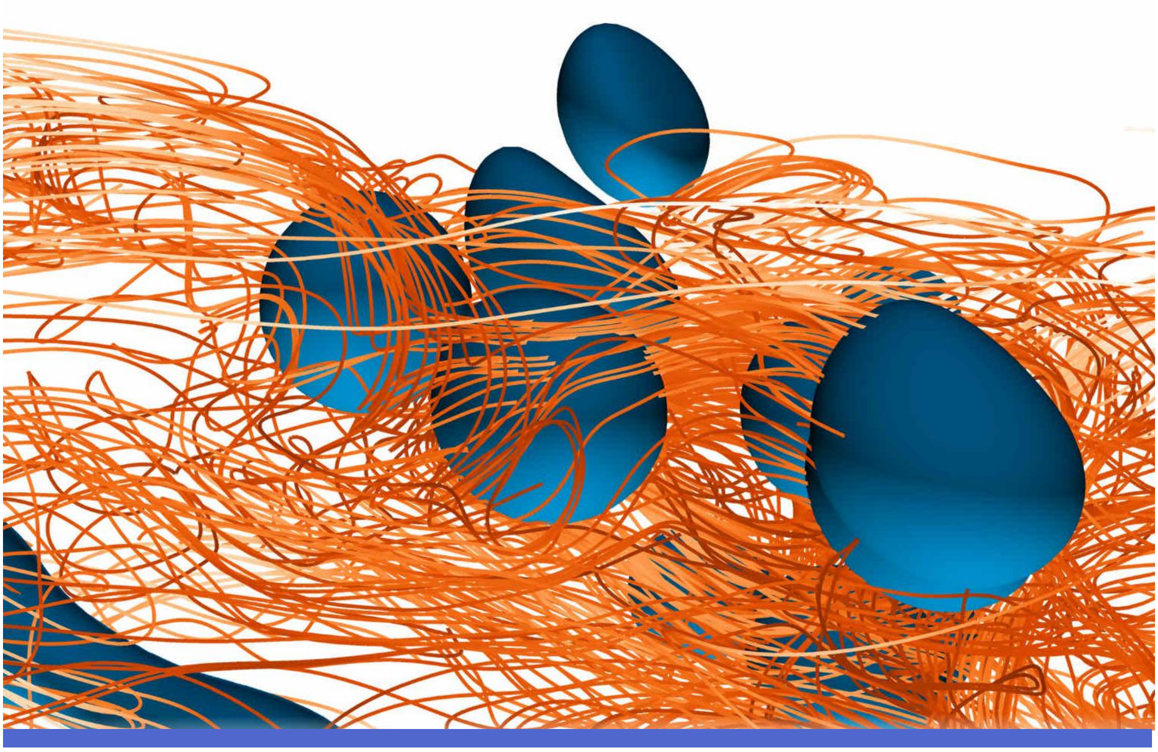
BICTAM-CISM Symposium on Dispersed Multiphase Flows: from Measuring to Modeling



Beijing, China

March 2-5, 2021

http://calliope.dem.uniud.it/BICTAM-CISM/

Cover image: Deformable oil droplets in turbulent channel flow of water (image credits: A. Roccon, A. Soldati, F. Zonta)

SYMPOSIUM SCHEDULE-AT-A-GLANCE

Tuesday, March 2, 2021

EU Time	CHINA Time	
8:15-8:30	15:15-15:30	Welcome Address
8:30-9:00	15:30-16:00	Keynote Lecture: Xiaojing Zheng, China
9:00-10:15	16:00-17:15	Session #1 (regular talks)
10:15-10:30	17:15-17:30	Coffee break
10:30-11:00	17:30-18:00	Keynote Lecture: Alfredo Soldati, Austria
11:00-13:00	18:00-20:00	Session #2 (regular talks)

Wednesday, March 3, 2021

EU Time	CHINA Time	
8:30-9:00	15:30-16:00	Keynote Lecture: Jianzhong Lin, China
9:00-10:30	16:00-17:30	Session #3 (regular talks)
10:30-10:45	17:30-17:45	Coffee break
10:45-11:15	17:45-18:15	Keynote Lecture: Christian Poelma, Netherlands
11:15-13:00	18:15-20:00	Session #4 (regular talks)

Thursday, March 4, 2021

EU Time	CHINA Time	
8:30-9:00	15:30-16:00	Keynote Lecture: Mingjiu Ni, China
9:00-10:30	16:00-17:30	Session #5 (regular talks)
10:30-10:45	17:30-17:45	Coffee break
10:45-11:15	17:45-18:15	Keynote Lecture: Eric Climent, France
11:15-13:00	18:15-20:15	Session #6 (regular talks)

Friday, March 5, 2021

EU Time	CHINA Time	
8:30-9:00	15:30-16:00	Keynote Lecture: Haitao Xu, China
9:00-10:45	16:00-17:45	Session #7 (regular talks)
10:45-11:00	17:45-18:00	Coffee break
11:00-11:30	18:00-18:30	Keynote Lecture: Wolfgang Schröder, Germany
11:30-13:00	18:30-20:00	Session #8 (regular talks)
13:00-13:15	20:00-20:15	Closing

WELCOME

On behalf of the Scientific and Organizing Committee we welcome you to the 1st BICTAM-CISM Symposium on Dispersed Multiphase Flows.

The Symposium aims to bring together experts from Europe and China in the complementary fields of physics, applied mathematics, chemistry and engineering to present and discuss progress in research, development, standards, and applications of the topics related to dispersed multiphase flows. The symposium will promote the exchange of new ideas, results and techniques by bringing together graduate students, postdoctoral researchers, faculty and researchers across government and industry.

To ensure a long-lasting scientific interaction between the two communities, the Symposium will be organized every 2 years, alternating between China and Europe. The first edition of the Symposium 2021 organized by BICTAM and Tsinghua University is held in Beijing. We have received 60 abstracts from 12 countries and we look forward to the 8 keynote lectures and 52 regular lectures.

Welcome to the BICTAM-CISM Symposium on Dispersed Multiphase Flows: from Measuring to Modeling!

Jiachun Li, BICTAM & Chinese Academy of Sciences
Chairman of the Symposium

Cristian Marchioli, CISM & University of Udine
Chairman of the Symposium

January 18, 2021

SYMPOSIUM SCOPE

The Symposium will provide the opportunity to compare and contrast the different available approaches, giving a global overview of the most significant advancements in the field. It will also serve the purpose of identifying the main open issues and research pathways that the community should focus on in the future. To these aims the Symposium will bring together internationally renowned scientists from all horizons (analytical, numerical, and experimental) to foster scientific exchange and strengthen interdisciplinary work among engineers, applied mathematicians, and physicists through invited keynote lectures and contributed talks.

TOPICS

The Symposium spans a wide selection of topics in the broad area of dispersed multiphase flows. The focus will be on generic aspects and physics of particulate flows (both viscous and turbulent), be it computer simulations, laboratory or field measurements, and theoretical studies. Among the topics to be included are: dynamics of particles, bubbles, and droplets in free and wall-bounded turbulence; rigid and deformable particle suspensions; non-Newtonian dispersed flows; reactive dispersed flows; advances in measurement and simulation techniques; modelling of collision, agglomeration and fragmentation/breakage phenomena.

ORGANIZATION

In view of the ongoing pandemic, the Symposium will be organised in the form of a hybrid event in which participants can attend either in-person or virtually by conference call. The Symposium's physical venue will be the Xijiao Hotel Convention Center (18 Wang Zhuang Road, Haidian Qu, Beijing, China, 100083). All talks will be live-streamed as they are delivered.

ACKNOWLEDGEMENT

NSFC

IUTAM International Union of Theoretical and Applied Mechanics

BICTAM

International Centre for Mechanical Sciences

Università degli Studi di Udine (Italy)

The Symposium is sponsored by IUTAM, BICTAM, CISM, Natural Science Foundation of China (NSFC), Institute of Mechanics of Chinese Academy of Sciences and School of Aerospace Engineering of Tsinghua University. The financial support by NSFC Basic Science Center Program for Multiscale Problems in Nonlinear Mechanics (No. 11988102) and NSFC Program for Academic Events (No. 11942218) is acknowledged.

SYMPOSIUM CHAIRMEN

- Professor Jiachun Li, BICTAM & Chinese Academy of Sciences (China)
- Professor Cristian Marchioli, CISM & University of Udine (Italy)

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- Professor Xiqiao Feng, Tsinghua University (China)
- Professor Kun Luo, Zhejiang University (China)
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- Professor Alfredo Soldati, TU Wien (Austria)
- Professor Chao Sun (co-chair), Tsinghua University (China)
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- Professor Lihao Zhao, Tsinghua University (China)
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- Mrs. Yanan Tang, Beijing Int. Center for Theoretical and Applied Mechanics (BICTAM)
- Professor Bing Wang, Tsinghua University
- Professor Chunxiao Xu, Tsinghua University
- Professor Lihao Zhao (co-chair), Tsinghua University

SYMPOSIUM VENUE

Xijiao Hotel　　北京西郊宾馆

Address: 北京海淀区王庄路 18 号　Phone: +86 10 6232 2288

From Beijing Capital International Airport (Terminal 1~3) to Xijiao Hotel:

- Taxi cost is 100 to 150 CNY (please show the Chinese name of Xijiao hotel to taxi driver in case he/she does not understand English).
- Subway (06:20-22:50, 30 CNY): Take Airport Line and transfer at Sanyuanqiao Station (三元桥) to Line 10. Then transfer at Zhichunlu Station (知春路) to Line 13. The destination is Wudaokou Station (五道口), from where it takes about 15 minutes to Xijiao Hotel by walking.

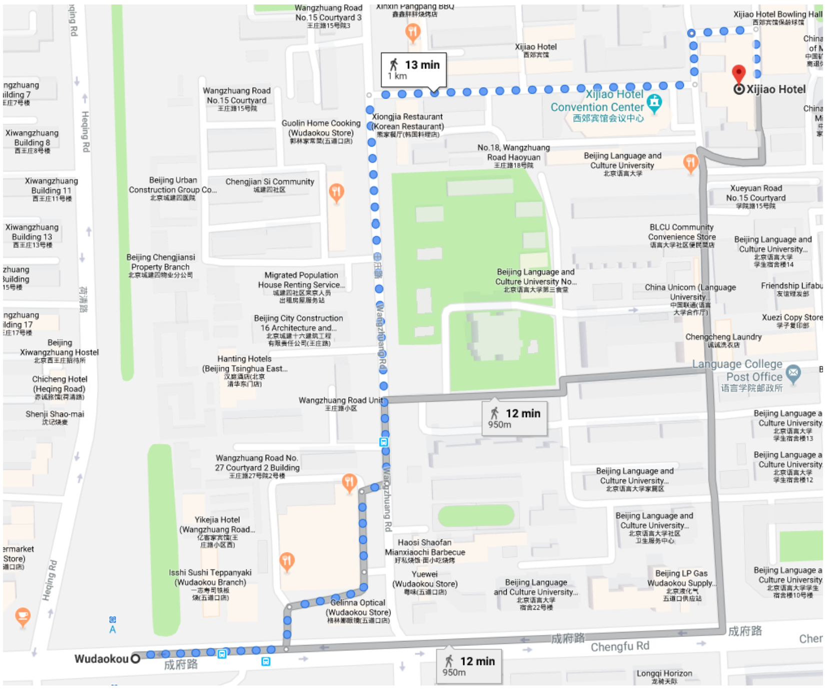

Fig. Walking routine from Wudaokou subway station to Xijiao Hotel.

- Airport Shuttle Bus (30 CNY): take Shuttle Line 5 to Tsinghua University Science Park (TusPark) (清华科技园).

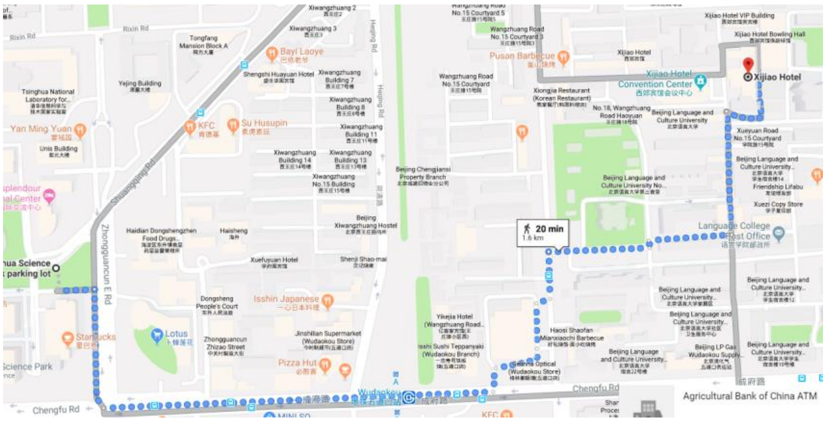

Fig. Walking routine from TusPark to Xijiao Hotel.

Beijing transportation:　www.travelchinaguide.com/cityguides/beijing/transportation/

Symposium Program

Tuesday March 2nd (Day 1)

EU time			CHINA time		CHAIRPERSON
From	To		From	To	
8:15	8:30	Welcome	15:15	15:30	Jiachun Li, Cristian Marchioli
8:30	9:00	**Modulation of very-large-scale motions by saltating particles** **Keynote speaker: Xiaojing Zheng, Xidian University, China**	15:30	16:00	Lihao Zhao
9:00	9:15	Measurements of the electrohydrodynamic fluctuation spectrum of dust storms Speaker: Huan Zhang, Lanzhou University, China	16:00	16:15	
9:15	9:30	Wave-induced scouring at a vertical cylinder: sediment transport, coherent structures and morphodynamics Speaker: Maurizio Brocchini, Università Politecnica delle Marche, Italy	16:15	16:30	
9:30	9:45	Layering and vertical mixing in double diffusive convection turbulence Speaker: Yantao Yang, Peking University, China	16:30	16:45	Maurizio Brocchini
9:45	10:00	Clustering and preferential sampling of micro-swimmers in laminar and turbulent flow Speaker: Guido Boffetta, University of Torino, Italy	16:45	17:00	
10:00	10:15	Turbulent Sedimentation of Phytoplankton Speaker: Filippo De Lillo, University of Torino, Italy	17:00	17:15	
10:15	10:30	Coffee break	17:15	17:30	
10:30	11:00	**Phase Field Simulations of Breakage, Coalescence and Drop Size Distribution in Turbulent Flows** **Keynote speaker: Alfredo Soldati, Vienna University of Technology, Austria**	17:30	18:00	Cristian Marchioli
11:00	11:15	Final Fate of a Leidenfrost Droplet Speaker: Chao Sun, Tsinghua University, China	18:00	18:15	
11:15	11:30	Experimental study of droplet dispersion in homogenous and isotropic turbulence Speaker: Huan Lian, Institute of Mechanics, Chinese Academy of Sciences, China	18:15	18:30	
11:30	11:45	Droplets in shear flows Speaker: Marco Edoardo Rosti, The University of Tokyo, Japan	18:30	18:45	
11:45	12:00	Droplet Generation via Bursting, Impacting, and Jetting, with Surfactants Speaker: Omar K. Matar, Imperial College London, United Kingdom	18:45	19:00	Chao Sun
12:00	12:15	Modeling a surfactant-covered droplet on a solid surface in three-dimensional shear flow Speaker: Haihu Liu, Xi'an Jiaotong University, China	19:00	19:15	
12:15	12:30	Bubbly flows instabilities in the Eulerian-Eulerian and Eulerian-Lagrangian frameworks Speaker: Gaetano Sardina, Chalmers University of Technology, Sweden	19:15	19:30	
12:30	12:45	Channel flow laden with neutrally-buoyant spherical particles: flow regimes and heat transfer efficiency Speaker: Luca Brandt, KTH Royal Institute of Technology, Sweden	19:30	19:45	
12:45	13:00	On the plug-to-slug transition in gas-liquid-solid three-phase flows Speaker: Paolo Sassi, Universitat Rovira i Virgili, Spain	19:45	20:00	

Wednesday March 3rd (Day 2)

EU time			CHINA time		CHAIRPERSON
From	To		From	To	
8:30	9:00	**Migration of particles in a confined shear flow of non-Newtonian fluid**	15:30	16:00	Limin Wang
		Keynote speaker: Jianzhong Lin, Zhejiang University, China			
9:00	9:15	Motion behaviour of heavy particles in bounded vortex flows	16:00	16:15	
		Speaker: Xiaoke Ku, Zhejiang University, China			
9:15	9:30	Modulation of turbulence intensity by heavy finite-size particles in upward channel flow	16:15	16:30	
		Speaker: Zhaosheng Yu, Zhejiang University, China			
9:30	9:45	Interface-resolved simulations of particle-laden turbulent channel flow	16:30	16:45	
		Speaker: Francesco Picano, University of Padova, Italy			
9:45	10:00	Large-scale Direct Numerical Simulation for Investigating the Effects of the Mesoscale Structure in Gas-solid Flow	16:45	17:00	Francesco Picano
		Speaker: Limin Wang, Institute of Process Engineering, Chinese Academy of Sciences, China			
10:00	10:15	Direct Numerical Simulation of turbulent transport and wall deposition of airborne particles on thermally active enclosed cavities	17:00	17:15	
		Speaker: Alexandre Fabregat, Universitat Rovira i Virgili, Spain			
10:15	10:30	Boundary layer models to predict particle wall deposition in enclosed turbulent natural convection flows	17:15	17:30	
		Speaker: Jordi Pallares, Universitat Rovira i Virgili, Spain			
10:30	10:45	Coffee break	17:30	17:45	
10:45	11:15	**Probing opaque flows: the cavitating Venturi benchmark**	17:45	18:15	Lianping Wang
		Keynote speaker: Christian Poelma, Delft University of Technology, Netherlands			
11:15	11:30	Experimental observation of the elastic range scaling in turbulent flow of dilute polymer solution	18:15	18:30	
		Speaker: Heng-Dong Xi, Northwestern Polytechnical University, China			
11:30	11:45	On μ(I) rheology of dense granular flows – can we get a mesh-independent solution?	18:30	18:45	
		Speaker: Srdjan Sasic, Chalmers University of Technology, Sweden			
11:45	12:00	Multi-way couplings between inertial particles and turbulence in a swirling flow	18:45	19:00	
		Speaker: Mickaël Bourgoin, University of Lyon, France			
12:00	12:15	Effect of electrostatic charges on the dispersion of inertial particles transported by a homogeneous isotropic turbulent flow	19:00	19:15	Mickaël Bourgoin
		Speaker: Athanasios Boutsikakis, Institut de Mécanique des Fluides de Toulouse, France			
12:15	12:30	Assessment of the Parcel model in LES of Turbulent Evaporating Sprays	19:15	19:30	
		Speaker: Jietuo Wang, University of Padova, Italy			
12:30	12:45	Mesoscale Model for Gas-Liquid Flow in Bubble Columns and Liquid-Liquid Flow in Rotor-Stator Mixers	19:30	19:45	
		Speaker: Ning Yang, Chinese Academy of Sciences, China			
12:45	13:00	Mesoscopic simulations of dispersed multiphase flows: recent results and open issues	19:45	20:00	
		Speaker: Lian-Ping Wang, Southern University of Science and Technology, China			

Thursday March 4th (Day 3)

EU time			CHINA time		CHAIRPERSON
From	To		From	To	
8:30	9:00	**Instability and control of a freely moving sphere affected by a magnetic field** **Keynote speaker: Mingjiu Ni, University of Chinese Academy of Sciences, China**	15:30	16:00	Guodong Jin
9:00	9:15	Interactions between two bubbles rising side by side under the influence of magnetic field Speaker: Jie Zhang, Xi'an Jiaotong University, China	16:00	16:15	
9:15	9:30	Modeling of non-equilibrium effects in intermittency region between two phases Speaker: Tomasz Waclawczyk, Warsaw University of Technology, Poland	16:15	16:30	
9:30	9:45	Multiscale modelling of disperse multiphase systems in VIMMP Speaker: Daniele Marchisio, Politecnico di Torino, Italy	16:30	16:45	Tomasz Waclawczyk
9:45	10:00	Wall model for large eddy simulations accounting for particle effect Speaker: Ping Wang, Lanzhou University, China	16:45	17:00	
10:00	10:15	Reproducing segregation and particle dynamics in Large Eddy Simulation of particle-laden flows Speaker: Roxane Letournel, EM2C-CentraleSupelec-CMAP, France	17:00	17:15	
10:15	10:30	A Structural Subgrid-Scale Model for LES of Particles in Turbulent Flows Speaker: Guodong Jin, Institute of Mechanics, Chinese Academy of Sciences, China	17:15	17:30	
10:30	10:45	Coffee break	17:30	17:45	
10:45	11:15	**History force on a fluid sphere (from particles to drops and bubbles)** **Keynote speaker: Eric Climent, University of Toulouse, France**	17:45	18:15	Guoqing Hu
11:15	11:30	The impact of interphase forces on the generation of turbulence in multiphase flows Speaker: Simon Schneiderbauer, Johannes Kepler University, Austria	18:15	18:30	
11:30	11:45	Fluid-Particle and Particle-Particle Drags of Bidisperse Gas-Solid Flows at Low Reynolds Number Speaker: Qiang Zhou, Xi'an Jiaotong University, China	18:30	18:45	
11:45	12:00	An ANN-based drag model and turbulence statistics from fully-resolved simulation of dense gas-solid flows Speaker: Kun Luo, Zhejiang University, China	18:45	19:00	
12:00	12:15	Prediction of inertial lift on particles for microfluidic applications Speaker: Guoqing Hu, Zhejiang University, China	19:00	19:15	Simon Schneiderbauer
12:15	12:30	Effect of fluid inertia on the orientation of a small particle settling in turbulence Speaker: Bernhard Mehlig, University of Gothenburg, Sweden	19:15	19:30	
12:30	12:45	The effect of hydrodynamics interaction (HI) on the dynamics and equilibrium configuration of colloidal aggregates in the quiescent flow regime Speaker: Mingzhou Yu, China Jiliang University, China	19:30	19:45	
12:45	13:00	Simulation of shock-particles interaction using conservative sharp interface methods Speaker: Hang Ding, University of Science and Technology of China, China	19:45	20:00	
13:00	13:15	Filtering effect of heavy particles in the three dimensional homogeneous and isotropic turbulence Speaker: Yongxiang Huang, Xiamen University, China	20:00	20:15	

Friday March 5th (Day 4)

EU time			CHINA time		CHAIRPERSON
From	To		From	To	
8:30	9:00	**Dynamics of inertial particles in an uniform unsteady flow at low Reynolds number** **Keynote speaker: Haitao Xu, Tsinghua University, China**	15:30	16:00	Junwu Wang
9:00	9:15	Dynamics of particles in viscoelastic liquids: numerical methods and microfluidic applications Speaker: Gaetano D'Avino, University of Naples Federico II, Italy	16:00	16:15	
9:15	9:30	Can the Rayleigh-Plesset equation describe nanoscale bubbles dynamics? Speaker: Zhan Gao, Tsinghua University, China	16:15	16:30	
9:30	9:45	Hydrodynamics of vapour bubble growth and detachment in a shear flow Speaker: Catherine Colin, Institut de Mécanique des Fluides de Toulouse, France	16:30	16:45	
9:45	10:00	Turbulent heat transfer of supercritical fluids: Fundamentals and models Speaker: Bofeng Bai, Xi'an Jiaotong University, China	16:45	17:00	Catherine Colin
10:00	10:15	Quantifying the non-equilibrium characteristics of heterogeneous gas-solid flows: kinetic theory analysis and CFD-DEM simulation Speaker: Junwu Wang, Institute of Process Engineering, Chinese Academy of Sciences, China	17:00	17:15	
10:15	10:30	Simulation of a reactive fluidized bed reactor using coupled CFD/DEM Speaker: Vincent Moureau, CORIA, France	17:15	17:30	
10:30	10:45	Marginal stability limits for a fluidized bed: theory and numerical simulations Speaker: Maoqiang Jiang, Huazhong University of Science and Technology, China	17:30	17:45	
10:45	11:00	Coffee break	17:45	18:00	
11:00	11:30	**Validation of drag correlations of ellipsoidal particles using fully resolved simulations** **Keynote speaker: Wolfgang Schröder, RWTH Aachen University, Germany**	18:00	18:30	Alain Pumir
11:30	11:45	A Numerical Investigation of Gas-Fluidized Bed of Flexible Fibers Speaker: Yu Guo, Zhejiang University, China	18:30	18:45	
11:45	12:00	Measurement of rigid fiber motion in a turbulent channel flow Speaker: Rene van Hout, Technion - Israel Institute of Technology, Israel	18:45	19:00	
12:00	12:15	Using fibers to measure flow properties Speaker: Andrea Mazzino, University of Genova, Italy	19:00	19:15	Guo Yu
12:15	12:30	Reconstructing the fluid flow by tracking of large particles Speaker: Francesco Romanò, Arts et Métiers ParisTech, France	19:15	19:30	
12:30	12:45	Turbulence-controlled evolution of particle patterns on the interface of large deformable drops Speaker: Arash Hajisharifi, University of Udine, Italy	19:30	19:45	
12:45	13:00	Importance of fluid inertia for the orientation of spheroids settling in turbulent flow Speaker: Alain Pumir, Ecole Normale Supérieure de Lyon and CNRS, France	19:45	20:00	
13:00	13:15	**Closing**	20:00	20:15	Jiachun Li, Cristian Marchioli

ABSTRACTS

Modulation of very-large-scale motions by saltating particles

Xiaojing Zheng[1]* **and Ping Wang**[2]

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Abstract

Modulation of very-large-scale motions by saltating particles was studied by large eddy simulations two-way coupled with point particle method at Reynolds number of Re_τ=3730, 4200, corresponding to wind-blown sand flows that take place in the atmospheric surface layer. In this case, saltating particle not only rebound but also eject other particles resting on the surface when it impacts the modeled granular bed. It is found that particles suppress the streamwise turbulence intensities and Reynolds stress in the near surface region, while significantly enhance the streamwise turbulence intensities and Reynolds stress in the region beyond the saltating layer, as compared to the particle-free case. Two-point correlation of streamwise velocity shows that saltating particles reduce the size of outer layer structure and enlarge the size of near surface structure. These trend will increase with Reynolds number. The transport equation of the two-point velocity correlation is further investigated in different length scales by applying a spectral analysis. Conditional averaging provides an ensemble-mean visualization of flow structures responsible for high particle concentration "event" and the reduced large/very large scale turbulent motions. Further, the effects of gravity and surface condition on turbulence modulation are emphatically discussed.

Keywords: turbulence modulation, very-large-scale motions, saltating particle, large eddy simulation

* National Natural Science Foundation of China (Grants No. 11490553)

Measurements of the Electrohydrodynamic Fluctuation Spectrum of Dust Storms

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[2] *Key Laboratory of Mechanics on Disaster and Environment in Western China, The Ministry of Education of China, Department of Mechanics and Engineering Science, College of Civil Engineering and Mechanics, Lanzhou University, Lanzhou 730000, PR China.*

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Abstract

Dust storms are the typical high Reynolds-number [up to $Re_\tau \sim O(10^6)$] electrohydrodynamic (EHD) turbulence heavily laden with charged dust grains, in which turbulent flows, dust grain movements, and electric fields are mutually coupled. To date, the fluctuation properties of such an EHD turbulence are still largely unknown. In this study, we present the first measurements of the fluctuation spectrums of wind velocity, dust concentration, and electric field in dust storms at the Qingtu Lake Observation Array. The results show that within the inertial wavenumber range, both wind velocity and PM_{10} dust concentration fluctuations show Kolmogorov's power law with indices of $\sim k^{-5/3}$. By contrast, there exist two power laws within the inertial wave number range of the electric field spectrum; that is, at low wavenumbers, the spectrum is $\sim k^{-5/3}$, while at high wavenumbers, the spectrum is $\sim k^{-11/3}$. This suggests that the energy cascade process of electric field fluctuation is probably governed by two distinct physical mechanisms. Furthermore, using the premultiplied power spectrum, we find that in addition to turbulent fluctuations, PM_{10} dust concentration and electric field fluctuations also have large-scale coherent structures with a size of about 3-4δ (δ is the thickness of the boundary layer). These results provide us with a wealth of experimental information for further understanding of EHD turbulence in multiphase flows.

Keywords: electrohydrodynamic, power spectrum, premultiplied power spectrum, dust storms

Wave-induced scouring at a vertical cylinder: sediment transport, coherent structures and morphodynamics

Sara Corvaro[1], **Francisco Alves Pereira**[2], **Maurizio Brocchini**[3], **Massimo Miozzi**[4]

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Abstract

The evolution of sediment transport, coherent structures and morphodynamics typical of the equilibrium stage of the scouring process forced by water waves at the toe of a vertical slender cylinder are analyzed through interpretation of dedicated laboratory experiments.

Keywords: water waves, vertical cylinder, scouring, sediment transport, coherent structures.

1. Introduction

We use the defocusing digital PIV technique (DDPIV) to obtain Lagrangian trajectories of sand particles and, through proper interpolation, the associated Eulerian fields. Fundamental dynamics – e.g. horseshoe vortex, lee-side vortices and their shedding – are, then, discussed on the basis of indicators typical of the evolution of coherent structures (Q-criterion) and of the local sediment density (see figures 1 and 2).

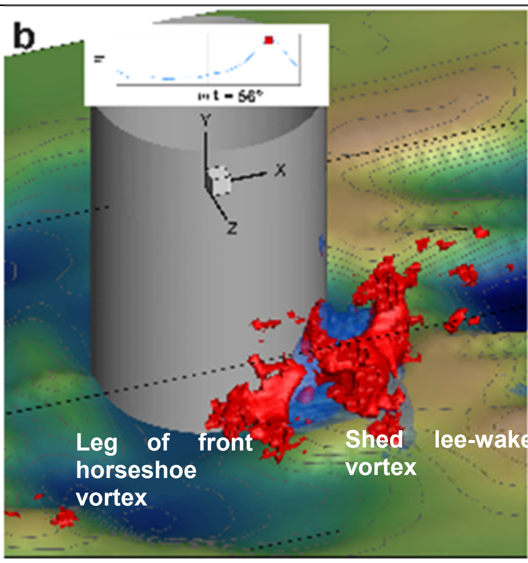

Figure 1: Isosurfaces at Q=80 (red) and $\rho_n = 1.3\,mm^{-3}$ (blue) at $\omega t = 56°$ (wave crest). Background represents the bathymetry measurements.

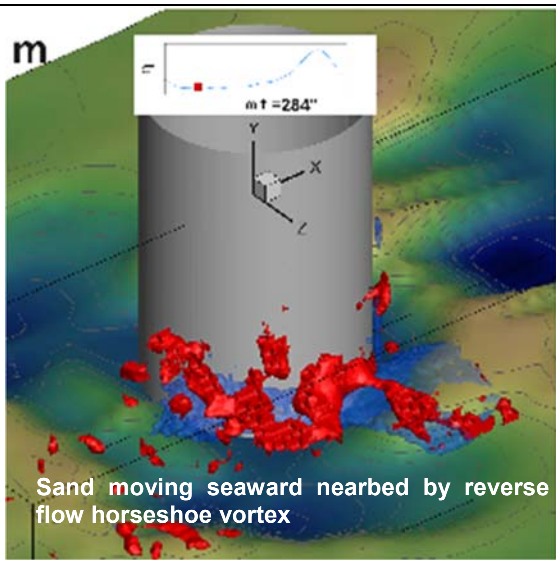

Figure 2: Isosurfaces at Q=80 (red) and $\rho_n = 1.3\,mm^{-3}$ (blue) at $\omega t = 284°$ (end of return flow stage). Background represents the bathymetry measurements.

A detailed analysis of the findings will be provided at the Symposium.

Layering and vertical mixing in double diffusive convection turbulence

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Abstract

Stratified fluid with density affected by more than one component is omnipresent in many natural environments and engineering applications. This is especially the case in ocean, such as the salinity-sediment system in estuaries where fresh water rushes into salty seawater, and the temperature-salinity system in the thermocline. In these systems, buoyancy-driven convection can happen in many different forms and play a crucial role in vertical mixing and transport process. One particular form is the double diffusive convection (DDC), which occurs when two components have vertical gradients with opposition directions.

Depending on the gradients of the two components, DDC can be in two distinct regimes. When the gradient of the slow-diffusing component drives the flow and that of the fast-diffusing one stabilizes the flow, DDC happens in the fingering regime, and the characteristic structure is the vertically aligned fingers with small horizontal width. When the flow is driven by the fast-diffusing component and stabilized by the slow-diffusing one, DDC is in the diffusive regime. In oceans, thermohaline DDC may exist in more than 40% of the total volume, thus has great impact on the heat and mass transfer in the vertical direction. Usually finger DDC happens in the tropic and sub-tropic oceans, while diffusive DDC in the polar oceans, respectively.

One intriguing feature of DDC is the so-called staircase state, in which well-mixed layers are separated by sharp interfaces with high component gradients, and the mean profiles of components exhibit staircase-like shape. Layering and staircases have been observed in many regions of oceans, ranging the sub-tropic oceans to polar regions. Such flow state has also been found in "the laboratory latte" and used for material manufacture. For ocean staircase, the vertical length scale is usually from ten to hundred meters, while the horizontal coherence of such structures is surprisingly large, covering hundreds of square kilometers, and existing for decades.

Here we present our recent studies on DDC both in fingering and diffusive regimes. By using a highly efficient, multiple-grid method we conducted systematic direct numerical simulations of DDC. We focus on the layering phenomena in such system and the transport behaviors. For fingering DDC, we show that at small Rayleigh numbers, finger structures grow and occupy the whole domain. When the Rayleigh number exceeds certain critical value, multi-layer state can be established and fingers do not extend over the whole height. Hysteresis happens during the transition between the single finger state and the multi-layer state. Thus, multiple states exist for the same global control parameters depending on the exact evolution history of the flow. Moreover, for Rayleigh number higher than the critical value, different configurations of staircases are achieved from different initial distributions. Single finger layer and the finger layers within staircases generate different fluxes even when they have the same density ratio, a parameter commonly used to describe the flux. We further show that for all finger layers, the flux follows a single scaling law of the apparent Rayleigh number. By using two-dimensional simulations with the same properties as seawater, we identified the parameter range where staircases exist.

We then investigate the layering in diffusive regime. Simulations reveal that layering can also appear when diffusive DDC interacts with vertical shearing. Analysis shows that the system is linearly stable. Therefore, layering has to be triggered by much stronger initial perturbation through a nonlinear mechanism. Very sharp diffusive interfaces emerge and separate well-mixed convection layers. These interfaces strongly oscillate in space and time. But they generate small heat flux compared to the convection layers after time average, thus serving as heat barriers in the vertical direction.

Keywords: multi-component stratified flow, double diffusive convection, thermohaline staircase, turbulent mixing

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Clustering and preferential sampling of micro-swimmers in laminar and turbulent flows

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Abstract

We present statistical properties of swimmers in laminar and turbulent flows in dilute conditions on the basis of numerical simulations of simple microscopic models. In general, the direction of swimming in our micro-organisms is determined by several factors including gravity (gyrotaxis), swimmers shape (Jeffery model), buoyancy. We study how these dynamical ingredients produces different statistical properties of the population of micro-swimmers, in particular clustering and preferential concentration.

Clustering is quantified by computing the correlation dimension of the spatial distribution of the population in stationary conditions and it is found to depend on the parameters of the dynamical model. We find that clustering is associated to a preferential concentration of the population in particular regions of the flow characterized in terms of the velocity or the vorticity statistics.

The conseguence of our finding for natural enviromental problems, such as micro-organisms in the ocean, and technological applications is discussed.

Keywords: micro-swimmers, turbulence, gyrotaxis

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Turbulent Sedimentation of Phytoplankton

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Abstract

We use numerical simulations of turbulent flows to study the distribution and sedimentation properties of phytoplankton transported by ocean turbulence and subject only to buoyancy. The effects of buoyancy regulation are investigated [1]. The latter is introduced via a simple model postulating that density varies (increases or decreases) continuously as a function of local shear stress. Buoyancy control produces several effects which are potentially relevant to plankton ecology, changing the probability distribution of sedimentation times (see fig.1 as well as clustering and segregation effects.

Keywords: phytoplankton, buoyancy control, sedimentation

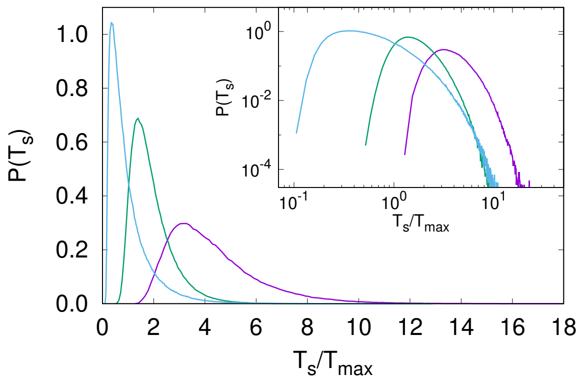

Figure 1: PDF of sedimentation times for particles whose density increases with local shear stress. Curves are shown for $Re_\lambda = 33$, 60, 165, increasing right to left. Times are normalized over the value $T_{\max}$ of the sedimentation time in still water.

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Phase Field Simulatins of Breakage, Coalescence and Drop Size Distribution in Turbulent Flows

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ABSTRACT

Droplets carried in turbulent fluids rely, for their existence, on tiny interfaces. Interfaces are not property of the drop or of the the carrier fluid and are inherently a non-place. However, in environmental and industrial processes, their role is enormously important since it is across the interfaces that momentum, heat and mass transfer fluxes coupling the drop to the carrier fluid occur: the accurate determination of their position, shape and interaction with the fluid turbulence is crucial to predict physical phenomena, and industrial and environmental processes. To this aim, Direct Numerical Simulation (DNS) of turbulence and accurate tracking of the interface are required, but the range of scales involved for most of practical environmental and industrial applications is so wide that performing this task is a formidable challenge for present day computers: The grid resolution for DNS of turbulence is of the order of the Kolmogorov scale, but of course physical interfaces have a much smaller scale (order of few molecules) making the direct resolution unfeasible.

In this talk, we will review the current computational methodologies used to describe the behavior of bubbles and drops entrained in turbulent flows, and we will present the phase-field approach: In this Eulerian approch, the phase distribution is described by the order parameter ϕ. We will examine several flow instances and a broad range of the parameter space examining turbulent dispersion of drops and bubbles. We will review the effects of varying viscosity and density contrast, and we will also consider the presence of a dispersed surfactant, which requires the use of a further order parameter ψ, and which will give further complexity to the problem, making the interplay among shear stresses, surface tension, and surface tension gradients even more intertwined.

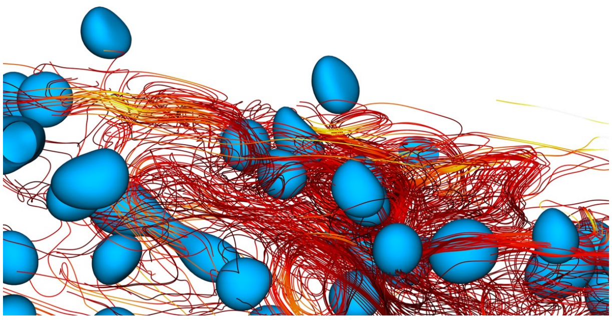

Figure 1: Instantaneous realization of drop-drop and drop-turbulence interaction. Turbulent flow outside the droplets is highlighted by the stream traces colored by turbulent kinetic energy ($E_{k,tot}$) level (yellow, low; red, high) (Taken from: A. Roccon et al. "Viscosity-modulated breakup and coalescence of large drops in bounded turbulence" Phys. Rev. Fluids **2**, 083603, 2017)

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Final Fate of a Leidenfrost Droplet

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Abstract

When a liquid droplet is placed on a very hot solid, it levitates its own vapor layer; a phenomenon commonly called the Leidenfrost effect. Although the mechanisms governing the droplet's levitation have been explored, not much is known about the fate of the evaporating Leidenfrost droplet. Here we report on the final stages of evaporation of Leidenfrost droplets. While initially small Leidenfrost droplets tend to take off and disappear, surprisingly, the initially large ones explode with a crack sound. We interpret these in the context of unavoidable droplet contaminations: as the droplet evaporates, the contaminants accumulate at the droplet-air interface, resulting in reduced evaporation rate and finally, contact with the substrate. We validate this hypothesis by introducing controlled amounts of (microparticle) contaminants within the droplet, and reveal a universal 1/3 scaling law for the dimensionless explosion radius as a function of contaminant fraction. Our findings open up new opportunities for controlling the duration and rate of Leidenfrost heat transfer and propulsion, by tuning the droplet's size and contamination [1].

Keywords: Leidenfrost, drop, evaporation

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Experimental study of droplet dispersion in homogenous and isotropic turbulence

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Abstract

Dilute dispersed droplets have been found to preferentially concentrate and form clusters (Maxey 1987) due to interactions with the carrier phase turbulence. To fully elucidate the governing mechanism with simplified form of turbulence, a facility was constructed to generate gaseous homogeneous and isotropic turbulence (Lian et al. 2013). Characteristics of the carrier phase turbulence including enstropy, velocity invariants and topological structures were acquired via the two-dimensional Particle Image Velocimetry (PIV) with quantifications of the experimental noise (Lian et al. 2017). Dispersion statistics of the identified turbulent structures and droplets are evaluated based on the Voronoï tessellation. The paper reports a new experimental finding that apart from the commonly acknowledged centrifugal mechanism, many of the velocity gradient based turbulent characteristics (enstropy, velocity invariants and topological structures) correlate with the droplet dispersion statistics, which seems to provide a positive support to the velocity gradient tensor driven explanation of (Bragg et al. 2018) in both of the inertial and the dissipation range with Direct Numerical Simulation (DNS) validation. The Mie scattering images of the dispersed droplets and PIV tracer particles in homogeneous and isotropic turbulence were recorded at the repetition rate of 1Hz and ultra-high sub-Komogorov spatial resolution with illumination by a 532nm Nd:YAG laser.

Keywords: droplet dispersion, velocity gradient tensor, homogeneous and isotropic turbulence

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Droplets in shear flows

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Abstract

The understanding of turbulent two-phase flows with bubbles and/or droplets is important in many natural and industrial processes, e.g. rain formation, liquid-liquid emulsion, spray cooling and spray atomization in combustors. In these flows the turbulence is altered by the droplet feedback on the surrounding fluid and by droplet-droplet interactions. We simulate the flow of two immiscible and incompressible fluids separated by an interface in laminar shear flows with a volume of fluid method. A random monodisperse distribution of droplets is initialized in a bi-periodic system and their motion driven by an applied shear rate. First, we examine the dependency of the effective viscosity on the volume fraction and the Capillary number for two different viscosity ratios; we show that the viscosity of the biphasic system decreases with the deformation and the applied shear while increases for low volume fraction and decreases for high volume fraction, exhibiting a maximum for an intermediate volume fraction. Next, we study the effect of a non-Newtonian inelastic carrier fluid modelled as simple power law fluids. Both shear-thinning and shear-thickening fluids are considered and their influence on the droplet coalescence analysed.

Keywords: multiphase flow, droplets, volume of fluid

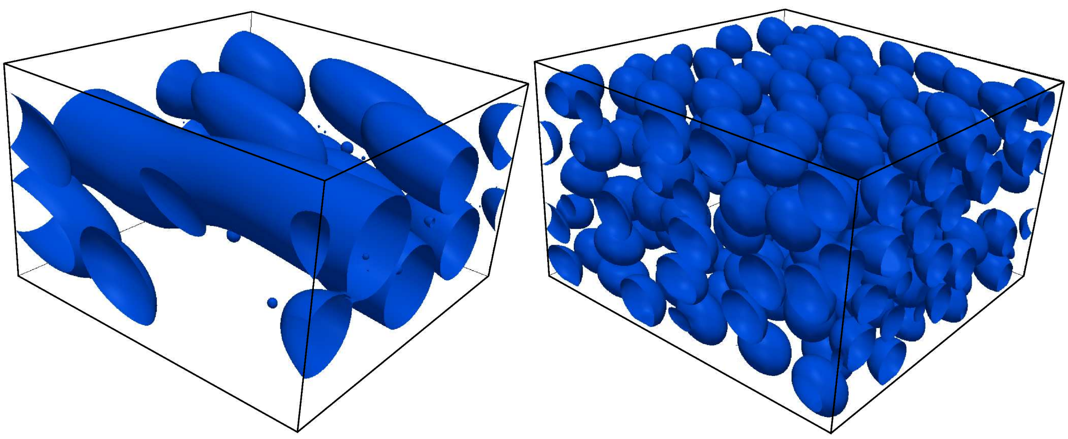

Figure 1: Instantaneous droplet distributions for emulsions with volume fraction 30% and capillary number Ca = 0.1 with high (left) and low (right) coalescence efficiency.

Droplet Generation via Bursting, Impacting, and Jetting, with Surfactants

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Abstract

We study a number of different flow situations using direct numerical simulations that employ interfacial-tracking methodology; these include turbulent jets of one liquid flowing into a stagnant phase of another, immiscible liquid, bubbles bursting through an interface, and droplets impacting on mobile interfaces. A particular emphasis is placed upon the effect of surfactant on droplet generation in all of these cases. The numerical results will be used to isolate the physical mechanisms underlying the observed complex phenomena.

Keywords: Multiphase flows, dispersions, emulsions, surfactants, droplets, CFD

1. Turbulent jets

Liquid atomisation processes are widely used to break down a liquid stream into smaller droplets to enhance its mixing with a stagnant phase. These streams may be contaminated with surfactants, whose concentration variations lead to surface tension gradients and Marangoni stresses. Here, we study the effect of surfactant on the complex interfacial dynamics associated with a turbulent jet. We use three-dimensional (3D) direct numerical simulations (DNS) and a hybrid front-tracking/level-set method [1] to capture the dynamics of the complex topological changes in this flow. The numerical method allows the natural tracking of the concentration of interfacial surfactant species and the faithful modelling of its spatio-temporal evolution. Our model also accounts for surfactant solubility and bulk-interface mass exchange. We perform a parametric study of the effect of surfactant properties on the dynamics. The effect of Marangoni stresses is analysed in terms of the mechanisms giving rise to the droplet size distributions depending on the elasticity number. An attempt to understand the interaction between the observed vortical structures accompanying the flow and the regions of elevated surfactant concentration will also be presented.

2. Bursting bubbles

Countless instances of bursting bubbles over the oceans contribute significantly to the exchange of heat and chemicals with the atmosphere. Understanding bursting bubble physics could be the key to tackling the ever-growing environmental problem. When a bubble is close to a free surface, it forms a hole which leaves an open unstable cavity that undergoes collapse; the change of the interface curvature leads to the formation of a central jet, which breaks into droplets according to the Plateau–Rayleigh instability. The surfactant-free interfacial dynamics are well understood, however, the surfactant-laden bursts are still unexplored. By neglecting gravity, the Laplace number is the only dimensionless control parameter measuring the relative importance of surface tension to viscous forces i.e. $La = \rho\sigma R/\mu^2$, where ρ, μ, σ, and R represent the liquid density, viscosity, surface tension, and the initial radius of the droplet, respectively. The fate of the central jet is analysed with help of a 3D DNS simulations, where the effect number of surfactant related non-dimensional parameter. Results regarding the importance of Marangoni stresses on the jet formation will be discussed.

3. Drop impact on interfaces

Finally, we consider the impact of drops on solid and fluid substrates whose rich phenomena have been the source of fascination for decades. Recent experimental work [2] has investigated the effect of surfactants on "crown" splashing and found that they affect significantly the propagation of capillary waves, the evolution of the crown, and the formation of secondary droplets. Here, we employ 3D DNS to examine drop impacts on thin surfactant-laden films. We couple the hybrid interface-tracking/level-set method for the interfacial dynamics to a convective-diffusion equation for the surfactant concentration to carry out the computations. We vary different surfactant properties (i.e. diffusion, elasticity, and solubility) to study their effect on the phenomena accompanying the drop impact.

The authors thank BP, EPSRC, PETRONAS, and the Royal Academy of Engineering (Research Chair in Multiphase Fluid Dynamics for OKM) for funding. The contribution of S. Shin, D. Juric, and J. Chergui to the numerical methods is also gratefully acknowledged.

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Modeling a surfactant-covered droplet on a solid surface in three-dimensional shear flow

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A surfactant-covered droplet moving on a solid surface subject to a three-dimensional shear flow is studied using a lattice Boltzmann and finite difference hybrid method. The hybrid method not only allows for contact line dynamics with contact angle dynamically varying with the local surfactant concentration, but also can deal with the surfactant concentration beyond the critical micelle concentration. We first focus on low values of effective capillary number (Ca_e) and systematically study the effect of Ca_e, viscosity ratio (λ) of droplet to ambient fluid, surfactant coverage and surface Peclet number on the droplet behaviour. Our results show that at low values of Ca_e, the droplet eventually reaches a steady deformation and moves with a constant velocity along the solid surface. The presence of surfactants is found to not only increase droplet deformation but also promote droplet motion, which are attributed to low interfacial tension at the droplet front and Marangoni-induced drag force acting on the droplet surface, respectively. For each value of λ, the contact-line capillary number of moving droplet linearly increases with Ca_e. Increasing λ always slows down the droplet motion, but changes the droplet deformation non-monotonically at relatively high Ca_e, where the largest deformation occurs at the viscosity ratio of around 1. In addition, increasing surfactant coverage or surface Peclet number enhances the droplet deformation and motion, although the surfactant distribution becomes less non-uniform when the surfactant coverage increases. We then increase Ca_e and study the droplet breakup for varying λ, where the role of surfactants on the critical Ca_e ($Ca_{e,c}$) of droplet breakup is identified by comparing with the results of clean droplet. Like in clean case, $Ca_{e,c}$ first decreases and then increases with increasing λ, but the minimum $Ca_{e,c}$ occurs at $\lambda = 0.5$ instead of $\lambda = 1$ in clean case. The presence of surfactants always decreases the value of $Ca_{e,c}$, and its effect is more pronounced at low values of λ. In addition, decreasing viscosity ratio is found to favour ternary breakup in both clean and surfactant-covered cases, and tip-streaming is observed at the lowest viscosity ratio in surfactant-covered case.

Bubbly flows instabilities in the Eulerian-Eulerian and Eulerian-Lagrangian frameworks

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Abstract

Bubbly flows are characterised by instabilities that appear in the form of elongated meso-scale structures aligned along the direction of gravity. The instabilities result in a non-homogeneous distribution of the gas fraction in the system where high-cluster and high-voidage regions coexist. The correct prediction of the meso-scale dynamics is fundamental to formulate more accurate closure models for coarse-grained simulations applied to design systems of industrial scale. Two different frameworks are compared to test their capability of capturing the characteristic meso-scale structures: the Eulerian-Eulerian two-fluid model and a Eulerian-Lagrangian approach. We show that the Eulerian-Eulerian simulations are affected at low bubble loadings by unphysical numerical instabilities appearing due to the lack of hyperbolicity of the governing equation system. Unfortunately, the occurrence of the numerical instabilities cannot be predicted a priori, but when they are not present in the solution, the two frameworks are able to predict the same meso-scale dynamics. Our analysis suggests that, concerning meso-scale simulations, the Eulerian-Lagrangian approach produces physically faithful results and represents an ideal framework to formulate new closure models.

Keywords: Bubbly flows, Eulerian-Lagrangian framework, Eulerian-Eulerian framework, Two-fluid model

Channel flow laden with neutrally-buoyant spherical particles: flow regimes and heat transfer efficiency

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We consider suspensions of neutrally-buoyant finite-size rigid spherical particles in channel flow and investigate the macroscopic behavior of the suspension in terms of pressure gradient (flow drag) and heat transfer in the solid and liquid phases. We examine bulk Reynolds numbers from the laminar to the turbulent regimes $500 \leq Re \leq 5600$ and particle volume fraction up to 35%. Two different particle sizes are considered, corresponding to 1/10 and 1/15 of the channel gap width. The analysis is based on the results of interface- resolved numerical simulations exploiting an efficient Immersed Boundary Method [1].

The momentum budget reveals the existence of three different regimes: laminar, turbulent and a particulate dominated regime, denoted as inertial shear-thickening depending on which of the stress terms, viscous, Reynolds or particle stress, is the major responsible for the momentum transfer across the channel. In addition, we show that the high-particle concentration the solid phase distribution is not uniform but presents two peaks: one at the wall and the second at the centerline with local volume fractions higher than 50%, see also [2]. The onset of the particulate-dominated regime is observed to occur at lower solid volume fractions in the case of larger particles.

We will also consider the heat transfer in the suspensions, for three different values of the Prandtl number. The numerical implementation, based on a volume of fluid approach enables us to solve for the temperature in the solid and fluid phase, i.e. the temperature does not need to be uniform inside each particle, see [3]. The results clearly indicate that heat transfer is enhanced by the presence of the particles in the laminar regime, monotonically with the increase of the solid volume fraction. In the turbulent regime, however, the presence of the particles increases the heat transfer when compared with the single-phase turbulent flow at the same bulk Reynolds number only at low volume fraction. Increase the number of particles, the global heat flux decreases below the single-phase values. This is explained by the particle migration towards the channel center: here the local volume fraction is high, particle move as a compact aggregate with weak relative velocity, the turbulence is quenched, the fluid velocity fluctuations are significantly reduced and so is heat transfer. The analysis of the heat flux budget confirms that the reduction observed at high Reynolds numbers and volume fractions is associated with the decrease of the turbulent heat flux, correlation between temperature fluctuations and the wall-normal velocity.

Keywords: particle-laden flows, multiphase turbulence, heat transfer, interface-resolved simulations.

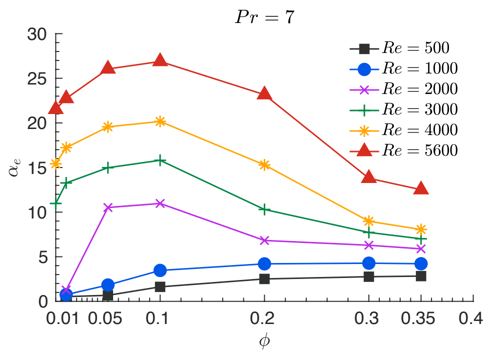

Figure 1: Effective heat transfer, normalised with the value in a laminar flow, versus the particle volume fractions for different bulk Reynolds numbers

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On the plug-to-slug transition in gas-liquid-solid three-phase flows

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Abstract

New experimental data have been obtained in a facility specially designed for analyzing three-phase gas-liquid-solid flows. Flow visualization has been performed for two and three-phase flows in horizontal 30 mm inner diameter and 4.5 meters long transparent acrylic pipes. A total of 134 flow conditions are analyzed and presented, including plug and slug flows in air-water two-phase flows and air-water-polypropylene three-phase flows.
The transition from plug to slug flow agrees with the flow regime maps available in the literature for two-phase flows. However, for three phase flows, a progressive displacement towards higher gas superficial velocities is found as the solid concentration is increased.

Keywords: Three-phase flows, Horizontal pipelines, Plug-to-slug flow transition, Flow visualization

1. Introduction

Three-phase flows are present in a wide range of industrial processes. However there is a lack of comprehensive studies regarding G/L/S mixtures because not all parameters or required measurements are reported in the available literature. Therefore, the current work aims to generate reliable database of three-phase G/L/S mixtures, flowing in horizontal 30mm ID pipelines for different flow regimes. Details of the experimental facility can be found in [1]. The G/L/S mixture is composed of air, water and polyethylene particles. The superficial velocity of the slurry phase is in the range of 0 to 2 m/s, with low concentrations of solids, in the range of 0 to 10%, and the air superficial velocity from 0 to 5 m/s.

2. Results and Conclusions

In fig. 1 the section of the regime map covered in the present study is displayed. Transition boundaries between plug and slug proposed by [2] and [3] for two-phase flows are indicated in the legend, as well as the proposed ones in the current study, for three-phase flows. Each test condition is plotted with a marker in the map, white marks correspond to air-water two-phase runs, grey marks to three-phase runs with 5% loading of solids and black marks to 10% loading; the flow regime visualized for each run is indicated with the shape of the markers, triangles for plug flow, diamonds for plug-to-slug transition and squares for slug flow.

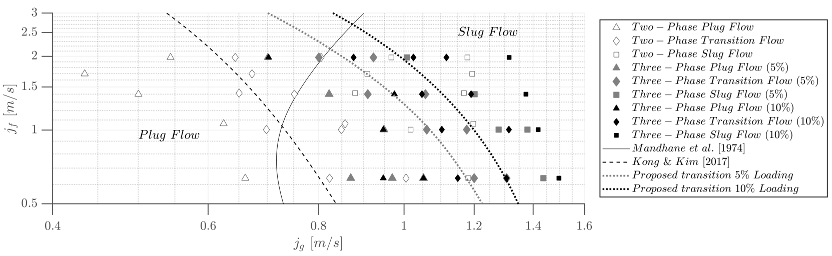

Figure 1: Flow regime map.

From the visual analysis of the two-phase runs it is observed that transition zones are wide, and they can hardly be expressed with a line. In any case, our measurements agree with the observations of [3] regarding the plug-to-slug transition. These authors claim that less air is required to reach slug flow at j_f above $1m/s$ and vice versa. For three-phase flows, it is observed that the accumulation of particles in the tail of plug flows, retards the small bubble detachment for increasing relative velocities, thus the transition from plug to slug flow is displaced towards higher gas superficial velocities.

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Migration of particles in a confined shear flow of non-Newtonian fluid

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ABSTRACT

Migration of particles in a confined shear flow of Giesekus fluid and power-law fluid is numerically studied. For the former, effects of the viscosity ratio, shear-thinning effect, Weissenberg number and wall confinement on the particle migration are examined. Results show that the particle migrates toward the wall, irrespective of whether the fluid is shear thinning. The wall confinement, shear-thinning and high Weissenberg number could respectively facilitate the particle lateral migration. While the effect of viscosity ratio on the particle migration is not monotonic, a separatrix value is found which divides the viscosity ratio into two ranges. The pattern of two particles migration can be roughly classified into returning and passing. The separatrix between returning and passing pattern is dependent on the initial vertical distance between two particles, Weissenberg number and shear-thinning effect. With other parameters fixed, the trajectories of particle change from the returning pattern to the passing pattern as the initial vertical distance between two particles and the Weissenberg number increase, but as the shear-thinning effect decreases. For the latter, single particle with different initial positions reaches the same equilibrium position for the same power-law index. The stable equilibrium position moves closer to the centerline under higher power-law index and blockage ratio. One-line of particles distributed initially at a vertical position will migrate to the vicinity of the wall and form single-line particle trains. The particle spacing is unstable and increased when particles migrate to the equilibrium position. The inertial focusing length is an important factor for analyzing the formation of particle trains, which will be longer with increasing the power-law index. The mean particle spacing will be reduced with increasing Re and blockage ratio. Two-lines of particles distributed initially and abreast along both sides of the centerline will migrate to the vicinity of the wall and form staggered particle trains. Final particle equilibrium position will deviate from the single particle equilibrium position. The particle spacing decreases with increasing the power-law index and blockage ratio, and with decreasing Re.

Keywords: Migration of particles, Giesekus fluid, power-law fluid, confined shear flow, numerical simulation

Motion behaviour of heavy particles in bounded vortex flows

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Abstract

An Eulerian-Lagrangian CFD model based on the discrete element method (DEM) and immersed boundary method (IBM) is adopted to numerically study the motion behaviour of heavy particles in circular bounded viscous vortex flows induced by one or two small rotating cylinders. Inter-particle and particle-wall collisions are considered by a hard-sphere collision model. Effects of Stokes number, Reynolds number, and the location of the small rotating cylinders are explored under both one-way and two-way couplings. Results show that, under one-way coupling, there is always a stable state for the accumulation of particles and various particle accumulation patterns are recognized. However, under two-way coupling, the stable accumulation points or closed trajectories appearing in cases under one-way coupling cease to exist, due to the intense interaction between particles and the gas phase. In addition, many more particles accumulate on the wall under two-way coupling than under one-way coupling at the same conditions and the percentage of particles accumulated on the wall increases with an increase in Reynolds number and Stokes number, whereas it decreases as the center-to-center distance between the circular domain and small rotating cylinder increases under both one-way and two-way couplings.

Keywords: Bounded vortex flows, one-way coupling, two-way coupling, particle accumulation pattern

Boundary layer models to predict particle wall deposition in enclosed turbulent natural convection flows

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Abstract

Understanding the transport and deposition of particles and aerosols in enclosed spaces is key in determining the preferential spatial location of the deposition and the rate at which particles accumulate on a given surface. This information has important implications in designing better buildings, public spaces; as exhibition rooms in museums; and display cases for art works. Here we focus on the deposition of particles transported by turbulent natural convection flows in confined spaces. We developed a simple model based on the boundary layer theory to predict the particle deposition in a prototypical configuration consisting in a closed cubical cavity where the bottom (floor) and one side (wall) are kept at a constant temperature higher than that of the top (ceiling) and opposite side wall. The remaining two lateral sides are thermally insulated. In this study we compare the predictions with measurements reported in the literature.

Keywords: Particle deposition, Turbulent natural convection, Thermophoresis, Brownian diffusion

The enclosed turbulent natural convection flow configuration considered was used by Thatcher et al. [1] to measure experimentally the particle deposition of particles of diameters from 0.1 μm to 2.5 μm at relatively large Rayleigh numbers ($Ra=5.4\cdot10^8$ and $Ra=3.6\cdot10^9$). At these Rayleigh numbers the horizontal and vertical boundary layers are well reproduced by mixed convection laminar boundary layers approximations, as recent direct numerical simulations of the flow have shown [2]. The forced convection flow is imposed by the large-scale flow circulation outside the boundary layers while the natural convection contribution originates from the buoyancy effect produced by the wall thermal boundary conditions. Under these flow conditions the size of the submicron particles is about 10000 times smaller than the boundary layer thickness and consequently the deposition process is governed by the flow within the thin boundary layers. The mixed convection boundary layer equations consider the hydrodynamic drag force, the Brownian motion, the thermophoretic force and the gravity force.

Figure 1 shows the deposition velocities measured by Tatcher et al. [1] in air at $Ra=5.4\cdot10^8$ and $Ra=3.6\cdot10^9$ using solid ammonium fluorescein particles with diameters of 0.1 μm, 0.5 μm, 0.7 μm, 1.3 μm and 2.5 μm. Measurements were performed in the four thermally active walls of the cubical cavity. In Figure 1, the dashed lines indicate the detection limit of the experiments and the red lines correspond to the model predictions. It can be seen that for the smallest particles the thermophoretic effect produces a larger deposition on the cold walls than on the hot walls. As the diameter of the particle increases gravity promotes the deposition mainly on the hot floor. Figure 1 shows that in general the predictions of the boundary layer models reproduce well the trends observed in the experiments. This indicates that, in principle, this model can be used to predict particle wall deposition in confined turbulent natural convection flows as those encountered in display cases for exhibition of art works.

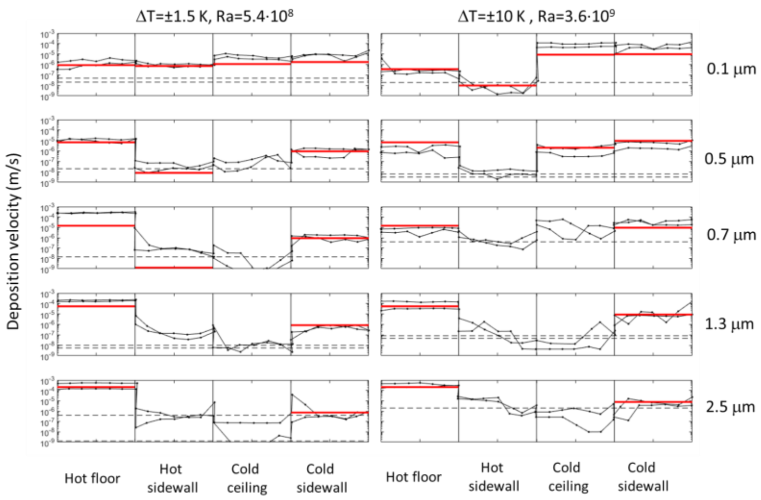

Figure 1. Comparison of the model predictions and measurements.

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Direct Numerical Simulation of turbulent transport and wall deposition of airborne particles on thermally active enclosed cavities

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Abstract

Our ability to understand the processes by which airborne particles are transported and settle on walls is key in a wide range of applications that include pollutant dispersion, aerosol deposition, public venue ventilation and soiling of valuable surfaces. In this work we have numerically investigated the transport and surface deposition of particles in a cubical cavity with differentially heated walls. The particles suspended in the turbulent flow are assumed to be transported by means of hydrodynamical drag, buoyancy, thermophoresis, lift and Brownian effects. Direct Numerical Simulations are used to obtain the hydrodynamic field at $Ra = 5.4 \times 10^8$ while particle trajectories are integrated using Exponential Tracking Schemes that alleviate the time step constrains associated to fully-explicit methods. Spatial distributions of deposition rate are reported for the horizontal and vertical pairs of 'hot' and 'cold' walls plus the two lateral adiabatic surfaces. The transport regime for the particle diameters considered here, 0.1 and 0.5 µm, is of special interest in applications where surface soiling and its minimization is critical. The comparison between numerical results and experiments suggests that this inertial particle model is capable of reproducing the transport and wall deposition in thermally active turbulent flows.

Keywords: turbulent transport, particle deposition, DNS

The transport equation of an idealized spherical and smooth particle can be derived from the balance of forces acting upon it. The position of a given particle x_i^* can be written as $dx_i^*/dt = u_i^*$ where the particle velocity u_i^* can be determined as:

$$\frac{du_i^*}{dt} = \underbrace{\frac{u_i - u_i^*}{\tau_p}}_{\text{Drag}} + \underbrace{n_g \delta_{i3}}_{\text{Weight}} + \underbrace{n_{th} \frac{\partial T}{\partial x_i}}_{\text{Thermophoresis}} + \underbrace{n_l \varepsilon_{ijk} \left[u_j^* - u_j \right] \omega_k}_{\text{Lift}} + \underbrace{n_i(t)}_{\text{Brownian}} \tag{1}$$

where u_i, ω_i and T are the background flow velocity, vorticity and temperature at the particle position, τ_p is the particle relaxation time and n_g, n_{th}, n_l and n_i are prefactors in the buoyancy, thermophoresis, lift and Brownian forces definitions respectively. Figure 1 shows an instantaneous flow velocity field at $Ra = 5.4 \times 10^8$ (left panel) [2], instantaneous positions and velocities for a small sample of particles (central panel) and deposition position over the two adiabatic walls in different colors over a time span of $\Delta t \approx 40$ time units (right panel). Despite this preliminary small number of deposited particles over the adiabatic walls, a pattern already emerges suggesting that particles tend to accumulate at the corners where 'hot' and 'cold' walls meet. These results provide detailed information about preferential deposition spots with a much larger detail than currently available experiments [1].

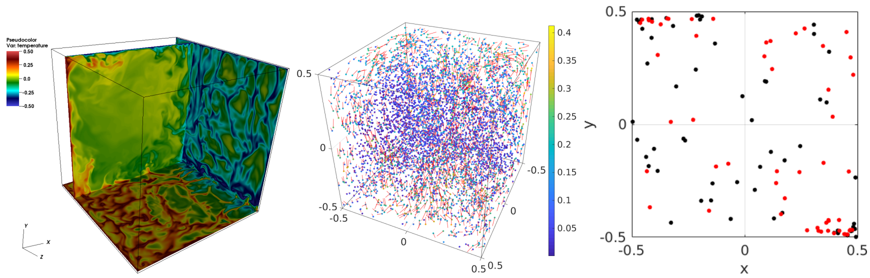

Figure 1: Instantaneous flow velocity at $Ra = 5.4 \times 10^8$ (left), position of 5000 particles (velocity magnitude shown in color and tail length) and particle deposition location over the adiabatic walls (right).

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Large-scale Direct Numerical Simulation for Investigating the Effects of Mesoscale Structure in Gas-solid Flow

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Abstract

A coupled lattice Boltzmann method and discrete element method (LBM-DEM) approach is usually a kind of particle-resolved direct numerical simulation (DNS) algorithms for modeling gas-solid flows, in which the size of fluid grid is generally one magnitude smaller than particle diameter and force acting on particles directly calculated by integrating both viscous force and pressure gradient force on the particle's surface. It has been regarded as the most accurate numerical method for simulation of gas-solid flow. However, the disadvantage is its huge computational cost resulting from small grid size and time step limited by Kolmogorov length and time scales. Only hundreds of particles scale is reported for DNS of gas-solid flow in the latest literature, which is far from the number of particles in the real gas-solid flows. In order to improve computational speed and scale for DNS of gas-solid flow, an immersed boundary method in framework of LBM has been adopt to realize the fluid-solid coupling to avoid a stair-step representation of the solid particles' surfaces [1, 2] and the multi graphics processor units (GPUs) parallel computing of LBM-DEM approach has been implemented. Taking advantage of the inherent parallelism of LBM and the attractive Flops/Price ratio of GPU, we have implemented 576 GPUs parallel computing on a Mole-8.5 system and conducted the largest-scale DNS of gas-solid suspensions so far, with 1,166,400 solid particles in an area of 11.5cm x 46cm for a two-dimensional system and 129,024 solid particles in a domain of 0.384cm x 1.512cm x 0.384cm for a three-dimensional system [3]. The scale of DNS data has been reached the statistical size in traditional computational grid, which implies the really meaningful statistical results from large-scale DNS of gas-solid flows were obtained for the first time. The effects of mesoscale structure on the interaction force between gas and solid phases [4] and the statistical properties of particles [5] were explored. Finally, a new drag correlation as the function of three variables: solid volume fraction, particle Reynolds number and Froude number is proposed with consideration of scale-dependence [6].

Keywords: Lattice Boltzmann method, Discrete element method, Direct numerical simulation, Mesoscale structure, Gas-solid flow

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Modulation of turbulence intensity by heavy finite-size particles in upward channel flow

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Abstract

It has been recognized that generally large particles enhance the turbulence intensity, while small particles attenuate the turbulence intensity. However, there has been no consensus on the quantitative criterion for the particle-induced turbulence enhancement or attenuation. In the present study, interface-resolved direct numerical simulations of particle-laden turbulent flows in an upward vertical channel are performed with a direct-forcing fictitious domain method to establish a criterion for the turbulence enhancement or attenuation. The effects of the particle Reynolds number (Re_p), the bulk Reynolds number (Re_b), the particle size, the density ratio and the particle volume fraction on the turbulence intensity are examined. Our results indicate that at low Re_p the turbulent intensity across the channel is all diminished, at intermediate Re_p the turbulent intensity is enhanced in the channel center region and attenuated in the near-wall region, and at sufficiently large Re_p the turbulent intensity is enhanced across the channel. The critical Re_p increases with increasing bulk Reynolds number, particle size and particle-fluid density ratio, while increasing with deceasing particle volume fraction particularly for the channel center region. The criteria of the enhancement or attenuation are provided for the total turbulence intensity in the channel and the turbulence intensity at the channel center, respectively, and both are shown to agree well with the experimental data in the literature. The particles attenuate the turbulence by inhibiting the large-scale vortices, while enhancing the turbulence by generating the wake vortices, and the critical Re_p for the turbulence enhancement or attenuation depends on the competition between the large-scale vortices and particle-induced wakes. The effects of the particle wakes are related to the interfacial term in the turbulent kinetic energy.

Keywords: Particle-laden flows, Vertical turbulent channel, Turbulence modulation, Interface-resolved direct numerical simulations

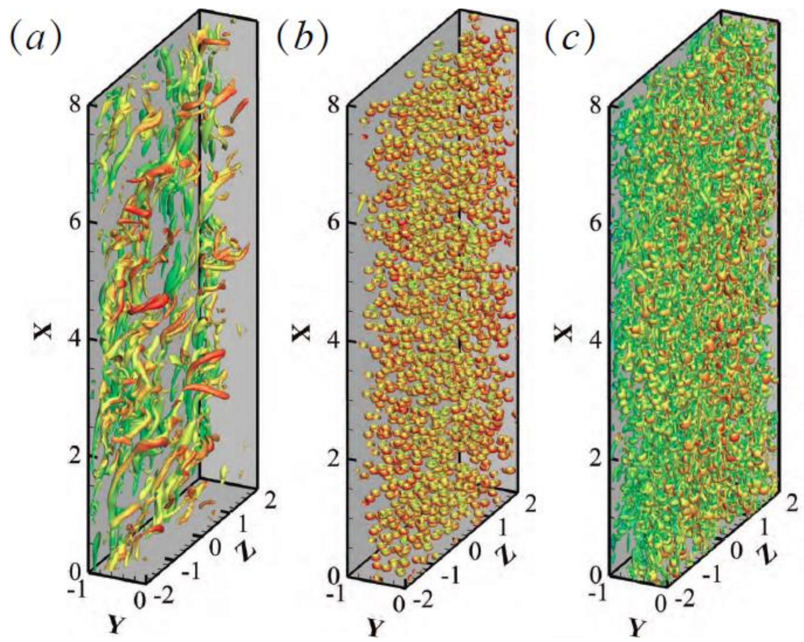

Figure 1: Vortex structures of the (a) single-phase flow and the particle-laden flows for: (b) u_i/u_b=0.25, (c) u_i/u_b =0.45. The colour of the vortices represents the fluid streamwise velocity.

Interface-resolved simulations of particle-laden turbulent channel flow

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Turbulent wall flows laden with small inertial particles are found in different contexts, from engineering devices to environmental flows. Dealing with very dilute conditions, the so-called one-way coupling regime takes place with particles transported by the fluid without back and mutual reactions. In the limit of high density ratio, the equations governing the particle dynamics are often simplified to a balance between inertia and drag [1]. Several numerical studies are based on this model. At present, it has become possible to simulate these flows without relying on the point-particle assumption. In other words, it is now possible to directly approximate the no-slip/no-penetration boundary condition on the surface of hundreds of thousands , or even millions of spherical particles [2]. In the present work we revisit the problem of particle-laden turbulent channel flow in the *point-particle limit*, with insights from interface-resolved direct numerical simulations. The numerical method uses an efficient immersed-boundary method, extended with closure models short-range particle-particle and particle-wall interactions [3].

We simulated different turbulent channel flow configurations with varying mass fraction, for fixed Reynolds number, $Re = 5600$, and particle size of about 3 viscous wall units. See figure 1-left for a visualization. The goal is to mimic the so-called 1-way, 2-way and 4-way coupling regimes. The number of particles was varied from 500 to 50 000 particles (volume fraction $O(10^{-3} \div 10^{-5})$), simulated on a mesh with 12 grid points over the particle diameter, corresponding to 13.5 billion grid points.

Concerning the most dilute regime, solid volume fraction $O(10^{-5})$, we observed that particle feedback on the flow is negligible so we compared the data with those of corresponding one-way-coupled point-particle simulations considering only the non-linear viscous drag. In the bulk of the channel, particle velocity statistics from the point-particle DNS agree well with those from the interface-resolved DNS, while major differences are found close to the wall. E.g. the local particle concentration of the point-particle simulation is more than twice the one of interface-resolved simulation, see figure 1-right panel. We show that the discrepancies are due to the intense shear of the near wall region and that using a proper lift model the predictions can be improved. In the final paper, we will also present results on the modulation of turbulence found at higher bulk volume fractions.

Keywords: DNS, turbulent channel flow, inertial particles, lift force

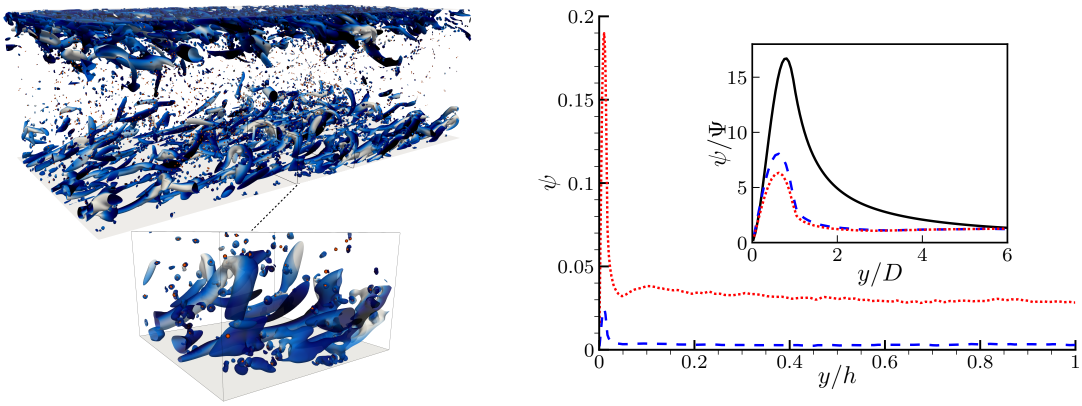

Figure 1: Left panel: visualization of the turbulent flow structures (Q-criterion) and interface-resolved particles. Right panel: local mass fraction ψ and normalized mass fraction ψ/Ψ (inset) of interface-resolved simulations in very dilute condition (blue), in dilute conditions (red), corresponding 1-way point-particle simulation in black.

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Probing Opaque Flows: the cavitating venturi benchmark

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Abstract

Flow measurement in (dispersed) multiphase flows is often hampered by the opacity of the medium. This means that traditional methods (such as laser-Doppler Anemometry and Particle Image Velocimetry) cannot be used, as they require a clean, transparent fluid. In this presentation, I will summarise our recent efforts to combine various measurement methods to extract as much information as possible from a number of benchmark cases. The main focus will be on cavitation in a converging-diverging 'venturi', a benchmark case showing complex partial cavitation dynamics [1]. A mobile test facility was constructed that allowed us to collect data at various laboratories equipped with specialised measurement equipment. High-speed imaging provided insight in the dynamics of the partial cavitation process (e.g. shedding frequency, growth rate of the cavity) [1]. Particle Image Velocimetry yielded velocity fields to predict where cavitation will first occur. Computed tomography using X-ray imaging provided accurate mean void fraction measurements, i.e. the local ratio of vapour and liquid [2]. Finally, Magnetic Resonance Velocimetry (MRV) also provided time-averaged velocity fields [3]. Importantly, this modality is expected to be insensitive to the presence of vapour bubbles. The four modalities each provide different information - or different parts of the puzzle; it is the combination that allows us to better understand cavitation dynamics.

During the Symposium, I will present the latest results and comment on what can be expected from these measurement techniques. I will also briefly report on experiences from another benchmark: particle-laden pipe flow. For this benchmark, we combined imaging (low volume fractions) and ultrasound imaging velocimetry (for volume fractions up to 20%). Again, the combination of techniques allowed an unprecedented insight in the dynamics of this complex flow [4].

Keywords: flow measurement, multiphase flow, cavitation

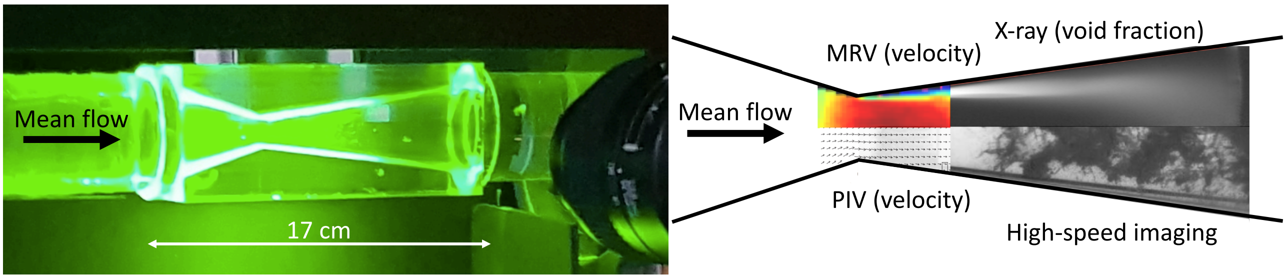

Figure 1: Cavitating flow in a venturi. To give an overview of the geometry, the left-hand side shows a photograph of the facility during PIV measurements. In the right-hand side, a composite image shows the data obtained using four modalities: (1) MRV provides the mean flow field, (2) PIV provides both instantaneous and mean flow fields, (3) x-ray tomography provides vapour void fractions, and (4) high-speed imaging provides the dynamics of the cavitation process. Note that this composite image serves to illustrate the project approach and data sets were obtained in separate experiments, not necessarily under the same conditions.

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Experimental Observation of the Elastic Range Scaling in Turbulent Flow of Dilute Polymer Solution

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Abstract

We present an experimental study of velocity scaling in the turbulent von Kármán swirling flow of dilute polymer solution. It is found that due to the addition of the polymers a new scaling range, referred as elastic range, emerges in between the dissipation range and the inertial range. In this new elastic range the second-order longitudinal velocity structure functions $S_L^2(r) \sim r^{1.38}$. The cross-over scales of the dissipation-elastic ranges, and the elastic-inertial ranges are determined by extending Batchelor's parameterization to turbulent flow with polymer additives. We propose that the energy flux through the elastic degree of freedom of polymers increases, while that through the turbulent flow decreases, with decreasing length scale r. This scale dependent energy flux model successfully shows that for turbulence of dilute polymer solutions the velocity structure function in the elastic range scales as $S_{L,p}^n \sim r^{(0.70\pm0.02)n}$ with intermittency correction.

Keywords: Turbulent flow, Energy Cascade, Polymer Solution

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On μ(I) rheology of dense granular flows – can we get a mesh-independent solution?

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Abstract

We deal in this work with continuum modelling of dense granular flow applied to handing of pharmaceutical particles. We use the μ(I) rheology model that makes the governing equations have the same structure as the Navier-Stokes equations, with the exception that the viscosity is here pressure- and strain-rate dependent. We first characterize the pharmaceutical particles in terms of the μ(I)-rheology model using a modified Malvern Kinexus rheometer. We then investigate a discharge of these particles from a hopper using a continuum Navier-Stokes solver based on the Volume-Of-Fluid (VOF) interface-capturing numerical method. We show that the framework is inherently ill-posed, i.e. that it exhibits a linear instability in which short-wavelength perturbations grow at an unbounded rate. Consequently, the numerical solutions will depend on the grid resolution and we argue that great caution is required when making a one-to-one comparison with experimental data. Finally, we discuss and test a number of approaches for regularizing this instability, in the first case by changing the formulation of the μ(I) function for both low and high inertial (I) numbers.

Keywords: granular flow, μ(I) rheology, ill-posedness, regularization

Multi-way couplings between inertial particles and turbulence in a swirling flow

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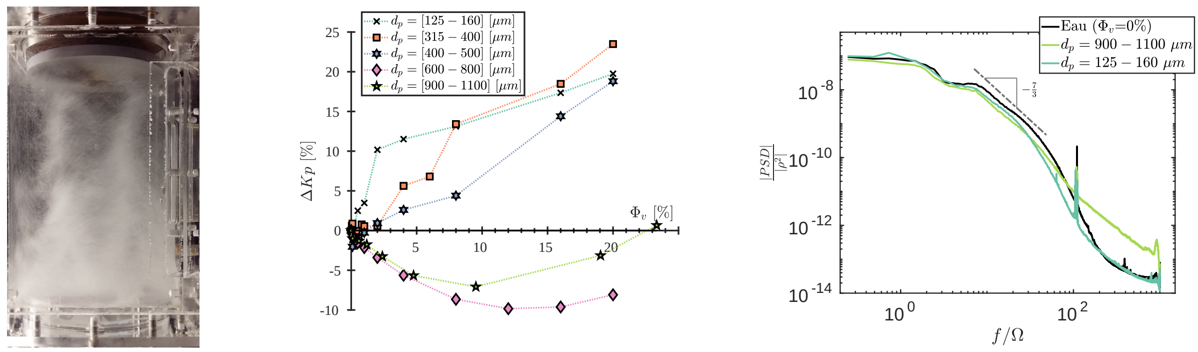
Abstract

Particle laden flows particles are ubiquitous in nature (pyroclastic flows, drops of water in clouds ...) and industry (industrial mixers, combustion of fuel droplets in a diesel engine, pollutants, etc.). In most situations the flow is turbulent and the interactions between the particles and the flow are complex due to both the random and multi-scale nature of the turbulence and the particles properties which involve additional effects due to inertia, gravitational settling and mass loading to mention just a few. The present work focuses on flows highly seeded with inertial particles. In this situation the flow and the particles are strongly coupled [1] as not only the flow transports the particles (one-way coupling), but particles modify the flow (two-way coupling) and possibly also interact between each-other (four way coupling).
We have explored these multiple couplings in a vertical swirling flow of water (Fig. 1a), seeded with glass spheres with diameter d_p ranging from 125μm to 1mm and volume fractions in the range $\Phi_v \in [0-20]\%$. For moderate seedings ($\Phi_v \lesssim 1\%$) , we have deployed optical diagnoses to characterize the spatial distribution of particles as they experience both gravitational settling and turbulent resuspension. This first study shows peculiar non-linear and non-monotonic effects, hints of the existence of subtle couplings between the dispersed and the continuous phases. We further explore these couplings by measuring the modulation of turbulence as the volume fraction of particles is increased up to 20%. In this situation the suspension is opaque and conventional optical diagnoses are useless. We have therefore implemented "multi-scale" indirect measurements: (i) a global measurement of the mechanical power required to suspend the particles (with an imposed average velocity) to explore global turbulence modulation and (ii) a measurement of turbulent pressure fluctuations to explore which scales of the flow are effectively impacted by the particles. Our measurements reveal that for a given volume fraction and average velocity, suspending small particles requires more power than suspending large particles (Fig. 1b) and more power than driving a single phase fluid with equivalent density. The multi-scale pressure diagnoses (Fig. 1c) suggest that these trends can be attributed to two different coupling regimes: (i) frictional for small particles with a modified effective rheology of the suspension and (ii) inertial for the large particles with reinjection of mechanical energy at particle scale through wake interactions.



(a) (b) (c)

Figure 1: (a) Swirling flow generated by an impeller rotating at the frequency Ω at the top of a vessel full of water. seeded with particles (b) Compensated mechanical power K_p as a function of volume fraction for various particle diameters. (c) Temporal spectrum of pressure fluctuations for small ($d_p \simeq 150\mu$m) and large ($d_p \simeq 1$mm) particles. Solid black line shows the reference case of pure water.

Keywords: particle laden flows, inertial particles, turbulence, suspensions, two-way coupling.

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Effect of electrostatic charges on the dispersion of inertial particles transported by a homogeneous isotropic turbulent flow

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Abstract

Particle-laden turbulent flows are found in a wide range of industrial of geophysical flows. In these flows many complex phenomena take place such as the turbulent dispersion, the inter-particle collisions, two-way coupling, particle-wall bouncing. In addition, the inter-particle collision and the particle-wall bouncing may lead the particles to be electrically charged. Once it happens, the forces due to the charges carried by the particle may have an effect on the particle dispersion [1]. Such a mechanism is in competition with the turbulent dispersion due to gas-particle interaction via the drag forces. The present study investigates how the particle dispersion is modified when the particles are charged. A pseudo-spectral approach is used to perform Direct Numerical Simulation (DNS) of turbulent flows coupled with a Lagrangian tracking of particles. The configuration is a statistically steady homogeneous isotropic turbulent flow. Hence a stochastic forcing is applied and periodical boundary conditions are applied The fluid flow is maintained statistically steady by a stochastic scheme [2]. The Navier-Stokes equations are solved by a pseudo-spectral method. The long- and short-range interaction forces are taken into account by a specific algorithm [3]. The numerical solver is parallel for the fluid and for the particles (including the collisions). The Fast Fourier Transform are operated by P3DFFT [4].

Two main results have been obtained. First, when the particles are charged the particle agitation decreases compared to the one obtained without charges. We show that this destruction of particle agitation comes not directly from the electrostatic forces but from the destruction of the fluid-particle covariance. Indeed, in the present configuration the particle agitation is directly linked to the fluid-particle covariance in the framework of the Tchen-Hinze's theory [5]. The effect of the charges on the fluid-particle covariance is analysed in terms of the Stokes number, defined as the ratio between the particle response time to the fluid turbulence characteristic time scale, but also in terms of Electrostatic Stokes number defined as the ratio between the characteristic time scale of the electrostatic forces to the particles response time. The second kind of results concerns the particle spatial distribution. Indeed, for a given range of Stokes number, the particles may accumulate in specific zones of the turbulent fluid flow leading to a non-uniform distribution of particles. We analysed how the charges modify this phenomenon also called preferential concentration.

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Keywords: electrostatic forces, particle dispersion, preferential concentration

Assessment of the Parcel model in LES of Turbulent Evaporating Sprays

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Evaporation and combustion of turbulent sprays are crucial processes in propulsive applications. In a turbulent spray, evaporating dispersed droplets are transported by the gaseous carrier phase exchanging mass, momentum and energy and determining a strong coupling between the two phases. To computationally address this problem two issues need to be tackled: The wide range of turbulent scales and The huge number of droplets. Given the multiscale coupling between the two phases the Large-Eddy-Simulation (LES) techniques where the most energetic large-scale motions are simulated appears a promising choice. In order to reduce the computational droplet number, it is necessary to represent a subset of droplets using the so-called parcel method, e.g. [1]. A computational particle represents a parcel which comprises a group of physical particles having same properties, e.g. velocity, temperature and diameter. In this context, the present work aims to investigate of role of parcel model in turbulent evaporating spray simulations focusing on the question: How large can we fix the parcel to droplet ratio (PR)? In order to answer to this point we use LESs of turbulent evaporating jets at Reynolds number $Re_D = 10^4$ with different PRs. These simulations have been compared with a corresponding fully resolved DNS simulation, see fig. 1. The numerical tool is a validated MPI parallel code which solves the low-Mach number formulation of the Navier-Stokes equations on a cylindrical domain coupled with a Lagrangian solver to account point-droplets position, radius and temperature, see [2] for more details. We initially focused on LES simulations with a mesh 4 times coarser than DNS for each direction that well captures the turbulent flow field. We show that the vaporization length slightly increases with the parcel ratio PR, i.e. evaporation is slower when less parcels are considered, see fig. 1. However, the overall dynamics are well captured up to PR=111, i.e. when 111 physical droplets are replaced with one parcel. We also performed LES with a coarser mesh (8 in each direction), and we found that the evaporation main features can be reproduced with an even larger parcel ratio. The results appear to indicate that the limit boundary of PR scales with the computational cell volume for LES of turbulent spray simulations. More details will be given in the final paper.

Keywords: spray dynamics, parcel, turbulent evaporation, DNS, LES

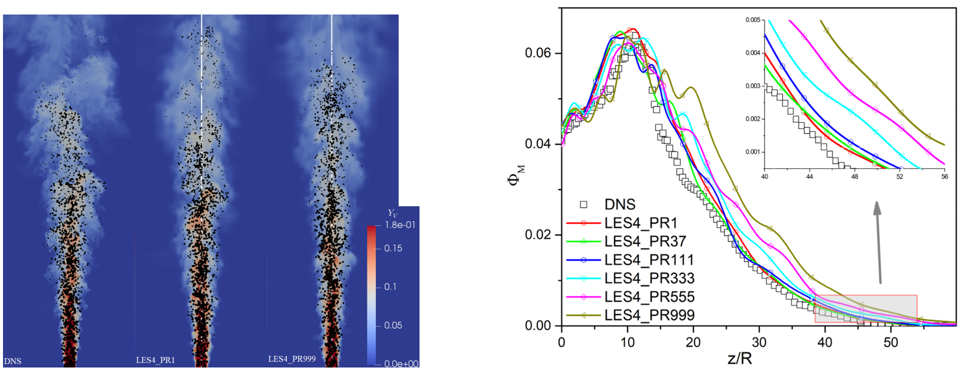

Figure 1: The left panel shows an axial-radial slices of the instantaneous vapour concentration field, Y_V , and droplets distribution for DNS, LES with PR=1 and LES with PR=999. The right panel shows evolution along the jet axis of the mean droplet mass fraction Φ_M for DNS and LES with different PRs.

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Modeling of Multiphase Reactors in Engineering: A Mesoscale Perspective

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Abstract

Mesoscale transport phenomena and mechanisms are essential to achieve a more fundamental understanding on the mass, momentum and heat transfer in the classical study of transport phenomena and on the mixing, residence time distribution and rate-limiting analysis in chemical reaction engineering, yet they are now beyond the scope of classical textbooks of chemical engineering. We highlight a heuristic mesoscale modeling approach starting from a conceptual Energy-Minimization Multiscale (EMMS) model and ending at the stability-constrained multifluid CFD model. While the stability condition determines the direction of system evolution, the stability-constrained CFD further describes the dynamics of structure evolution. We establish the Dual-Bubble-Size (DBS) model, an extended EMMS approach for gas-liquid systems. Stability condition is formulated as the minimization of the sum of two energy dissipations, reflecting the compromise of a liquid-dominant regime at which smaller bubbles prevail and a gas-dominant regime favoring the existence of larger bubbles. It supplies a mesoscale constraint for conservation equations, and a mesoscale perspective to understand the macroscale regime transition. The model calculation for gas-liquid and gas-solid systems demonstrates the intrinsic similarity of the two systems: the system evolution at macroscale is driven by stability conditions. Theoretically stability condition may offer closure laws for CFD simulation, leading to the stability-constrained multifluid CFD model. While direct integration is difficult, we propose various simplified approaches to derive the closure models for drag, bubble-induced turbulence and correction factors for coalescence rate in population balance equations. The stability-constrained multifluid CFD model shows much advantage over traditional closure models. We will also show how this model is applied in complex liquid-solid flow of swelling particles in olefine polymerization and in predicting the drop size in liquid-liquid emulsification.

Keywords: Multiphase Flow, Fluidized Bed, Bubble Column, Mesoscale, Reactor

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1. Introduction

The increasing tempo of change in human life, society, economics and environment creates a correspondingly urgent need for scientists and engineers seeking for new perspectives for traditional problems some of which may be longstanding, or posing new questions and offering new answers. For example, although new catalysts and chemical technologies can be invented or patented in laboratory every year, process scaleup from laboratory to industrial application remains a troublesome or challenging issue. Successful cases are limited and risky, relying on the empirical correlations and the engineers whose knowledge and experience is acquainted through the long-term case study of previous well-established processes. It is generally acknowledged that the main technical problem, among others, is how to create an ideal transport environment for reactions and separation, and hence chemical reactions could be compatible with their carrier, i.e., the fluid flow, mass and heat transfer in multiphase reactors. A new angle to achieve a fundamental understanding and then seek efficient solutions of these classical problems is to reveal the mystery on mesoscales, i.e., the mesoscale transport phenomena and mechanisms relevant to bubbles, droplets and particles. Actually, mesoscale problems are essential to a more fundamental understanding of momentum, mass and heat transfer in the classical study of transport phenomena, and to the mixing, residence time distribution and rate-limiting analysis in the chemical reaction engineering, yet they are beyond the scope of those classical textbooks of chemical reaction engineering. Basically, there are two kinds of meso-scale problems in chemical reaction engineering, i.e., the mesoscales at the interfacial/material level and the mesoscales at the reactor level, each of which displays diverse mesoscale structures and phenomena, but some common principles may reside. Understanding the two mesoscale problems and their coupling is of great significance to the rational control and optimization of chemical processes[1-4].

2. Methods

Despite the complexity of mesoscale structures and mechanisms, we highlight a heuristic mesoscale modeling approach for multiphase reactor systems, starting from a conceptual Energy-Minimization Multiscale (EMMS) model and ending at the stability-constrained multifluid CFD model. While the stability condition determines the direction of system evolution, the stability-constrained CFD further describes the dynamics of structure evolution. By resolving the structures and dominant mechanisms, it is possible to establish a stability condition reflecting the compromise between different dominant mechanisms for multiphase reaction systems, and the stability condition supplies a mesoscale constraint in addition to mass and momentum conservation equations.

We establish the Dual-Bubble-Size (DBS) model, an extended EMMS approach for the gas-liquid flow in bubble column systems. The total energy dissipation in gas-liquid systems can be resolved into three parts, i.e., Nsurf, Nturb and Nbreak. The former two are directly dissipated at microscales. The third reflects a kind of mesoscale energy dissipation, i.e, the energy stimulated from the interaction of turbulence eddies with bubbles and then stored temporarily as surface energy generated from bubble breakage and finally released to the liquid bulk phase during bubble coalescence. The mesoscale dissipation is used to sustain the formation and evolution of mesoscale structures and serves as a buffer for energy dissipation. Stability condition is formulated as the minimization of energy directly dissipated at microscales (Nsurf+Nturb → min) or equivalently the maximization of energy consumption at mesoscales (Nbreak → max). It reflects the compromise between two dominant mechanisms: Nsurf → min represents a liquid-dominant regime and in this case larger bubbles are likely to break into those smaller bubbles which prevail in the system. Nturb→ min represents a gas-dominant regime to favor the coalescence of smaller bubbles and the existence of larger bubbles. Stability condition in the DBS model is used to close the simplified conservation equations and hence the structure parameters can be obtained.

3. Results and Discussion

Stability condition provides a mesoscale perspective to understand the flow regime transition at macroscale in bubble columns. The transition can be interpreted as the jump change of the global minimum point of micro-scale energy dissipation in the 3D space of structure parameters. The calculation of EMMS model demonstrates also that it is the stability condition that drives the structure variation and system evolution at macroscales, which may be the intrinsic similarity of gas-solid and gas-liquid systems. Theoretically stability condition may offer closure laws for CFD simulation, leading to the stability-constrained multifluid CFD model. While the direct integration is difficult, we propose various simplified approaches to derive the closure models for drag, bubble-induced turbulence and the correction factors for the kernel functions of bubble coalescence or breakup for population balance equations. The stability-constrained multifluid CFD model shows much advantage over current closure models. This theory is applied to gas-solid fluidization [5-6] and gas-liquid bubble column reactors, with further extension to gas-liquid-solid three phase flows and stirred tanks[7-9]. Several industrial applications on meso-scale modeling in liquid-solid polyethylene reactors and liquid-liquid emulsification systems will also be highlighted.

4. Conclusions

Mesoscale transport phenomena and mechanisms indeed offer new angles to achieve a more fundamental understanding on the traditional problems in chemical engineering. Despite these explorations and knowledge on mesoscales, mesoscale transport phenomena and mechanisms would continue to be a challenge for multiphase reaction systems. For example, there are currently no general guidelines to identify the dominant mechanisms and formulate the stability condition for different specific systems. Although we establish mesoscale models for gas-liquid and gas-solid systems, the presence of particles in gas-liquid-solid systems and the internals used to intensify the mixing in multiphase reactors have great influence on mesoscale structures, which requires further investigation. The adsorption of surfactant on bubble or droplet surface constitutes another mesoscale problem at the interfacial level, and it is necessary to bridge this mesoscale problem and the mesocale at the reactor level before we could completely understand the complexity of multiphase reaction systems..

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Mesoscopic simulations of dispersed multiphase flows: recent results and open issues

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Abstract

Turbulent flows laden with finite-size solid particles, liquid droplets, and gas bubbles are encountered in a variety of industrial and environmental applications. The rigorous approach to study details of such dispersed multiphase turbulent flows is to numerically resolve the disturbance flow around each particle, known as the interface-resolved simulations (IRS). The key of conducting IRS is to enforce no-slip boundaries on the particle surfaces accurately and efficiently. Due to its flexibility in boundary treatments, in recent years mesoscopic methods based on the Boltzmann equation, such as the lattice Boltzmann method and gas kinetic schemes, have been developed and applied to these flows. In this talk, we discuss how a sharp interface representation of moving fluid-solid interfaces can be achieved with a good numerical stability and computational efficiency. To further illustrate the potentials of mesoscopic simulation methods as well as challenging issues, we consider three specific examples: (a) single-phase turbulent channel flow, (b) turbulent channel flow laden with a few finite-size fixed particles near the channel walls [1], (c) turbulent channel flow laden with neutrally buoyant finite-size moving particles [2]. In the first example, we focus on the proper treatment of the no-slip boundary condition on the channel wall, in order to be consistent with the Chapman-Enskog expansion required for flow hydrodynamics. In the second example, we investigate how the wall generated turbulence interacts with the fixed particles and how as a result the global turbulence statistics are modified. All terms in the budget equations of total and component-wise turbulent kinetic energies (TKEs) are explicitly computed using the data from direct numerical simulations. Particles are found to modify turbulence by two competing mechanisms: the reduction of the intrinsic turbulence production associated with a reduced mean shear due to the resistance imposed by solid particles, and an additional TKE production mechanism by displacing incoming fluid. In the third example, we focus on turbulence modulation by finite-size moving solid particles, the distribution of solid particles, and mean-field equations of the flow. Two particle sizes are considered, with diameter equal to 14.45 and 28.9 wall units. To understand the roles played by the particle rotation, two additional simulations with the same particle sizes but no particle rotation are also presented for comparison. Particles of both sizes are found to form clusters. Under the Stokes lubrication corrections, small particles are found to have a stronger preference to form clusters, and their clusters orientate more in the streamwise direction. As a result, small particles reduce the mean flow velocity less than large particles. Particles are also found to result in a more homogeneous distribution of TKE in the wall-normal direction, as well as a more isotropic distribution of TKE among different spatial directions. To understand these turbulence modulation phenomena, we analyze in detail the total and component-wise volume-averaged budget equations of TKE with the simulation data. This budget analysis reveals several mechanisms through which the particles modulate local and global TKE in the particle-laden turbulent channel flow. Through the above examples, we hope to encourage discussions on the advantages and open issues of mesoscopic simulation methods when compared to the Navier-Stokes solvers [3]. Specifically, the no-slip boundary treatment methods in LBM, including the immersed boundary method (IBM) and the bounce-back schemes (BBS), and their advantages and potential problems will be discussed.

Keywords: particle-laden flow, turbulent channel flow, lattice-Boltzmann method, direct numerical simulation

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Interactions between two bubbles rising side by side under the influence of magnetic field

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Abstract

A series of three-dimensional numerical results are reported about the interactive behaviours between a pair of bubbles rising side by side in different liquids, and through fully solving the three-dimensional Navier-Stokes equations, different interactions between the two bubbles are reproduced, such as the repelling, the attracting coalescence, the attracting bounce, and the repeated bounce, which are also observed in the experiments. After that, different magnetic fields are imposed to investigate the magnetohydrodynamics (MHD) effects on the bubble interactions. We find that the vortex developments in the bubble wakes play a key role during the collision of the two bubbles, and the magnetic fields are observed to have significant influences on the vortex structures while such impacts are highly dependent on the direction of the magnetic field. To be more specific, for an originally bounced bubble pair, a streamwise magnetic field tends to make them coalesce by weakening the vortex interactions between the bubble pairs. However, a horizontal magnetic field produces anisotropic effects with respect to the angle between the bubble centroid line and the magnetic field lines: a transverse magnetic field always brings the bubble pair to coalesce while a spanwise magnetic field leads to more complex influences on the bubble interactions. Besides, more detailed investigations are carried out on the physical mechanisms for the MHD influences on the vortex interactions.

Keywords: vortex structures, bubble interactions, magnetohydrodynamics

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Instability or control of a freely moving sphere affected by a magnetic field

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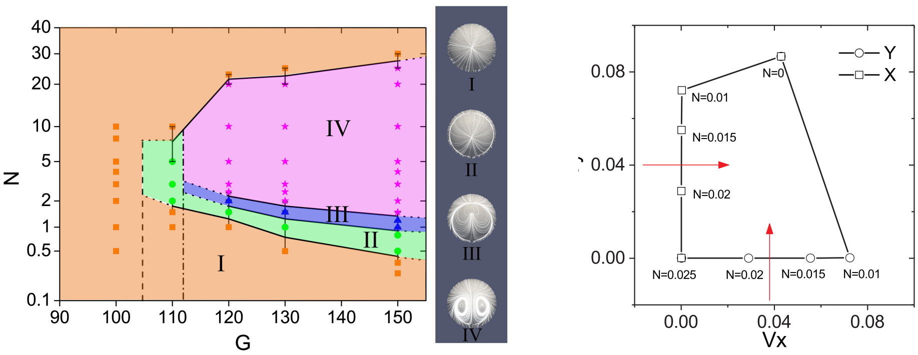
Abstract

To understand the motion of a free, electrically insulating sphere under the simultaneous actions of gravity, buoyancy, hydrodynamic force and Lorentz force is one of the most important issues in magnetohydrodynamics (MHD) particle two-phase flows.

When the Galileo number is below the first bifurcation, instability and transition of a vertical ascension or fall of a free sphere affected by a vertical magnetic field are investigated numerically. A compact model is used to explain that the magnetic field can destabilize the fluid-solid system. When the interaction parameter exceeds a critical value, the sphere trajectory is transitioned from a steady vertical trajectory to a steady oblique one. Furthermore, the trajectory will remain original one at a sufficiently large magnetic field, because of a double effect of the magnetic field on the fluid-solid system. Under the influence of an external vertical magnetic field, four wake patterns at the rear of the sphere are found and the physical behavior of the free sphere is independent of the density ratio. The wake or trajectory of the free sphere is only determined by the Galileo number G and the interaction parameter N. An interesting "agglomeration phenomenon" is also found, which describes the vertical velocities are agglomerated into a point for a certain magnetic field regardless of the Galileo number and satisfies a scaling law $V_z \sim N^{-1/4}$, when $N > 1$. The principal results are summarized in a map of regimes in the $\{G, N\}$ plane, see figure 1(a).

A free rising sphere case at $G = 165$, $m^* = 0.5$ in the absence of a magnetic field is chosen, which wake is plane symmetric with a double-threaded structure. After the free rising sphere reaches its stable state, a transverse magnetic field is imposed to show the magnetic field control feature to the trajectory of such free rising sphere. The horizontal velocity of the free rising sphere, which is within in the symmetric plane of the wake structure, is used to represent the moving direction of the sphere in the horizontal plane. Under the influence of a transverse magnetic field, the horizontal velocity tends to be perpendicular to the magnetic field, see figure 1(b). The reason is that the transverse magnetic field will rotate the wake structure behind the free rising sphere to be perpendicular to itself.

Keywords: magnetohydrodynamics, particle/fluid flows, instability, control



(a) (b)

Figure 1: A freely moving sphere affected by a magnetic field. (*a*) Map of regimes for wake patterns at the rear of the sphere in the $\{G, N\}$ plane. (*b*) Transverse velocity $V_x - V_y$ plot for $x-$ and $y-$directional magnetic field. The initial orientation is located at $N = 0$.

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Modeling of non-equilibrium effects in intermittency region between two phases

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Abstract

Recently, the present author has shown [1, 2] known in literature models of the sharp and diffusive interface all approximate the intermittency region: domain where the interface defined on the molecular level can be found with non-zero probability. Moreover, it has been argued when non-flat interface remains in the equilibrium state, it can be described by the cumulative distribution function (c.d.f.) and quantile of the logistic distribution. This c.d.f. approximates regularized Heaviside and its quantile function is the signed distance from the expected position of the interface. The latter result, allows to write equations assuring theoretical convergence of both interface and its curvature [1, 2]. In the present work, we note the classical models of the interface assume the intermittency region (interface) remains in the state of equilibrium. However, open systems are unlikely to be and remain in the state of its maximum entropy. For this reason, motivated by modeling of the turbulence-interface interactions [3, 4, 5], we introduce non-equilibrium effects into the intermittency region evolution model, see Figure 1. The presentation concerns incorporation of variable characteristic length/times into the numerical model, discusses required assumptions and further modeling possibilities.

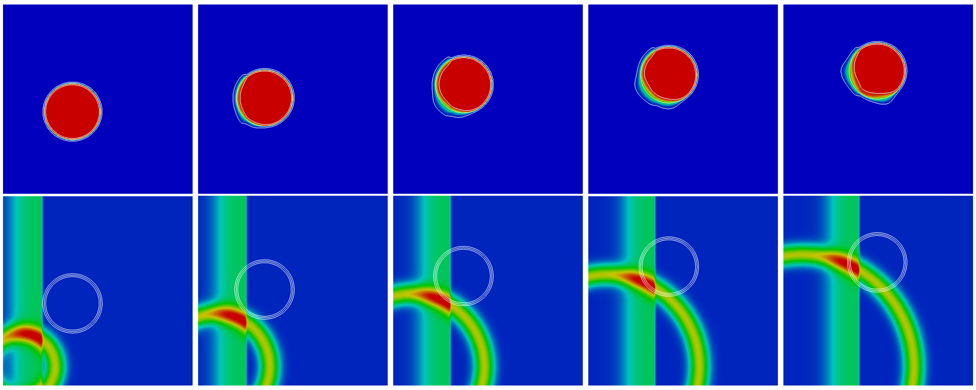

Figure 1: Advection (from left to right) of the intermittency region affected by variable characteristic length scale field. The top figures depict evolution of the intermittency region in time, white contours of cumulative distribution function, colors volume fraction. The bottom figures shows variable, arbitrary field of characteristic length scale and contours of the signed distance function.

Keywords: statistical model of the interface, interface capturing, evolution of the intermittency region

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Multiscale modelling of disperse multiphase systems in VIMMP

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Abstract

The Virtual Materials Marketplace (VIMMP) is a research initiative of the European Union's Horizon 2020 programme aiming at the development of a marketplace for computational models, applied to materials and chemical engineering. One of the items offered by the marketplace is the so-called "simulation-as-a-service" (SAAS) based on the implementation of numerous computational tools into an open-simulation platform (OSP). The effectiveness of the approach is being demonstrated on several user-cases and this contribution illustrates two of them: the simulation of (1) dispersive mixing of carbon-black aggregates into a polymer matrix and (2) formation of turbulent (food) liquid-liquid emulsions.

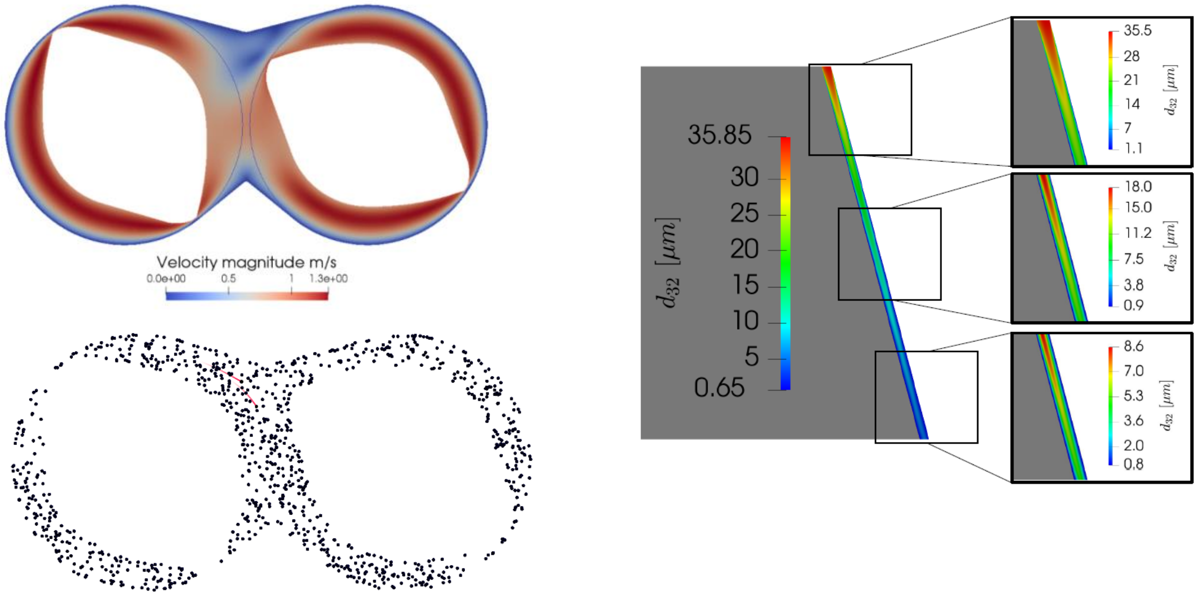

Figure. 1. Left: contour plot of velocity magnitude and particle trajectories for a two-wing internal mixer for rubber compounding; right: mean droplet size in a cone mill high-shear device for the production of stable food emulsions.

As far as the first example is concerned, this is a disperse multiphase flow encountered in the process of rubber compounding, which is here simulated by using different computational models, namely: computational fluid dynamics to simulate the flow field and particle trajectories in the internal mixer (where carbon-black particles are dispersed and mixed in the polymer) and discrete element method to predict the fate of each carbon-black aggregate. The second example refers instead to another disperse multiphase systems encountered in the production of food emulsions, where an oily phase is dispersed into an aqueous phase by using high-shear mixing devices, such as the cone mill mixer. In this case the disperse multiphase flow is simulated by using computational fluid dynamics to simulate the flow field in the device, a population balance model to describe the evolution of the oil droplets and molecular models to predict the relevant interfacial phenomena.

Figure 1 reports some typical results obtained with code_Saturne and Ansys Fluent (left) and with OpenFOAM (right) for the two above mentioned examples. The different computational codes are linked and coupled together by using the OSP Salome (https://www.salome-platform.org). The different codes are interfaced with the OSP thanks to the use of standardized wrappers developed within the project. Our results show that the coupling and linking of the different models is the key to gain a deeper understanding of these complex flows.

This Project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907 (https://vimmp.eu/).

Keywords: emulsions, droplets, fractal aggregates, elastomers, multiscale modelling, computational fluid dynamics

Wall model for large eddy simulations accounting for particle effect

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Abstract

Computational investigations of high Reynolds number turbulent multiphase flow is rather time-consuming even in large eddy simulation (LES) framework. The integral wall model (iWM) for large eddy simulation of particle-free wall-bounded turbulent flows proposed by Yang et al (2015) is further improved to include the body forces that particles exert on the fluid. The slightly modified iWMLES method is tested in the context of a finite-difference LES code for turbulent two phase flow. For model testing, the data from wall-resolved LES of particle-laden flow at Reynolds number of $Re\tau$ =550 ~ 4200 are treated as "standard data". The results show that the mean velocity profiles, particle concentration, particle mean velocity and mass flux profiles compare well with "standard data" once particle force is properly included in WMLES of particle-laden flow. Meanwhile, it allows significant reduction of the required CPU time over simulations of turbulent two phase flow in which no-slip conditions are applied.

Keywords: large eddy simulation, two-phase flow, wall stress model

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Reproducing segregation and particle dynamics in Large Eddy Simulation of particle-laden flows

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The Large Eddy simulation (LES) is now widely used as an investigation tool to understand and predict turbulent particle-laden flows. The most classical way consists in combining a single-phase LES model for describing the gas phase, with a LES model for the particulate phase. The objective of the latter is to recover the lost interactions between the particles and the unresolved scales. Several studies have shown the impact of subgrid turbulence and spatial filtering on particle dynamics (see for example [1]) pointing the need of suitable models for two-phase flows reduced-simulations.

Models have been proposed in the literature (see review of Marchioli [2]), that can be classified into two categories: (1) Structural models that aims at reconstructing the subgrid scales of the flow. Among them are the approximate deconvolution (ADM), the fractal interpolation or kinetic simulations; (2) Stochastic models which objective is to mimic the effect of subgrid-scale flow on particle paths (with a Lagrangian approach) using additional random process on the particle trajectory. In [1], the authors investigated the uses of stochastic Langevin models, and concluded that they can produce the right amount of particle kinetic energy and any one-point statistics by construction. However, they suggested that two-points statistics can only be found in structural models, to insure particle-fluid and particle-particle velocity correlations.

In the present work, we want to explore modelling strategies for LES of particle-laden flows in the scope of capturing two-way coupled dynamics. Such dynamics requires a correct description of the particle localisation (preferential concentration) as well as particle acceleration. Looking at the conclusion of [1], we would expect that stochastic models are not an acceptable choice because they lack a correct prediction of preferential accumulation. This conclusion is based on a specific strategy for validation: the authors validate LES models on the DNS statistics. However, this choice is open to discussion since one can also decide to validate the LES models on the filtered DNS statistics. These two options differ by the objective of the model in sight: describing the PDF or the filtered PDF.

In Fig. 1, we perform a DNS simulation of particle-laden turbulent flows, and we show the unfiltered (a) and filtered (b) Particle Number Density (PND) fields, which are the two possible references. In Fig. 1(d) which shows the distribution of PND for several simulations, we can see that the LES without stochastic particle model presents less segregation than the DNS, and adding a "diffusive-like" stochastic model will not recover the missing segregation. However, looking at the Filtered DNS, we have now an excessive segregation for the LES, and adding a stochastic process permits to reduce the segregation and eventually to recover the missing physics. On the other hand, if we want to recover the unfiltered DNS statistics, as suggested by [1], we can rely on structural models such as kinetic simulations. Our work is thus devoted to the investigation of these two paths: using stochastic model to recover the filtered DNS statistics such as segregation, particle acceleration, and intermittency; or using structural models to recover the unfiltered DNS statistics by explicitely incorporating turbulent structures in our simulations.

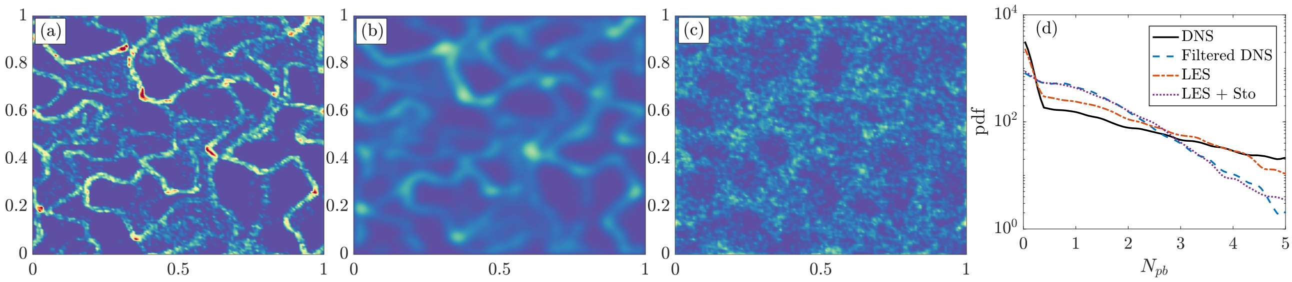

Figure 1: Particle number density field for (a) DNS, (b) Filtered DNS, (c) LES with stochastic modeling and (d) probability distribution function of number of particles per bin.

Keywords: Particle dynamics, turbulence, stochastic modelling, intermittency, kinetic simulations

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A Structural Subgrid-Scale Model for LES of Particles in Turbulent Flows

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Abstract

A kinematic simulation with an approximate deconvolution (KSAD) coupled model is proposed to predict the Lagrangian relative dispersion of fluid and inertial particles in a large eddy simulation (LES) of isotropic turbulent flows. In the model, a physical connection between the resolved and subgrid scales is established via the energy flux rate at the filter width scale. Due to the lack of subgrid-scale (SGS) turbulent structures and SGS model errors, the LES cannot accurately predict the two- and multi-point Lagrangian statistics of the fluid particles [1, 2]. To improve the predictive capability of the LES, we use an approximate deconvolution model (ADM) to improve the resolved scales near the filter width and a kinematic simulation (KS) to recover the missing velocity fluctuations beneath the subgrid scales. To validate the proposed hybrid model, we compare the Lagrangian statistics of two- and four-particle dispersion with the corresponding results from the direct numerical simulation (DNS) and the conventional LES. It is found that a significant improvement in the prediction of the Lagrangian statistics of fluid particles is achieved through the KSAD model (See Fig. 1). Furthermore, a parametric study regarding the wavenumbers and orientation wavevectors is conducted to reduce the computational cost. Good results can be obtained using a small number of wavenumber modes and orientation wavevectors. Thus, we can improve the prediction of the Lagrangian dispersion of fluid particles in the LES by applying the KSAD hybrid model at an acceptable computational cost [3].

Keywords: two-phase turbulent flows, relative dispersion, large-eddy simulation, particle subgrid scale model

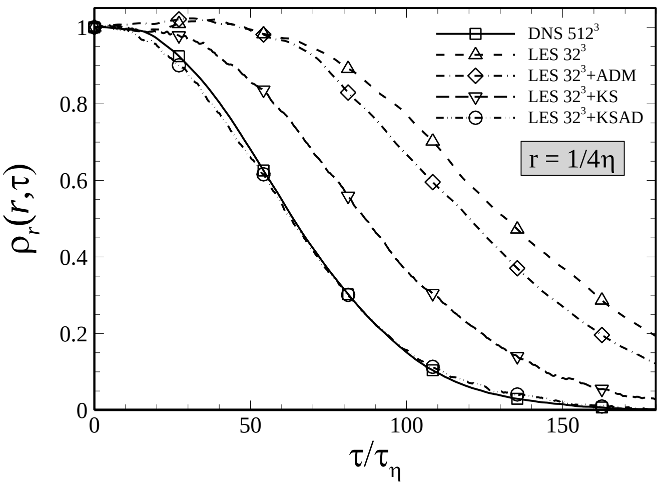

Figure 1.Two-point, one-time Lagrangian correlation function obtained by using DNS (solid line with squares) and the proposed KSAD model (dash-dot-dotted line with circles). The conventionally approximate deconvolution method (dash-dotted line with diamonds) and kinematic simulation method (dashed line with down triangle) are not enough to recover the DNS results, while the proposed KSAD model well recover the DNS results.

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History force on a fluid sphere (from particles to drops and bubbles)

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Abstract

We consider the Basset-Boussinesq (history) force experienced by a spherical fluid sphere (varying the viscosity from bubbles to drops and particles). The kernel of the Basset-Boussinesq force has not been determined so far when internal circulation of the fluid occurs. We first characterize the slip at a fluid sphere interface by direct numerical simulations. Under both steady and unsteady conditions, the corresponding slip length is remarkably uniform along the fluid sphere interface and is directly related to the viscosity ratio.

Combining the analytical expression of the Basset- Boussinesq kernel obtained for a solid sphere with interface slip and the description of the slip at the fluid-fluid interface, we were able to describe for the first time the Basset-Boussinesq history force acting on a spherical drop. This expression has been validated over a wide range of viscosity ratio from bubbles to viscous drops and particles.

Keywords: particles, drops, bubbles

The impact of interphase forces on the generation of turbulence in multiphase flows

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Abstract

Many multiphase systems involve either interfacial flows, such as the two-phase flow of immiscible fluids, or liquid-solid flows. These are ubiquitous in many environmental and industrial flows. Especially, fluidised gas-particle systems are inherently unstable and are characterised by fluctuations over a wide range of time and length scales. At moderate solids volume fractions these fluctuations manifest, for example, in the formation of clusters or bubbles.

These turbulent two-phase flows feature different mechanisms for production and dissipation of turbulent kinetic energy (TKE) compared to the single-phase flows. However, this difference is usually neglected in developing eddy viscosity-based sub-grid scale (SGS) models for the two-phase large eddy simulation (LES). In this study, the impact of the presence of interphase forces on the generation of turbulence in multiphase flows is shown. In the case of liquid-solid flows, the interphase force acts as a source of the continuous phase turbulence due to the work done by the liquid-solid drag force [2]. Particularly, this leads to turbulence enhancement in regions of low strain (figure 1). Subsequently, drag further transfers a part of this energy to the solid phase increasing its TKE. In the case of liquid-liquid flows, the work done by surface tension features a dual behaviour depending on the length scale. Surface tension acts either as a sink of TKE for large scale deformations and breakup process and extracts (damps) the kinetic energy at such scales or it provides this energy back to the flow at the small scales (figure 1), where it behaves as production mechanism during the events like droplets coalescence [1]. However, at high strain the common shear production, which is well known from single phase flows, dominates the production of TKE (figure 1). Finally, turbulent energy spectra and the corresponding decay of turbulence are discussed.

Keywords: surface tension, drag force, volume of fluid (VOF) method, two-fluid model (TFM)

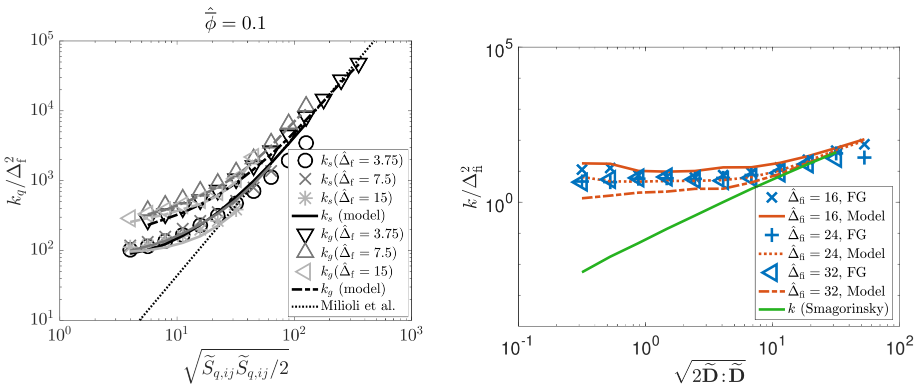

Figure 1: Turbulent kinetic energy as a function of the strain rate. The left hand figure corresponds to a fluidized gas-solid system for and averaged particle volume fraction of 0.1 [2], while the right hand side figure is derived from a liquid-liquid phase inversion problem [1].

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Fluid-Particle and Particle-Particle Drags

of Bidisperse Gas-Solid Flows at Low Reynolds Number

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Abstract

Particle-resolved direct numerical simulations (PR-DNSs) of bidisperse gas-solid flows in cubic periodic domains over a range of total solid volume fractions, solid volume fraction ratios and particle size ratios are employed to develop new models for the fluid-particle and particle-particle drags at low particle Reynolds numbers. The most important difference distinguishing the present work from previous works is that the particle phase is allowed to move according to the Newton's law, and therefore the slip velocity between two particle types can be developed. The scaled slip velocity, defined as the ratio of the slip velocity of one particle type to the mean slip velocity of the mixture, varies profoundly depending on the specific properties of the mixture. For large particles, the drag force, scaled by the mean drag force of the mixture, is reasonably predicted by the models obtained from fixed beds. While for small particles, these models underestimate the scaled drag force, especially when the scaled slip velocity is small. By introducing the scaled slip velocity, a new model for the fluid-particle drag on each particle type is proposed and agrees well with the PR-DNS data. The proposed model is also validated against the experimental data for a large particle settling in a suspension of small particles. It is observed that the proposed model gives much better predictions than previous models. In dilute suspensions, due to the strong influence of surrounding fluids on the particle phase, the simulated particle-particle drag is significantly smaller than the predictions of models based on kinetic theory of granular flow (KTGF). Based on the PR-DNS results, new relations for particle-particle drag are also proposed.

Keywords: fluidization, bidisperse gas-solid suspension, fluid-particle drag, particle-particle drag, direct numerical simulation

An ANN-Based Drag Model and Turbulence Statistics from Fully-resolved Simulation of Dense Gas-Solid Flows

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Abstract

Since the fidelity of simulation of dense gas-solid flows using TFM or CFD-DEM depends strongly on the accuracy of the drag model, the fully-resolved simulation of a shallow bubbling bed (SBB) and a deep bubbling bed (DBB) using IB method was performed. There are 384 inertial particles in SBB and 1152 in DBB, whose collision is modelled using a soft-ball collision model. With the void fraction ε_f, particle Reynolds number Re_s, particle velocity fluctuation Reynolds number Re_T and void fluctuation ς taken as input and the dimensionless drag force F taken as output, an ANN-based drag model is proposed a priori from a statistical grid perspective. The correlation coefficients for the ANN-based drag model are all greater than 0.93 for different data sets, whereas that for Gidaspow drag model is 0.83, with the fitted lines for the former closer to the 45-degree line than that for the latter, showing that the ANN-based drag model allows a more accurate prediction of real values (see Fig. 1 and Fig. 2). Variance-based sensitivity analysis shows that ε_f has the greatest importance to F, followed by Re_s, Re_T and ς. Turbulence statistics show that there exists a clear anisotropy both in gas phase and in solid phase, and that the turbulent kinetic energy for the gas phase is higher inside the beds than that outside the beds.

Keywords: gas-solid flows, ANN, drag model, turbulence

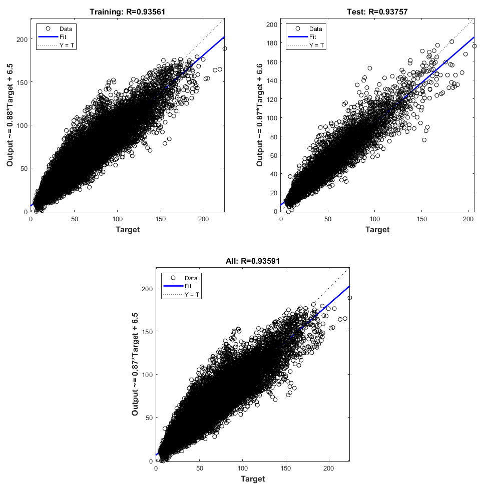

Figure 1: The lines fitting points of F_{ANN}-F_{DNS} for different data sets

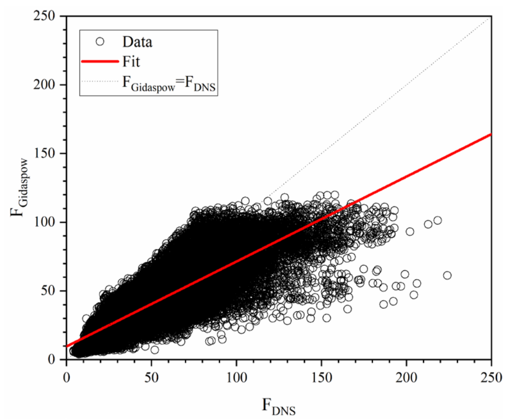

Figure 2: The line fitting points of $F_{Gidaspow}$-F_{DNS} for all the samples

Prediction of inertial lift on particles for microfluidic applications

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Abstract

Inertial migration has been extensively used for manipulation and separation of engineered particles and bioparticles in microfluidic platforms. Inertial lift stems from the asymmetry of pressure and viscous stresses on the particle surface in a Poiseuille flow with finite Reynolds numbers. To design inertial microfluidic devices for particle manipulation, researchers need to predict the focusing positions of the targeted particles under various operating conditions, mainly by estimating the lift forces acting on the particles. Direct numerical simulations can provide more direct and realistic images of the particle migration, but they could become dramatically burdensome for the long microchannels encountered in the practical devices. Here we use three-dimensional direct numerical simulations to calculate nearly 8,000 cases to determine the inertial lift distribution under different operating conditions in rectangular microchannels. Based on these simulation data, we build a database of inertial lifts over a wide range of parameters. The interpolation is then performed to apply the database to obtain the inertial lift within the parameter space, by simply specifying Reynolds number, particle blockage ratio, and channel aspect ratio. We then implement the interpolated lift in the Lagrangian tracking method to predict the particle trajectories in two typical microchannels for the inertial microfluidic applications, yielding good agreement with the experimental observations.

Keywords: microfluidics, microparticle, inertial lift, numerical simulation

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Effect of fluid inertia on the orientation of a small particle settling in turbulence

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Ice crystals settling through a turbulent cloud are rotated by turbulent velocity gradients. In the same way, turbulence affects the orientation of aggregates of organic matter settling in the ocean. In fact most solid particles encountered in Nature are not spherical, and their orientation affects their settling speed, as well as collision rates between particles. Therefore it is important to understand the distribution of orientations of non-spherical particles settling in turbulence. Here we study the angular dynamics of small prolate spheroids settling in homogeneous isotropic turbulence. We consider a limit of the problem where the fluid torque due to convective inertia dominates, so that rods settle essentially horizontally. Turbulence causes the orientation of the settling particles to fluctuate, and we calculate their orientation distribution for prolate spheroids with arbitrary aspect ratios for large settling number Sv (a dimensionless measure of the settling speed), assuming small Stokes number St (a dimensionless measure of particle inertia). This overdamped theory predicts that the orientation distribution is very narrow at large Sv, with a variance proportional to Sv^{-4}. By considering the role of particle inertia, we analyse the limitations of the overdamped theory, and determine its range of applicability. Our predictions are in excellent agreement with numerical simulations of simplified models of turbulent flows. Finally we contrast our results with those of an alternative theory predicting that the orientation variance scales as Sv^{-2} at large Sv.

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Keywords: Turbulence, settling particles, non-spherical particles, orientation distribution, ice crystals, clouds

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The effect of hydrodynamics interaction (HI) on the dynamics and equilibrium configuration of colloidal aggregates in the quiescent flow regime

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Abstract

Some authors claimed that hydrodynamic interactions (HI) between colloids should be able to reduce the colloid volume fraction for gellation to occur and probably alter the structure of a colloidal gel. There is no agreement in the literature on this possibility, which might be falsified by computational works. In this work, we used our own Inertial Coupling Method (ICM) (a Langevin dynamics and Stochastic Immersed Boundary Method using our open code FLUAM which includes hydrodynamics between particle units (blobs)) as well as other two methods, namely Brownian Dynamics (BD) (without HI) and Monte Carlo (MC) (NVT, without HI), to study the effect of HI on the dynamics and equilibrium configuration of colloidal aggregates. Three different scale-level systems, composed by 3 particles, 296 particles, and 2108 particles, were investigated. Non-bonded force between particles, i.e. Lennard-Jones-Yuwaka pontential with varying $\kappa = 0.5$, 1.0, 2.0, 3.0 and 4.0, were employed in the calculation with volume fraction, 0.04. Some key quantities including radial distribution function, structure factor, bond number per particle, time to approach 90 degree for triple particle system, were analyzed. We found that: (1) hydrodynamic delays the formation of the equilibrium configuration and that the bond formation time is governed by a Kramer escape time ruled by the jump in the (angle dependent) free energy; (2) all three types of computational techniques produce the same final equilibrium configuration, regardless of the system level. No any evidence was found that HI affects the final equilibrium configuration. Our conclusion support the very recently work from Graaf et al. (De Graaf, Poon, Haughey, & Hermes, 2019).

Keywords

Hydrodynamics; colloidal aggregate; Brownian dynamics; Monte Carlo method; Langevin dynamics

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Simulation of shock-particles interaction using conservative sharp interface methods

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Abstract

We present a conservative sharp interface method for direct numerical simulation of flow-particle interaction in compressible inviscid flows. The moving rigid particles are represented by level set functions, and are reconstructed on a background Cartesian mesh by line segments. In such a way, unstructured body-fitted meshes are generated near the particle boundaries while structured meshes keep unchanged in the rest of the domain. The boundary condition at the surface of the particles are resolved by solving a local Riemann problem, thereby giving an accurate prediction of the forces exerted on the particle. Using finite volume method in the arbitrary Lagrangian-Eulerian framework, we ensure that the conservation of mass, momentum, and energy are satisfactorily maintained during the computation. The collisions among particles are modeled by perfectly elastic collisions. The method is validated by comparing against benchmark solutions or experimental data available in the literature. Good agreement has been achieved both qualitatively and quantitatively. The method is also used to investigate the dynamic process of a planar shock impacting onto a cloud of particles, and to reveal the complicated but interesting flow structures and particle dynamics. One such example is shown in figure 1.

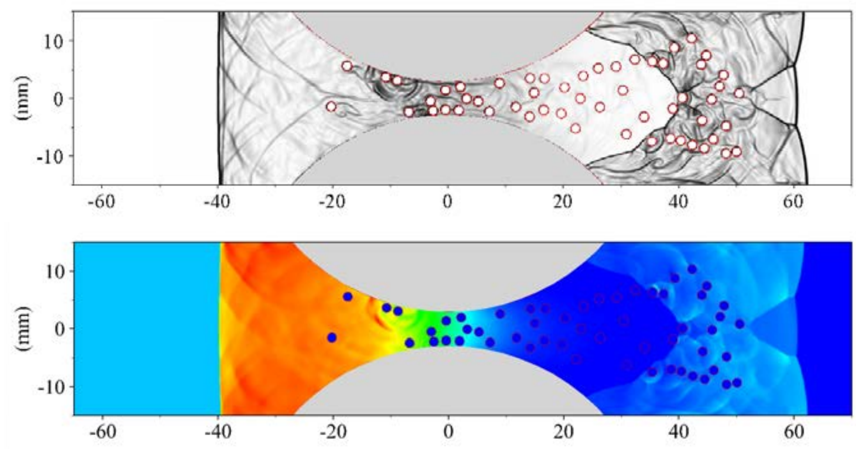

Figure 1: Dynamics of clustered particles in high-speed flow: numerical schlieren (upper) and pressure contour (lower).

Keywords: Sharp interface method, rigid particles, shock wave, arbitrary Lagrangian-Eulerian

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Filtering effect of heavy particles in the three dimensional homogeneous and isotropic turbulence

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Abstract

A quantitative understanding of the interaction between heavy point particles and turbulence is still lacking [1]. It has been found that the heavy particle acts as a low-pass filter and they will detect less and less small scales fluctuation when the inertial effect, which is characterized by the Stokes number St, is increasing. In this work, we quantify this filtering effect via both the intermittency parameter μ from the lognormal statistics and empirical filtering function from the Fourier spectral analysis. A state-of-art high resolution DNS database with 2048^3 grid points and a Taylor microscale based Reynolds number $Re_\lambda = 400$ is mainly considered with Stokes number $St \in [0, 70]$. A coarse-grained statistics of the instantaneous power along the Lagrangian trajectory, i.e., $M_q(St, \tau) = \langle P_\tau^q(t) \rangle_t$, where $P_\tau = \frac{1}{\tau} \int_{0 \le t' \le \tau} |P(t + t')dt'|$ and τ is the coarse-grained scale, is performed. Power-law behavior e.g., $M_q(St, \tau) \propto \tau^{-K(St,q)}$, is evident on the inertial range, i.e., $10 \le \tau/\tau_\eta \le 100$, where τ_η is the Kolmogorov time scale. For the tracer case, i.e., $St = 0$, one has $K(0, q)$ agree well with the one for the energy dissipation rate ϵ along the tracer particles, which can be further modeled by the lognormal formula, i.e., $K(St, q) = \frac{\mu(St)}{2}(q^2 - q)$, where $\mu(St)$ is the so-called intermittency parameter [2], See Fig.2 (a). It is found that the measured intermittency parameter $\mu(St)$ is logarithmically decreasing on the range $0.1 \le St \le 7$ due to the filtering effect of heavy particles. A linear reduction of the intermittency parameter is evident on the range $St \ge 10$, see Fig.2 (b) [3].

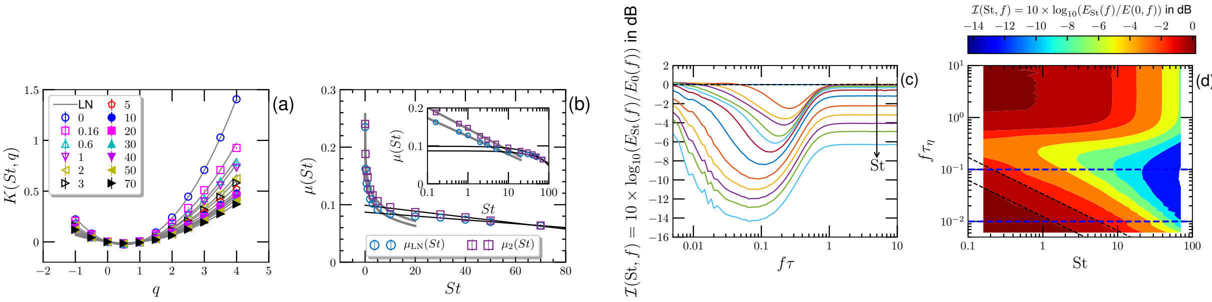

Figure 1: (a) Measured $K(St, q)$ versus St numbers. The lognormal formula fitting is illustrated by a solid line. (b) Experimental intermittency parameter $\mu(St)$ provided by the lognormal formula fitting $\mu_{\mathrm{LN}}(St)$ and $\mu_2(St) = K(St, 2)$. Two regimes are identified respectively for a log-law (thick solid line) on the range $0.1 \le St \le 7$ and a linear relation (thin solid line) on the range $St \ge 10$ with slight different slopes. (c) Measured empirical filtering function $\mathcal{I}(St, f)$. (d) Contour plot of the empirical filtering function $\mathcal{I}(St, f)$. Power-law behavior is observed on the range $0.01 \le f\tau_\eta \le 0.1$ and $0.1 \le St \le 10$ with a scaling exponent 0.70 ± 0.02.

We then consider the filtering effect in the Fourier space. We first illustrate that the Kolmogorov-Landau spectrum of the Lagrangian tracer particle , i.e., $E(f) \propto f^{-2}$, is valid on the inertial range $0.01 \le f\tau_\eta \le 0.1$ [4]. The experimental results show a strong reduction of the energy spectrum due to the inertial effect. An empirical filtering function, i.e., the ratio of the Fourier power spectra between the one of inertial particle and that of the tracer particle, i.e., $\mathcal{I}(St, f) = \log \frac{E(St,f)}{E(0,f)}$, is obtained, see Fig.2 (c). Power-law behavior is observed on the inertial range $0.01 \le f\tau_\eta \le 0.1$ and $0.1 \le St \le 10$ with a scaling exponent 0.70 ± 0.02, see Fig.2 (d). Additionally, an $\mathcal{I}$-dependent power-law is observed on the inertial range when $St \ge 10$, which may an effect of the box-size [4]. The methods employed here is in general, and is applicable for other problems.

Keywords: intermittency, scaling behavior, filtering effect

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Dynamics of inertial particles in an uniform unsteady flow at low Reynolds number

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Abstract

Many natural and industrial flows are ladened with dispersed small particles. Most often these particles are with density larger than the fluid and hence do not follow the fluid exactly due to the inertial effect. Well known examples of such particle-laden flow include clouds, dust in storms, particulate matters in the exhaust of coal-burning power plants, and others. Our ability to analyze such multiphase flows is, however, hindered, by the lack of understanding of the particle dynamics in this complex flow. In many flows, the particles are tiny and the Reynolds number based on the particle size is small, the fluid inertia could be ignored. For these cases, the equation of motion of a single particle in a general flow field has been widely studied [1,2,3] and several experiments has been carried out to measure the motion of single particle in an unsteady flow [4,5,6,7]. These experiments, however, are all for particle-fluid density ratio of the same order, i.e., with solid particles in liquids. There is a lack of experimental data for large particle-fluid density ratios that are relevant to, e.g., clouds and dust in storms. Here we report our measurement of the motion of single water droplets in a periodic air flow created by sound waves. We compare our data with those calculated from theoretical solutions [7,8]. Moreover, as it was found that particles could agglomerate under the action of sound waves [9], there have been intensive studies on the interaction between particles in an acoustic field [10,11,12], but there is very few quantitive experimental data on the dynamics of two or more particles in an acoustic field. Here we will also report data of the motion of two particles in an acoustic wave and compare against existing theoretical calculation.

Keywords: particle dynamics, unsteady flow, acoustic wave

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Dynamics of particles in viscoelastic liquids: numerical methods and microfluidic applications

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Abstract

Solid particles suspended in viscoelastic fluids are encountered in a variety of industrial applications such as reinforced polymers, detergents, inks, paints, foods. It is well-known that the viscoelasticity of the suspending medium has a strong influence on the particle motion leading to phenomena not observed in Newtonian fluids, affecting, in turn, the rheological behaviour of the suspension [1]. Our group has developed efficient numerical methods based on the Arbitrary Lagrangian-Eulerian technique to accurately compute the flow and stress fields around rigid or deformable particles of arbitrary shape immersed in a viscoelastic fluid subjected to a general flow field [2, 3]. The simulation tool has been successfully applied to study the rotation and migration of spherical and spheroidal rigid and deformable particles in shear and pressure-driven channel flows, with specific interest in microfluidics applications [4, 5].

In this contribution, we present an overview of the numerical methods for simulating viscoelastic suspensions of rigid or deformable particles, and recent results on the dynamics of particle trains in microfluidics channels. We show that fluid elasticity can promote self-assembly of aligned particles and the formation of equally-spaced microstructures. The effect of fluid rheology, confinement ratio, and particle shape on the train dynamics is also discussed.

Keywords: viscoelasticity, suspensions, numerical simulations, microfluidics

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I will focus on experiments that could be carried out in a turbulent cloud chamber. Turbulence is generating by either pulsating jets of fans, each driven independent and randomly to generate homogenous isotropic turbulence in the center region of the sphere. Care is taken is ensure that the pumping causes negligible in/out flow between the chamber and the surrounding. Taylor micro-scale Reynolds number, R_λ, of up to 400 and Kolmogorov micro-scale in the range of 150 to 500 microns can be typically achieved. The energy injection scale is about 10 cm. Droplets in modern version of such experiments are produced using a spinning disc droplet generator [2]. Liquid is fed to a high speed spinning disc (faster than 30,000 rpm), at the disc edge, centrifugal force causes small drops (of order 10 microns in diameter) to be ejected together with some small satellite drops (few times smaller in diameter). To observe the droplets, one could employ the back-lighted imaging method, where a white light source is shined directly into a camera fitted with macro lens. In the focal volume of the camera, particle appear as black round dots in white background. By taking a high speed movie (>10,000 fps) of the particle field, one could study the distribution and motion of the droplets using the method of Lagrangian particle tracking (LPT) [3]. Since 3 dimensional information of the droplets motions is needed, one employs two or more cameras with identical illumination. If time permit, I will briefly present the latest version of such experiment in our current institute.

Focus of the studies is primarily on the statistics of relative particle (droplet) velocities and how this depends on the Stokes number, St, which characterizes the importance of particle inertial compared to the advective forces it experiences in turbulence and of the Reynolds Number of the background flow. In particular, we are interested in how relative particle statistics scale with separation distance between particle in the dissipation range. We are also interested in the study of droplet collision and coalescence in turbulent flow, in particular how collision rate depends on various flow parameters, the relative particle velocity statistics and inertial clustering statistics of the particles. We will also look at how well results of modern computational simulation compares with the experiments.

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Can the Rayleigh-Plesset equation describe nanoscale bubbles dynamics?

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Abstract

It still remains unclear whether the Rayleigh-Plesset (RP) equation could describe nanoscale bubbles dynamics. To shed light on this, this research performs molecular dynamics (MD) simulations of heterogeneous cavitation in water in nano-scale, and the bubble evolutions are analyzed and compared with solutions of RP equation. The results indicate that the Tolman's equation should be introduced into RP equation to describe the correct bubble dynamics in nano-scale but the coefficient in the Tolman's equation is the critical parameter. This study confirms that the negative correction of Tolman length has a better prediction for nanoscale bubbles in water.

Keywords: Rayleigh-Plesset equation, nanobubble, bubble dynamics

Rayleigh-Plesset (RP) equation is a classical bubble dynamics theory and is suitable for macroscopic situations, but whether it could predict the bubble evolution in nano-scale still remains unclear. To shed light on this question, this study performs molecular dynamics (MD) simulations of heterogeneous cavitation stimulated by ultrasonic standing wave in water, and the temporal variations of bubble size are compared with solutions of RP equation and corrected RP equation.

The surface tension is sensitive to the radius of the droplet when the droplet is minute, so combine Tolman's equation with RP equation should be considered to extend RP equation to nano-scale.

RP equation could be expressed as

$$\frac{p_B - p_L}{\rho_L} = R\frac{\mathrm{d}^2 R}{\mathrm{d}t^2} + \frac{3}{2}\left(\frac{\mathrm{d}R}{\mathrm{d}t}\right)^2 + \frac{4\nu_L}{R}\frac{\mathrm{d}R}{\mathrm{d}t} + \frac{2\sigma}{\rho_L R}, \tag{1}$$

where p_B is the pressure in bubble, p_L the pressure in liquid, ρ_L the density of liquid, R the bubble radius, υ_L the kinematic viscosity of liquid, and σ is the surface tension. Tolman's equation describes the radius dependence of the surface tension. Under the condition of a vapor bubble, it could be expressed as

$$\sigma / \sigma_{\mathrm{bulk}} = 1 + 2\delta_T / R, \tag{2}$$

where σ_{bulk} is surface tension of plain interface, and δ_T is the Tolman length and it describes the planar limit of separation between the equimolar surface and the surface of tension. Previous studies give either positive or negative Tolman length for water, and its sign and magnitude remain unclear either.

The MD simulation results and solutions of original/corrected RP equation under four different conditions are presented in Fig. 1. It can be seen that the present corrected RP equation predict bubble evolution better. This study suggests that when Tolman length $\delta_T = -0.413$ nm (1.5 times of the water molecule diameter), the corrected RP equation could describe bubble evolution in nano-scale well. Thus, Tolman length is confirmed to be negative for the nanoscale cavitation bubble in water.

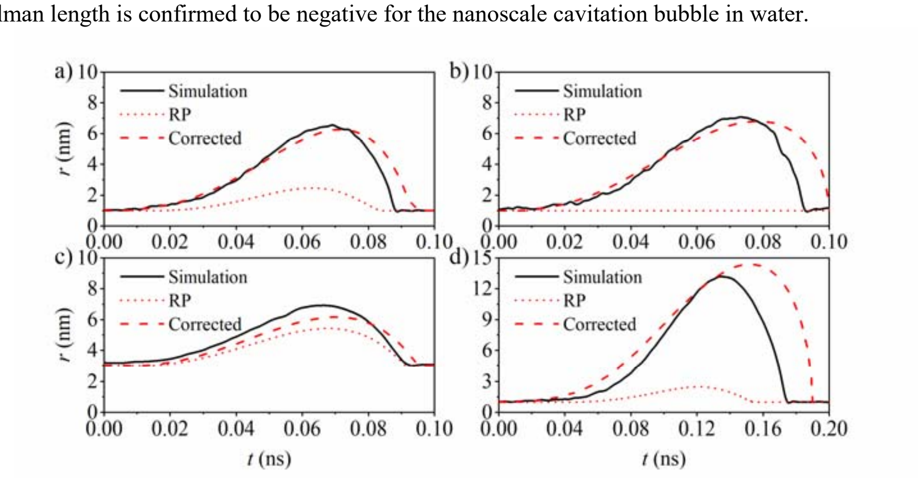

Figure 1. Bubble radius-time evolution in 4 typical conditions. a) water temperature $T = 298$ K, bubble's initial radius $r_0 = 1\,nm$, ultrasonic amplitude $A = 420$ MPa, ultrasonic period $\tau = 0.2$ ns. b) $T = 450$ K, $r_0 = 1\,nm$, $A = 150$ MPa, $\tau = 0.2$ ns. c) $T = 298$ K, $r_0 = 3\,nm$, $A = 210$ MPa, $\tau = 0.2$ ns. d) $T = 298$ K, $r_0 = 1\,nm$, $A = 340$ MPa, $\tau = 0.4$ ns.

Hydrodynamics of vapour bubble growth and detachment in a shear flow

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Abstract

The prediction of heat transfer coefficient in convective nucleate boiling remains an open question. Advanced models are based on the heat flux partitioning [1,2] taking into account the contribution of phase change, rewetting of the wall after bubble lift-off or in the wake of the sliding bubble, convection between the nucleation sites. These models require a good prediction of the diameter and frequency of bubble detachment. The prediction of the bubble radius at detachment is often based on point force models [3,4]. The main difficulty is the lack of knowledge in the hydrodynamic forces for a deformed bubble growing on a wall for a large range of bubble Reynolds numbers (20 to 1,000). Another problem is the modeling of the capillary force acting at the bubble foot. To improve the modeling of the static and hydrodynamic forces, a detailed analysis at the scale of individual bubbles is required. In this context, several dedicated experiments on isolated bubble nucleation and growth have been performed. First, bubbles are injected in a pool liquid on an inclined plate to provide a new modelling of the capillary force [5]. Then quasi static air bubbles injection at the lower wall of a horizontal channel allowed to determine the drag force. Finally experiments on bubble vaporization on a heated plate in a shear flow have been performed with the RUBI* (Reference mUltiscale experiment for Boiling Investigation) test cell on ground and in microgravity conditions aboard the International Space Station. Experiment provides measurements of wall temperature and heat flux distribution underneath vapour bubbles with high spatial and temporal resolutions by means of IR thermography(Figure 1). These data are synchronised with the bubble shape observation by a high-speed video (Figure 2). Experiments in microgravity allow to observed larger bubbles than on ground with a longer growth time. From Image processing, the geometrical characteristic parameters of the bubble are determined: bubble equivalent radius, height, position of the centre of gravity, width of the bubble foot and contact angles on both sides of the bubble. From these data, the forces acting on the bubble are evaluated (Figure 3). In the flow direction the drag force F_D and inertia force F_I tend to detach the bubble and the capillary force F_C acts against the detachment. A force balance model for a vapour bubble growing on a heated wall is validated. This is the first step toward the prediction of the bubble detachment diameter.

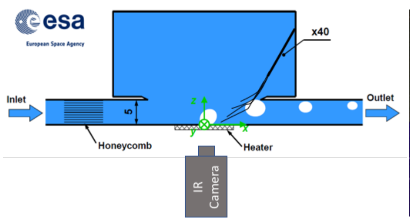

Figure 1: RUBI test cell

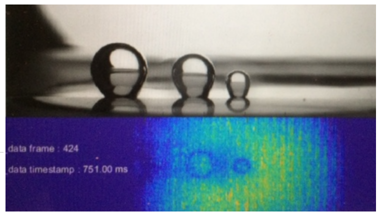

Figure 2: bubble visualisation / IR image

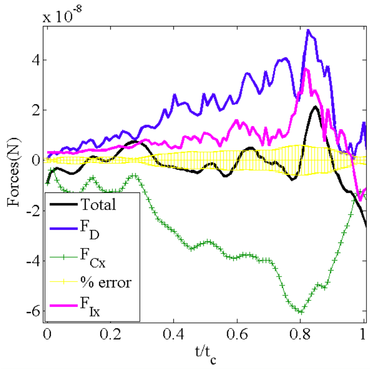

Figure 3: forces on the bubble in the flow direction

Keywords: bubble dynamics, heat transfer, boiling, microgravity

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Turbulent heat transfer of supercritical fluids: Fundamentals and models

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Abstract

Supercritical fluids have become promising working mediums in many industrial fields such as the coal-fired power generation, nuclear power system, hydrogen production, and distributed energy. The accurate estimation of the turbulent heat transfer of supercritical fluids is of critical for the design and optimization of the systems and devices. The thermo-physical properties of supercritical fluids vary significantly in the pseudo-critical region, leading to very complex turbulent heat transfer characteristics. In the previous researches, the compressibility and buoyancy force have been found to influence the turbulence properties. The compressibility is significant in the pseudo-critical region and the buoyancy effect is believed to be responsible for the heat transfer deterioration phenomenon at high heat flux. Unfortunately, the existing compressible turbulent theories fail to describe supercritical fluids turbulence, and the traditional models could not give satisfying predictions. In this lecture, we will introduce the progress we made in the fundamentals and eddy viscosity model (EVM) of supercritical fluid turbulence.

The turbulence properties of the supercritical fluid are firstly introduced, including the turbulent transport, scaling law, turbulent cascade and budgets. Based on the direct numerical simulation, we find that due to the strong density fluctuations, the Morkovin's hypothesis is invalidated in the pseudo-critical region, and the statistical properties are quite different from those of the conventional compressible turbulence. The Van-Driest scaling law in the conventional compressible turbulence which only considers the mean density variation is invalidated. The effect of the compressibility on the turbulent large scale is obvious, while the dissipation region is hardly influenced by the compressibility and this phenomenon is quite different from that of the conventional compressible turbulence. The turbulent production is nearly identical with the turbulent dissipation, which indicates that the local equilibrium property is not broken even in the pseudo-critical region with strong compressibility.

Then we will present our modelling theory on the compressibility of supercritical fluid turbulence. Due to the invalidation of the Morkovin's hypothesis, the second-order and third-order statistics related with the density fluctuation should be considered in the governing equations of EVM. Based on this conclusion, we proposed the two-mode compressible eddy viscosity model. The Helmholtz decomposition is employed to decompose the fluctuating velocity into the solenoidal mode and the compressive mode, and the mathematical framework of the compressive mode (including the governing equations of the velocity spectrum, the second-order spectral tensor and the energy spectrum) are proposed. The physical parameters describing the compressive mode such as the turbulent kinetic energy, turbulent dissipation rate and eddy viscosity are obtained by numerically solving these governing equations, and the new eddy viscosity formula of the supercritical fluid turbulence is obtained. The prediction capability of the new model on the statistical properties in the pseudo-critical region is obviously improved.

Furthermore, we present our new modelling approach on the supercritical fluid turbulence with the buoyancy effect. The DNS results reveal that the linear hypothesis of the Reynolds stress constitutive equation in the EVM is invalidated. Moreover, the local equilibrium hypothesis used in the EVM is also invalidated, the pressure strain term in the Reynolds stress transport equation are significant thus these factors should be taken into consideration. The new model is investigated from two aspects: i) we proposed a new constitutive equation of the Reynolds stress based on the non-linear relationship between the Reynolds stress and the mean velocity strain rate. ii) The mathematical description of the effect of the pressure strain is added into the constitutive equation. The analytical solution of the pressure strain term is obtained by solving the Poisson equation of the pressure fluctuation in the compressible flow, then the modelling of the slow term and rapid term in the analytical solution are proposed according to the redistributive properties of the pressure strain. On the basis of the new Reynolds stress constitutive equation, the modified expression for the turbulent Pr number is finally developed. We find that the predictive deviation of our model on the turbulent heat transfer and turbulence statistics can be significantly reduced.

Keywords: supercritical fluid, turbulence properties, two-mode compressible eddy viscosity model

QUANTIFYING THE NON-EQUILIBRIUM CHARACTERISTICS OF HETEROGENEOUS GAS-SOLID FLOWS: KINETIC THEORY ANALYSIS AND CFD-DEM SIMULATION

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Abstract

Navier-Stokes order continuum theory (NS theory) established on the basis of local thermodynamic equilibrium (LTE) postulate has been widely used to study gas-solid flows. Qualitatively, the postulate is valid for systems sufficiently close to equilibrium, however, continuum theory provides no information on how small these deviations from equilibrium should be in order to guarantee the validity of LTE. To this end, kinetic theory analysis was carried out to formulate an entropy criterion and extensive CFD-DEM simulations were performed to quantify the non-equilibrium characteristics of heterogeneous gas-solid flow, by systematically studying the bubbling, turbulent and circulating fluidization of Geldart A, B and D particles. Kinetic theory analysis showed that (i) the entropy density up to the NS order is exactly the same as the one at the LTE condition, meaning that the LTE postulate is only valid for linear non-equilibrium regime, although NS theory and the LTE postulate are logically self-consistent; (ii) an entropy criterion (I_s) characterizing the importance of nonlinear effects is derived, which should be small in order to make sure that the LTE postulate is valid and also sets the boundary of validity of NS theory; and (iii) the proposed entropy criterion is not only a function of granular temperature gradient and velocity gradient, but also a function of restitution coefficient that characterizes the inelasticity of particle-particle collisions. It is more complex and systematic than the traditional criterion based on the Knudsen number. CFD-DEM simulations showed that (i) except at the centre of bubbles where the solid concentration is quite low, NS theory for discrete particles was valid for bubbling fluidization irrespective of the breakdown criterion. Even at the boundary of the bubbles, values of Is and Kn were small; and (ii) the conclusion depended on the criterion used in turbulent and fast fluidization. If solid volume fraction based Knudsen number was used, NS theory would be generally valid. If the entropy criterion was chosen, NS theory would be still valid but with lower confidence. However, if solid velocity based Knudsen number or granular temperature based Knudsen number was selected, NS theory broke down. Because Is includes the non-equilibrium effects caused by the gradient of hydrodynamic fields and particle inelasticity, we may conclude that NS theory was valid for all tested cases. This means that the continuum description of discrete particles is not the main source of the breakdown of NS theory.

Simulation of a reactive fluidized bed reactor using coupled CFD/DEM

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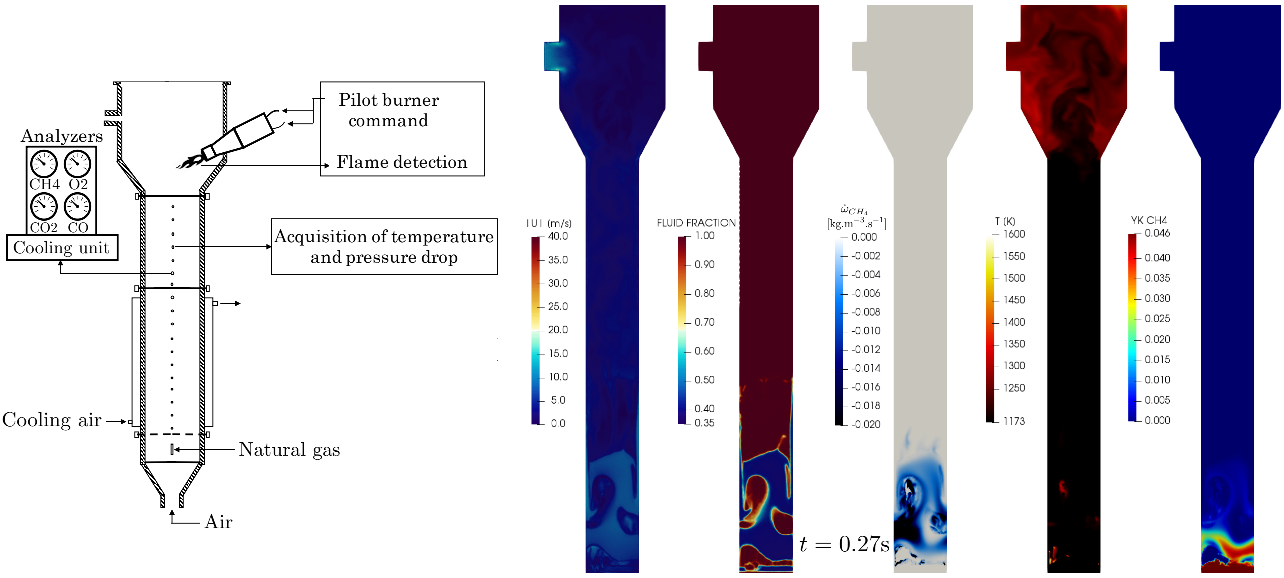
Abstract

Fluidized-bed reactors (FBR) are found in a large variety of industrial processes ranging from coal gasification to water treatment. In reactive FBR processes, gas-solid mixing and interactions can be enhanced as well as the chemical reaction rate. These properties are particularly interesting to achieve low-temperature combustion with high conversion efficiency and low pollutant emissions such as nitrogen oxides.

The objective of this study is to achieve simulations of a FBR at mesoscopic scale using a coupled CFD/DEM (Discrete Element Method) approach in order to gain insight into the physics of such processes and to extract information to be used in the modeling at macroscopic scale. The chosen configuration is a semi-industrial FBR fed with a mixture of natural gas and air containing 50 million sand beads with a mean diameter of 550 microns. Experimental data show a shift in the combustion regime above a critical temperature of 750°C. Two different values of temperature above and below this critical temperature are investigated to gain insight into the two combustion regimes.

Large-Eddy Simulations (LES) are performed using the finite-volume code YALES2 (www.coria-cfd.fr), a low-Mach number solver based on unstructured meshes. Its DEM solver has been designed to perform simulations in arbitrarily complex geometries and optimized for massively parallel computing. It features a dynamic collision detection grid for unstructured meshes, packing/unpacking of the halo data for non-blocking MPI exchanges and a dynamic load balancing algorithm for particle-laden flows.



Keywords: fluidized bed reactors, DEM-CFD, dynamic load balancing

Marginal stability limits for a fluidized bed

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Abstract

Fully resolved direct numerical simulations (FR-DNS) combined with a linear stability analysis are performed for getting the marginal stability limits for a monodispersed fluidized bed undergoing hydrodynamic interactions at finite particle. The instabilities by hydrodynamic interactions and elastic collisions at high particle inertia predicted in previous theories are shown and confirmed by the present numerical simulations. The FR-DNS is based on a boundary-thickening based direct forcing immersed boundary-lattice Boltzmann method. Several statistical quantities representing the macroscopic properties of the sedimenting particles are examined extensively by the simulations, such as the average sedimenting velocity, the velocity fluctuation, the structure factor, the radial distribution function, the correlation time, the self-diffusivity, the volume fraction fluctuation and the kinematic wave speed. The effect of Reynolds number (Re=1-50), solid-to-fluid density ratio (ρ*=1-1000) and solid volume fraction (φ=0.01-0.5) on above quantities are studied in detail. Then the particle velocity, velocity fluctuation and diffusivity are introduced to the Batchelor theory to get the predications of the marginal stability limits by a linear stability analysis. The competing roles of the particle inertia (destabilization term) and the particle diffusion (stabilization term) for the particle stability are also analysed. At last, the simulations are used again to confirm and refine the critical density ratio point where marginal stability occurs by exhibiting the transition to an inhomogeneous structure at small wave number, which is corresponding to a large computational box size.

Keywords: instability, fluidized bed, kinematic wave, FR-DNS, IB-LBM

Validation of drag correlations for ellipsoidal particles using fully resolved simulations

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A popular method to analyze particle dynamics in turbulent flows is the Lagrangian point-particle method where the motion of the particles is modeled via semi-empirical expressions. For heavy rigid particles, these expressions are mostly reduced to the drag force. In the case of spherical particles, a huge data base and an established "standard drag curve" is available. Such a data base is missing for non-spherical particles and recently proposed drag correlations for ellipsoidal particles show significant deviations [1]. Available ellipsoidal Lagrangian point-particle methods are largely restricted to particle Reynolds numbers $Re_p \ll 1$.

In this contribution, correlation functions for the drag, lift, and torque acting on a fixed non-spherical particle in uniform flows are presented. Therefore, a numerical parameter study is performed, which covers the range $Re_p \leq 100$ for aspect ratios $1 \leq \beta \leq 8$ and inclination angles $0 \leq \phi \leq 90$. In total, more than 4,000 simulations are performed to provide sufficient data points for the models. A conservative discretization on locally refined Cartesian meshes is used, where the fluid-solid interface is sharply resolved via a cut-cell representation [3]. Figure 1 shows one of the conducted simulations, i.e., an ellipsoidal particle with $\beta = 8$, $Re_p = 50.0$, and an inclination angle $\phi = 45°$. The computational effort of such simulations is significantly reduced by solution-adaptive mesh refinement, which is controlled by local velocity gradients and the distance to the fluid-solid interface. The generated data set shows that the drag coefficient follows

$$C_{D,\phi} = C_{D,\phi=0^\circ} + (C_{D,\phi=90^\circ} - C_{D,\phi=0^\circ}) sin^2\phi \tag{1}$$

for the analyzed parameter space, which confirms the study [2]. To provide a shape-specific drag correlation, the data set is used to derive a drag correlation based on

$$C_{D,\phi=0^\circ} = C_{D,Stokes,\phi=0^\circ} \cdot f_{d,0}(Re_p, \beta), \qquad C_{D,\phi=90^\circ} = C_{D,Stokes,\phi=90^\circ} \cdot f_{d,90}(Re_p, \beta), \tag{2}$$

with the analytical drag coefficient $C_{D,Stokes,\phi}$ valid for creeping flow conditions, and the correction terms $f_{d,0}$ and $f_{d,90}$. Figure 2 shows the data points and the correlations of the correction terms for $\beta = \{1, 2, 4, 8\}$. Motivated by the good agreement of model and data, a similar approach is conducted to develop a correlation for the lift coefficient C_L and the torque coefficient C_T (not shown here). For the final contribution, it is planned to expand a common ellipsoidal Lagrangian point-particle model by the semi-empirical correlations for C_D, C_L, and C_T and to validate against large-scale benchmark simulations of fully-resolved particle-laden turbulence [4]. It is expected that the correlations significantly improve the accuracy of ellipsoidal point-particle models.

Keywords: non-spherical particles, fully resolved simulations, particle-laden turbulence

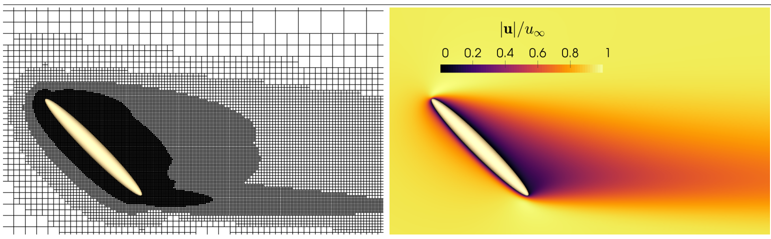

Figure 1: A sample configuration of the parametric study with $Re_p = 50.0$, $\beta = 8.0$, and $\phi = 45°$: solution-adaptive Cartesian grid (left) and absolute normalized velocity magnitude (right).

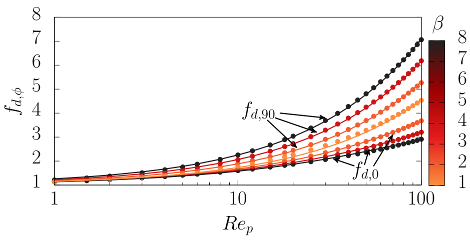

Figure 2: Drag correction term $f_{d,\phi}$ for particles with $\phi = 90°$ and $\phi = 0°$. Selected simulation values (points) and correlations (lines) are visualized.

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A Numerical Investigation of Gas-Fluidized Bed of Flexible Fibers

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Abstract

Gas fluidized bed of flexible fibers is investigated using the coupled approach of discrete element method (DEM) and computational fluid dynamics (CFD). In the numerical simulation, a flexible fiber is formed by connecting a number of spheres using elastic bonds. The fiber can deform as the bonds undergo stretching/compressive, bending, and twisting deformations. The resultant drag on a fiber by a gas is a collection of drag forces on each sphere component. The fibers of the same volume but various aspect ratios are examined for the effect of fiber elongation. It is observed that the minimum fluidization velocity increases with increasing fiber aspect ratio (AR) for AR ⩾2, due to the increase in porosity. However, the minimum fluidization velocity for the spheres (AR = 1) with the same volume as the elongated fibers is between those of AR = 3 and AR =4 fibers, because the sizes of the voids are larger for the spheres compared to the AR=2 and 3 fibers and also the effect of gas drag on the fiber motion is reduced as the sphere component size increases. At last, the effects of fiber flexibility and cohesive liquid bridge force on the fluidization behavior are reported.

Keywords: flexible fibers; gas-fluidized bed; DEM; CFD

Measurement of Rigid Fiber Motion in a Turbulent Channel Flow

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Abstract

The orientation dynamics of fibers in turbulent flows are important in various geophysical, biological, environmental and industrial processes. Flow induced fiber motion is a combination of translation and rotation, and fiber orientation depends on the history of velocity gradients experienced along fiber trajectories. In many cases, fibers are transported in channel flows and are immersed in turbulent boundary layers. While many numerical studies on fiber dispersion in wall-bounded turbulence exist [**?**], there is a lack of high quality experimental results [**?**]. We present measurements of nylon fiber, 3D rotational and translational motion in a turbulent channel flow focusing on inertial and length effects. These are quantified by the Stokes number, St, and the aspect ratio, $\beta = L/D$, repectively, where L is the fiber length and D its diameter. St is defined as the ratio between the fiber response time and the viscous time scale. Three sets of nylon fibers characterized by: β = [30.7, 47, 68.2], St = [0.22, 0.34, 0.04], and L/δ_v = [27.7, 50.6, 25.2], were investigated; $\delta_v = \nu/u_\tau$ denotes the viscous length scale, u_τ the friction velocity and ν the kinematic viscosity. Experiments were performed in a horizontal, closed-loop square water channel (50 $\times$ 50 mm^2 internal cross-section) at a distance of 1.3 m from the channel entrance, where the turbulent flow was fully developed. The corresponding bulk and friction Reynolds numbers were 7353 and 435 respectively. The 3D fiber motion in the volume of interest (VOI = 35$\times$25$\times$35 mm^3) was tracked using two orthogonal view, digital inline Fraunhofer holographic cinematography. The VOI was centered and extended from the bottom of the channel (Fig. **??**). Holograms were acquired at 500 Hz, i.e. an order of magnitude greater than the fiber response frequency. In order to acquire substantial statistics, more than 40,000 individual fibers were tracked (average track length: 10 instances) in the VOI for each fiber type. Acquired holograms were numerically reconstructed and by combining the information from the two cameras, fiber 3D orientations were determined (Fig. **??**c). Using the temporally resolved data sequences, in-plane fiber orientation rates as well as 3D fiber tumbling rates were determined as a function of wall normal distance. Results indicate a large effect of wall proximity on the orientation and orientation rates. Close to the wall fibers strongly preferentially orient themselves with the mean stream wise flow direction. In addition, fiber rotation rates strongly increase upon approaching the wall (Fig. **??**c). As far as the authors are aware, these are the first temporally and spatially resolved, 3D measurements of fiber motion in a turbulent boundary layer.

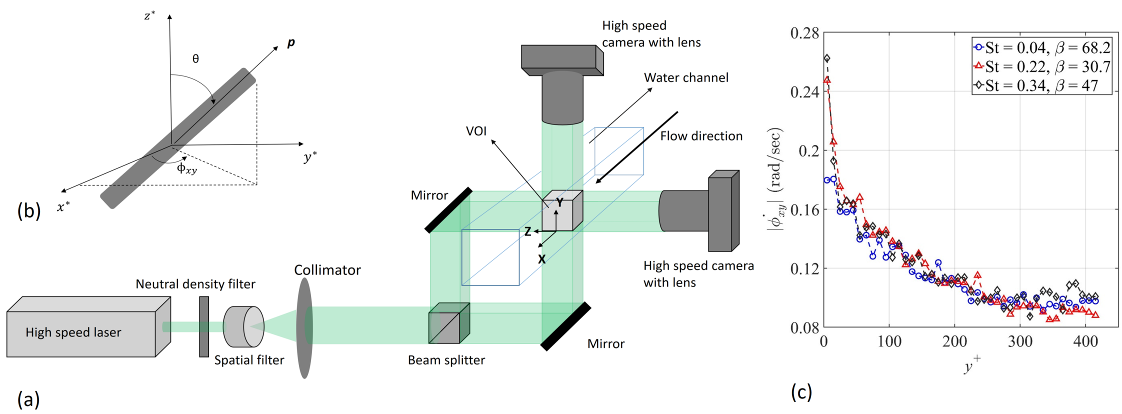

Figure 1: a) Schematic digital holography set-up (not to scale), (b) fiber with co-moving coordinate system; ϕ_{xy}: fiber's in-plane orientation, θ: polar angle, $\mathbf{p}$: unit orientation vector, (c) in-plane fiber rotation rate as a function of wall-normal position.

Keywords: Fiber rotation and translation, Channel flow, Digital holography

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Using fibers to measure flow properties

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Abstract

We present results showing how fiber-like objects (elastic [1, 2] or rigid [3]) can be used to measure relevant flow properties in both laminar and turbulent conditions. Numerical and experimental analysis are used in concert for this aim.
As far as the turbulent environment is concerned, we focus on homogeneous isotropic turbulence (HIT) and show how elastic fibers can be conveniently exploited to measure the statistics of longitudinal (flow) velocity fluctuations. Rigid fibers turns out to be suitable objects to measure the statistics of transverse velocity fluctuations.
Our evidences gave birth to a new experimental technique, the Fiber Tracking Velocimetry (FTV), which we introduce and test against 'standard' PTV measurements of the same two-point inertial range statistical observables.
The possibility of tracking assemblies of rigid fibers to access the whole flow velocity gradient is analyzed numerically for simple cellular flows with encouraging results [4].
To illustrate the potential of the new approach, we show in Figs. 1b and 1d the accuracy of the method to measure the probability density function of velocity increments both in terms of numerical experiments (via a suitable IBM) and laboratory experiments.

Keywords: flexible and rigid fibers, turbulence, Lagrangian tracking, two-point observables

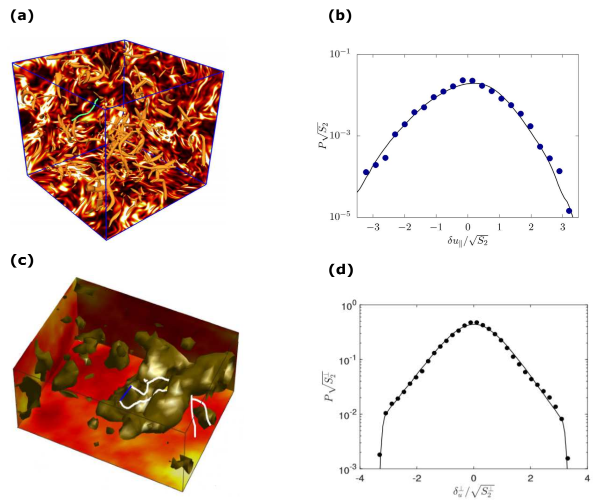

Figure 1: (a) flexible fiber (green line) immersed in a homogeneous isotropic turbulent flow; (b) probability density function (pdf) of longitudinal velocity increments; line: Eulerian pdf; bullets: pdf from the fiber. (c) rigid fiber (blue line) in turbulent flow; (d) pdf of the transverse velocity differences; line: PTV; bullets: pdf from the fiber. Panels (a) and (b) refer to the numerical experiments while panels (c) and (d) to the laboratory experiments.

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Reconstructing the fluid flow by tracking of large particles

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Abstract

The motion of a particle immersed in an unbounded fluid flow depends on the acceleration of the fluid, the instantaneous relative velocity of the particle, the history of its relative acceleration, as well as on its Stokes, Froude and Reynolds number, and on the particle-to-fluid density ratio [1]. When a suspension of particles is considered, collective effects may play an important role on the particle motion [2]. Moreover, for confined fluid flows, the presence of a wall or a free surface affects the particle trajectory by enhancing the particle drag and torque, as well as by inducing a normal-boundary lift force on the particle [3].

The particle velocity, therefore, differs from the fluid velocity. Estimating the latter from the former is a challenging task of experimental measurement techniques such as the particle image velocimetry. The particles employed in such techniques have a low Stokes number St $\ll 1$ in order to approximate the tracer limit and the suspensions formed by such particles are diluted enough to limit collective effects [4]. Under such conditions, the particle velocity is a good approximation of the fluid flow if the particle moves far away from the boundaries, i.e. its radius a is much smaller than its distance from the wall or from the free surface h. Hence, measuring the fluid flow velocity at small distance from the boundary requires very small particles, i.e. $a \ll h \ll L$, where L is the characteristic length scale of the far-wall fluid flow. As a result, the challenge of classic measurement techniques increases and so does the costs of the experimental apparatus.

In our study we propose to employ a few large density-mismatched particles in order to efficiently and accurately reconstruct the background fluid flow. Since their Stokes number is not St $\ll 1$, their velocity will not be representative of the fluid flow. However, the particles velocity can be used to approximate the particulate phase space. Taking the limit of vanishing Stokes numbers St$\rightarrow 0$, we will demonstrate how to accurately reconstruct the background flow [5]. Our approach will be numerically tested for steady, laminar flows in paradigmatic configurations. Its advantages and potentials will be discussed. Moreover, we will highlight how our approach overcomes the shortcomings faced by classic experimental measurements for particles tracked near a boundary. Extensions to time-dependent turbulent flows will be discussed.

Keywords: particle-laden flow, reconstruction of the unperturbed fluid flow, particulate phase space

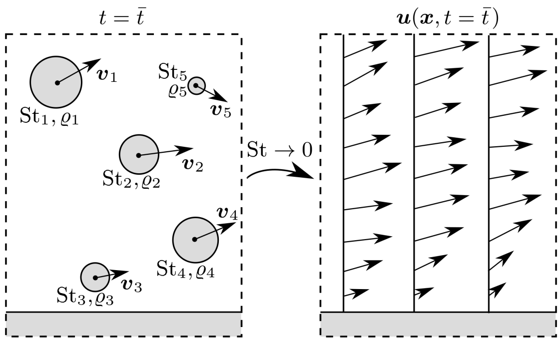

Figure 1: Approximating the particulate phase space and taking the limit of vanishing Stokes number (St $\rightarrow 0$), the background flow $\boldsymbol{u}$ is reconstructed (right) by using relatively large particles (left).

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Turbulence-controlled evolution of particle patterns on the interface of large deformable drops

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Abstract

In this paper, the process of particle capture and trapping by large deformable drops in turbulent channel flow is investigated numerically. An Eulerian-Lagrangian approach specifically developed for this three-phase flow is used: The flow field in the carrier fluid and inside the droplets is obtained from Direct Numerical Simulation of the Navier-Stokes equations; the drop interface dynamics are provided by a Phase Field Model; and particle trajectories are calculated via Lagrangian tracking. Drops have the same density and viscosity of the carrier fluid in order to mimic a liquid-liquid dispersion of water and low-viscosity oil. Particles are modelled as neutrally-buoyant, sub-Kolmogorov spheres that interact with each other through collisions (excluded-volume interaction). Simulation results allow a detailed characterization of the particle dynamics during the interface capture and trapping stages. Particle capture is driven by the capillary forces of the interface in combination with near-interface turbulent motions: Particles are transported towards the interface by jet-like turbulent motions and, once close enough, are captured by interfacial forces in regions of positive surface velocity divergence. These regions appear to be well correlated with high-enstrophy flow topologies that contribute to enstrophy production via vortex compression or stretching [1]. Examining the turbulent mechanisms that bring particles to the interface, we have been able to derive a simple transport model for particle capture. The model is based on a single turbulent transport equation in which the only parameter scales with the turbulent kinetic energy of the fluid measured in the vicinity of the drop interface, and its predictions of the overall capture efficiency agree remarkably well with numerical results [1]. Upon capture, particles sample preferentially regions of positive surface velocity divergence, which correlate with jet-like fluid motions directed towards the interface. At later times, however, particles are observed to move away from these regions under the action of the tangential stresses acting on the interface: Eventually, excluded-volume interactions bring particles into regions of vanishing surface divergence, where two-dimensional clusters are formed. Clustering into one-dimensional, highly-concentrated filaments is less likely to occur and this hampers particle accumulation into regions of negative surface divergence, which correlate with jet-like fluid motions directed away from the interface. Regions of long-term trapping and high particle concentration correlate well with portions of the interface characterized by higher-than-mean curvature. This finding is important since the presence of tiny particles at the interface is known to affect locally the surface tension, particularly in the presence of concentration gradients: present results suggest that particle-induced modifications of the surface tension should be stronger where the curvature of the interface is higher.

Keywords: Particle-interface interaction, clustering, interface topology, excluded-volume effects

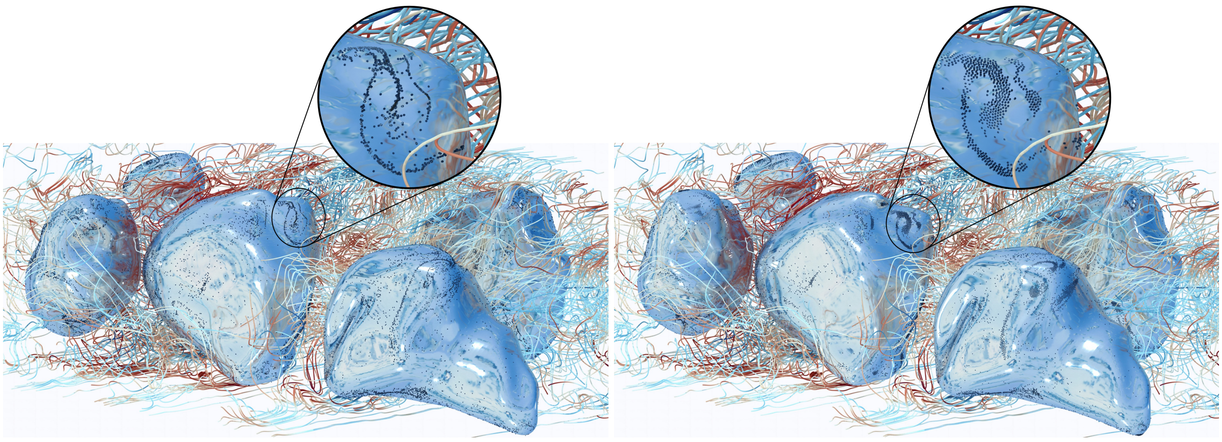

Figure 1: Snapshot of $St = 0.1$ particle distribution on the drop surface. Non-interacting trapped particles form highly-concentrated filamentary clusters (left), but appear more evenly distributed when excluded-volume effects are accounted for (right).

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Importance of fluid inertia for the orientation of spheroids settling in turbulent flow

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Abstract

How non-spherical particles orient as they settle in a flow has important practical implications in a number of scientific and engineering problems. In a quiescent fluid, a slowly settling particle orients so that it settles with its broad side first. This is an effect of the torque due to convective inertia of the fluid that is set in motion by the settling particle, which maximises the drag experienced by the particle. Turbulent fluid-velocity gradients, on the other hand, tend to randomise the particle orientation. Recently the settling of non-spherical particles in turbulence was analysed neglecting the effect of convective fluid inertia, but taking into account the effect of the turbulent fluid-velocity gradients on the particle orientation. These studies reached the opposite conclusion, namely that the particle tends to settle with its narrow edge first, therefore minimizing the drag on the particle. Here, we consider both effects, the convective inertial torque as well as the torque due to fluctuating fluid-velocity gradients. We ask under which circumstances either one or the other dominates. To this end we estimate the ratio of the magnitudes of the two torques. Our estimates suggest that the fluid-inertia torque prevails in high-Reynolds number flows. In this case non-spherical particles tend to settle with orientations maximising drag. But when the Reynolds number is small then the torque due to fluid-velocity gradients may dominate, causing the particle to settle with its narrow edge first, minimising the drag.

Keywords: BICTAM-CISM Symposium, instructions, formatting, abstract

[*] Footnotes may be used to indicate research grant, sponsoring agency, etc. These should not be numbered but referred to by symbols, e.g. *,+. The footnote text may be produced in a small font.