24.45 (▽). The results stand for the domain average solid volume fractions $\langle\phi_s\rangle = 0.15$, for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y}/v_t = 0.47$, and for the dimensionless filter size $\Delta_f/(v_t^2/g) = 4.112$.

for $P_{fil,s}$ and $\mu_{fil,s}$. Again, as $\langle\phi_s\rangle$ rises from 0.05 to 0.25, both $P_{res,s}$ and $\mu_{res,s}$ decrease by at least one order of magnitude, the effect being much stronger at higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$. The dropping on $P_{res,s}$ and $\mu_{res,s}$ at higher $\langle\phi_s\rangle$ comes as a result of the observed lower solid velocity fluctuations (as illustrate in Fig. 4c, as already mentioned).

All the previous analyses were performed for the solid phase. Most of the discussions, however, also stand for the gas phase. This is so for the gas velocity fluctuations in Fig. 4b and d, which are just alike and of the same order of magnitude as those for the solid velocity fluctuations given in Fig. 4a and c. The residual pressures and viscosities of the phases given in Figs. 6 and 7 present some resemblances as well as disagreements. Both ($P_{res,g}$ and $\mu_{res,g}$) and ($P_{res,s}$ and $\mu_{res,s}$) considerably decrease at higher $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$, while the parameters for the gas phase are of lower order of magnitude. Also, while ($P_{res,s}$ and $\mu_{res,s}$) naturally grow at larger filtered solid volume fractions, the opposite naturally happens for ($P_{res,g}$ and $\mu_{res,g}$) owing to the relatively lower presence of gas. The lower order of magnitude of ($P_{res,g}$ and $\mu_{res,g}$) is a consequence of the lower order of magnitude of the residual stresses on the gas phase, as observed in Fig. 9, as compared to those for the solid phase, given in Fig. 8. Regarding the effect of $\langle\phi_s\rangle$ over ($P_{res,g}$ and $\mu_{res,g}$), the same behavior is observed as that for the solid phase, as seen in Fig. 10.

A number of additional issues may be raised regarding the current results. i. A feature showed in many graphs (Figs. 1–3, 6–9) is

Fig. 10. $P_{res,\epsilon} / (\rho_s v_t^2)$ (a), $\mu_{res,\epsilon} / (\rho_s v_t^3 / g)$ (b), as a function of the filtered solid volume fraction, ϕ_s , for the domain average solid volume fractions $\langle\phi_s\rangle = 0.05$ (gray symbols), 0.15 (black symbols) and 0.25 (white symbols), for gas Reynolds number ratios $\langle Re_g \rangle / \langle Re_g \rangle_{susp} = 1$ ($\circ$) and 20.34 ($\square$). The results stand for the dimensionless filtered axial slip velocity $\tilde{v}_{slip,y} / v_t = 0.47$, and the dimensionless filter size $\Delta_f / (v_t^2 / g) = 4.112$.

that profiles mostly approach each other at both very high and very low filtered solid volume fractions (as compared to the domain average). This reveals an inside-filter topology that becomes independent of the domain average gas Reynolds number as the filtered solid volume fraction goes to extremes. ii. There is a particular behavior among the various profiles of the various filtered parameters that deserve some thought. Such behavior can be observed by comparing the (b) against the (c) graphs of Figs. 1, 2, 6 and 7 (the same trend is seen in graphs for various other filtered slip velocities and filter sizes, not showed). The (b) graphs stand for a domain average solid volume fraction of 0.15, while the (c) graphs stand for 0.25. In the (b) graphs a gap arises between the profiles of the filtered parameters when $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ reaches 12.23, while in the (c) graphs this gap is anticipated and arises when $\langle Re_g \rangle / \langle Re_g \rangle_{susp}$ reaches 8.15. This change of behavior among the profiles may come as a result of some topology evolution towards a more homogeneous condition, which would happen at different domain average gas Reynolds numbers depending on the domain average solid volume fraction. iii. As largely evidenced in the previous analyses, field fluctuations become quite attenuated at high gas Reynolds number conditions, leading to lower filtered and residual stresses. At higher gas flow rates there is a growing damp effect by the gas affecting interparticle interactions that define properties of the solid phase, ultimately leading to decreased stresses. It should be noted that such a behavior is opposite to what happens in mono-phase turbulence. iv. Some non-systematic behavior is seen among the results, specially for the higher domain average gas Reynolds number ratios (above 20.34) and also for the lower domain average solid volume fraction (0.05). This possibly means that the markers that were considered (filtered solid volume fraction and filtered slip velocity), which provide for systematicity in most of the present situations, seem to fail as approaching more extreme conditions.

5. Summary and conclusions

The hydrodynamic simulation of large-scale gas-solid fluidized flows can be performed through filtered two-fluid formulations, which require sub-grid closures to deal with filtered interphase momentum exchanges as well as filtered and residual stresses. While momentum exchanges are of outmost relevance since providing for the actual flow driving force, stresses also play a role on shaping the heterogeneous topology that develops (length and time scales associated to coherent structures considerably depend on phase stresses). Clearly, filtered stresses cannot be disregarded in large-scale simulations, and must be correlated to sub-grid parameters alongside with any filtered interphase momentum exchanges.

Literature brings sub-grid closure models that are derived by filtering over results of meso-scale highly resolved simulations with microscopic two-fluid modeling, where filtered and residual stresses (alongside with other relevant filtered parameters such as the effective drag coefficient) are correlated to other filtered parameters that are assumed as independent variables. Those models usually correlate filtered parameters to other inside filtered parameters alone, taking no account of any macro-scale conditions from the outside of the filtered region. This assumption is consistent with the scale separation hypothesis which, nevertheless, is known not to stand for fluidized gas-solid flows. In this work an analysis was advanced aiming to reveal the extent at which filtered and residual stresses are affected by the outside filter micro-scale conditions. Following literature, highly resolved simulations with microscopic two-fluid modeling were performed, whose results were taken for the derivation of the concerning sub-grid filtered parameters. In the simulations, two macro-scale parameters associated to flow topology were controlled, namely the domain aver-

age solid volume fraction and the domain average gas flow Reynolds number. The macro-scale parameters were enforced in ranges characteristic of dilute rapid flows, for a particulate typical of fluid catalytic cracking widely studied in previous works.

The simulations were performed over 2D periodical domains with the MFIX's microscopic two-fluid model, with fluid properties for the solid phase provided by Lun's kinetic theory of granular flows (Lun et al., 1984), and interphase momentum exchanges provided by Wen and Yu's drag model (Wen and Yu, 1966). Filtered data were derived from results collected at statistical steady state conditions, covering the whole domain and through a suitable time interval for providing robust statistics. For a particular filter size, the filtered data were then classified and statistically averaged by narrow ranges of assumed independent variables (filtered solid volume fraction and filtered slip velocity, following previous works). Such results were provided for each pair of macro-scale conditions (i.e. domain average solid volume fraction and domain average gas flow Reynolds number) that were imposed.

Results were presented for filtered and residual pressures and viscosities, and very significant effects of both the macro-scale imposed conditions were observed. For both phases, variations of up to two orders of magnitude arose for domain average gas Reynolds numbers varying between suspension conditions and very high gas flow rates approaching pneumatic transport, and domain average solid volume fractions varying between 0.05 and 0.25. The effect of the macro-scale conditions over the velocity fluctuations of both phases was found the one factor responsible for the observed behavior of the filtered and residual pressures and viscosities. It was seen that as the filtered solid volume fraction goes to extremes as compared to its domain average, the filtered and residual stresses become independent of the macro-scale conditions. Changes of topology towards homogeneity, that were observed at higher domain average gas Reynolds numbers, were found to affect the relative systematic behavior among profiles of filtered and residual stresses. Higher domain average gas Reynolds numbers caused lower filtered and residual stresses, owing to lower velocity fluctuations, which opposes mono-phase turbulence behavior. Finally, some non-systematic behavior among profiles was observed both at higher domain average gas Reynolds numbers and lower domain average solid volume fractions, suggesting that, at least for those conditions, the filtered solid volume fraction and the filtered slip velocity require revision as suitable markers for the concerning filtered and residual stresses related parameters.

A final remark is made on the qualitative character of the current results, which were based on 2D simulations. Even though gas-solid fluidized flows are 3D in nature, 2D simulations are widely practiced for their hydrodynamic prediction. This is so owing to two main reasons: i. 2D simulations are recognized as useful tools for qualitative analysis; ii. 3D simulations are frequently unaffordable owing to high computational costs. Qualitative issues aside, it is recognized that the current results require revision on the basis of complementary 3D simulations before new improved sub-grid closure models can be advanced.

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