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Events

Fundamental Research

Physical Sciences Transfer and transport physics Engineering sciences Solid mechanics Fluid mechanics Chemical engineering and process engineering Mathematics and IT High performance computing

25 - 26 April 2017

The workshop took place from 25st to 27st of April 2017 in the Roscoff biological station.

The main objective was to bring together researchers, scientists, engineers and students in the same event to exchange and share their experiences, ideas and research results in numerical, theoretical and experimental studies about all aspects of particulates flows: particles sedimentation and dispersion, fluidized beds, heterogeneous combustion, blood flows… with applications in fields as environmental fluid mechanics, petroleum industry, paper industry, energy storage, aeronautics, biomedical sciences.

33 people attended this event. The format consisted of invited lectures within one session established to motivate scientific discussions and to enhance future collaborative research activities. The different contributions were related to the following topics:

- Multi-scale modelling and simulations of dense particulate flows
- Dynamics of particles in turbulence
- Non-spherical particles

- Heat and mass transfers in dense particulate flows
- New technologies and industrial applications

The Organising Committee is part of the two French ANR projects: MORE4LESS and CODSPIT

Thanks to all participants, speakers, authors and partners. You made the event a success!

Keynote Speaker

Sticky and tricky: Cohesive-particle flows

Cohesion between particles is widespread in nature and industrial applications alike. It can arise from a number of sources – van der Waals forces, liquid bridging, and electrostatics, to name just a few. Predicting cohesive effects is challenging at both the particle-particle level (micro) and for many-particle systems (macro). In this talk, a new framework for describing cohesive particle flows, which relies on bridging the micro-level effects to macro-level systems via a combination of experiments, DEM simulations, and continuum theory, will be presented. Demonstration of the new framework and an assessment of its performance will also be given.

Prof. Christine M. Hrenya
Chemical and Biological Engineering
Univ. of Colorado
Boulder, USA

Challenges of CFD modeling in the chemical industry: an example of multi-scale modeling of dense liquid/solid suspensions

Industrial scale processes can be challenging to improve. Amongst the usual tools used in chemical industry, CFD is more and more becoming a valuable tool for diagnosis and design. CFD models that can be used are sometimes limited in comparison to available academic tools. For instance, an LES of a few cubic meter device is still challenging, thereby limiting the turbulence modeling approach to RANS or URANS.

One option is to use a downsizing strategy in order to define a 'numerical lab reactor' (Farcy et al., Chemical Engineering Science 139, 285-303). Another possible strategy consists of doing multiscale modeling: small scales are resolved with DNS, then the information is used to calibrate/validate higher scale models. This approach has been chosen for the MORE4LESS ANR project. It has been applied to dense solid-liquid suspensions in stirred tanks. For dense liquid/solid suspension at 20% of solid volume fraction, this approach was used during a collaboration between TU Delft, University of Aberdeen and Solvay: particle-resolved elementary simulations have been done on a canonical problem and on a small tank (Derksen, AIChE J, vol 58, n°10). On the same device, a procedure using particle-unresolved simulation is validated and then applied to a higher scale in 1liter reactor. At this scale, comparisons with experiments and Euler-Euler URANS models from commercial software are done.

This allows to qualify the Euler-Euler approach that can be later be used more confidently on industrial scale reactors.

Dr. Nicolas Perret
Solvay R&I
Lyon, France

Rotation of non-spherical particles in shear

If inertia is present, the rotational motion of ellipsoids in Stokes flow derived by Jeffery (Proc. Roy. Soc. A, 102; 1922) is modified so that the particles no longer move in closed orbits but instead drift towards a preferential orbit or steady orientation. The inertial effects are determined by a rotational Reynolds number and the particle motion exhibits a number of bifurcations as this number is increased. A series of works, together presenting a combination of numerical and theoretical considerations, have been performed during the last years and the insights from these studies will be summarized in this talk.

Prof. Fredrik Lundell
KTH Mechanics

Stockholm, Sweden

Paths of Bodies Freely Rising or Falling in Fluids

Even such an ideal body like a sphere can be observed not to fall (or rise) vertically in common Newtonian fluids like air or water. The same holds for bodies of other shapes (discs, cylinders, spheroids) intuitively expected to follow vertical paths. Direct numerical simulations and the bifurcation theory make it possible to demonstrate that, as soon as the stabilizing effects of viscosity become weak enough, the vertical paths of ideally axisymmetric bodies moving in ideally quiescent fluid under the action of gravity and buoyancy become unstable and give way to a rich variety of regimes. The talk will focus on flat objects like discs, flat cylinders and spheroids presenting the most intriguing behavior.

Prof. Jan Dušek
ICube
Strasbourg, France

Flow past a yawed cylinder of finite length using a Finite Volume/ Fictitious Domain Method

Fluidized beds are frequently encountered in various industrial processes such as catalyze and biomass gasification. Despite the large numbers of studies describing the fluidization of spherical particles, much less is known concerning cylindrical particles, which are frequently used in bubbling fluidized bed. In this work, the flow past a short yawed cylinder is studied as a first step to understand the motion of many of them. To this aim the Distributed Lagrange Multiplier / Fictitious Domain (DLM/FD) method developed in the PeliGRIFF code (Wachs et al. 2015) is intensively used. This method is validated using numerical results of the literature for a cylinder of finite length in cross flow (Inoue & Sakouragi 2008). Drag and lift forces as vortex-shedding frequencies are carefully analyzed giving strong confidence in the numerical methodology. A detail study of the flow past a short cylinder at moderate Reynolds numbers (O(100)) is also carried out. The influence of the yawed angle on the wake as on the hydrodynamic force is identified. The threshold for wake instability appears for a smaller Reynolds number when the flow direction is perpendicular to the cylinder than when it is parallel. Otherwise the principle of independence which states that the normal force on the cylinder only depends on the normal component of the velocity (Sears 1948), does not seem to be valid in those regimes.

Dr. Jean-Lou Pierson
???????IFP Energies nouvelles
Solaize, France

Development of filtered particulate Eulerian modeling approach for the prediction of bi-disperse gas-solid fluidized bed

Due to computational resource limitation, Eulerian gas-solid fluidized bed simulations of industrial processes are usually performed with mesh sizes much larger than the smallest meso-scale structure size. Thus, these effective simulations do not fully account for the particle segregation effect (cluster or bubbles formation) and neglecting these structures generally lead to poor prediction of bed hydrodynamic. According to previous numerical studies, this effect seems to be very effective in bi-solid mixture with large inertia difference between the solid species.

Following Igci et al., filtered approach may be developed where the unknown terms accounting for the influence of unresolved structures, called sub-grid contributions, have to be modelled in terms of the computed (filtered) variables. In the work presented here, the development of such modelling approach is based on a priori analysis of 3D periodic circulating bi-disperse gas-solid fluidized bed simulations using computational grids cell size of a few particle diameters. Using the 3D N-Euler multiphase code NEPTUNE_CFD, separate transport equations are computed for the number density, velocity and random kinetic energy of the two solid species, coupled by collisions terms developed in the frame of kinetic theory of granular media supplemented by interstitial gas effect. The mesh-independent results obtained are filtered using volume average to analyse the effect of the subgrid scales on the terms of the momentum and the particle kinetic agitation equations. Thanks to those results, closure models are developed for the subgrid fluid-particle and particle-particle interactions terms in bi-disperse gas-solid fluidized beds. Those closure models include parameters, which may depend on the particle and gas properties and are dynamically adjusted using a multi-level filtering procedure. Several monodisperse and bi-disperse fully resolved simulations have been performed and enable to test the models for a wide range of diameter and density.

Prof. Olivier Simonin
President INP Toulouse
???????IMFT, Toulouse, France

Development of Numerical Approach for Gas-Solid Flows with Complex Particle-Particle Interactions

Euler-Lagrange (E-L) approach has been developed to take into account complex particle/ particle interactions such as; van der Waals force, forces due to liquid bridge, electrostatic forces, for gas-solid flow simulations. Highly resolved E-L simulations of periodic and wall-bounded fluidization cases have been then performed to investigate flow characteristics and propose constitutive models for standard and coarse-grained Euler-Euler approach.

Dr. Ali Ozel
Chemical and Biological Engineering
Princeton University
???????Princeton, USA

Modulation of the onset of turbulence by finite size particles

Particle-resolved numerical simulations based on the Force Coupling Method are carried out to study the effect of finite-size particles on the onset of turbulence in wall-bounded shear flows. The study particularly considers the effect of concentration, particle size and particle-to-fluid density ratio on the mixture flow features.

A specific emphasis is devoted to the cycle of regeneration of turbulence for two specific configurations, plane Couette flow and plane Poiseuille flow. Indeed, the shape of the streaks and the intermittent character of the flow (amplitude and period of oscillation of the modal fluctuation energy) are all altered by the presence of particles.

Prof. Eric Climent
???????Director of IMFT
Toulouse, France

Euler-Lagrange Modeling of Strongly Coupled Particle-Laden Flows

High fidelity simulation tools that leverage large-scale computational resources are now capable of making quality predictions of disperse two-phase flows involving a large number of particles under a wide range of operating conditions. In this talk, we present recent insights on multiphase flows with significant momentum coupling between disperse and carrier phases. Of particular interest are configurations dominated by clustering dynamics such as cluster-induced turbulence (CIT), homogeneously sheared CIT, and vertical particle-laden channel flows. Computational data from such canonical flow problems as well as from realistic engineering flows are used to inform the development of multiphase turbulence models at the macro-scale.

Prof. Olivier Desjardins
???????Sibley School of Mechanical and Aerospace Engineering
Cornell University
Ithaca, USA

Recent advances in the multi-scale simulation of mass, momentum and heat transfer in dense particulate flows

Dense particulate flows involving coupled mass, momentum and heat transfer are frequently encountered in large scale industrial processes involving granulation, coating and production of base chemicals and polymers. In dense gas-particle flows both (effective) fluid-particle and (dissipative) particle-particle interactions need to be accounted for because (the competition between) these phenomena to a large extent govern the prevailing flow phenomena, i.e. the formation and evolution of heterogeneous structures. These structures have significant impact on the quality of the gas-solid contact and as a direct consequence strongly affect the overall performance of the process. Additional complexities arise due to enhanced dissipation due to wet particle-particle collisions.

In dense particulate flows phenomena (effective) fluid-particle and particle-particle interactions have to be properly accounted for because the large scale system behavior (i.e. impact of heterogeneous flow structures on reactor performance) is sensitively influenced by the these interactions. In the multi-scale approach detailed models, taking into account the relevant details of fluid-particle interaction (DNS) and particle-particle interaction (DEM) are used to assess and develop closure laws to feed continuum models (TFM) which can be used to compute the flow structures on a much larger (industrial) scale. In this presentation recent advances in the multi-scale modeling of dense gas-particle flows will be highlighted with emphasis on coupled mass, momentum and heat transfer. In addition, areas that need substantial further attention will be discussed.

Prof. J.A.M. (Hans) Kuipers
???????Department of chemical Engineering and Chemistry
Eindhoven University of Technology
Eindhoven, The Netherlands

Micro/meso numerical simulations of fluidized beds

We perform particle-resolved micro-scale and Euler/Lagrange meso-scale numerical simulations of two fluidized beds. The former is representative of a liquid/solid fluidization with a moderate density ratio and a small Reynolds number leading to a homogeneous bubbling regime while the latter corresponds a gas/solid fluidization with a higher density ratio and a higher Reynolds number. The 2 data sets from particle-resolved and Euler/Lagrange simulations are compared on the basis of a detailed statistical analysis in order to identify potential deficiencies of Euler/Lagrange models to predict the right dynamics. We suggest a correction of the classical deterministic drag force correlation by introducing a stochastic term whose parameters are determined from particle-resolved simulation results. We discuss different research directions to further improve the predictions of Euler/Lagrange models.

Prof. Anthony Wachs
Chemical and Biological Engineering
The university of British Columbia
???????Vancouver, Canada

Theoretical modeling and three-dimensional unsteady numerical simulations of reactive fluidized beds

Natural gas combustion in two different configurations, 1) a dense fluidized bed reactor, operating with lean premixed methane-air mixture, and 2) a CLC system using perovskite as oxygen carrier is investigated. An Eulerian-Eulerian approach is used to compute both the gas and the solid phases in an Eulerian fashion accounting for specific closures in order to model interphase mass, momentum and energy transfers. Combustion is modeled using a two-step mechanism for homogeneous (gas-gas) reactions (Dryer & Glassman, Sym. (Int) on Combustion, 1973). A grain model, which accounts for both the competing mechanisms of chemical reaction at the particle surface and gaseous diffusion through the particle layer, is instead retained for heterogeneous (particle-gas) reactions (de Diego et al., Ind. Eng. Chem. Res., 2014). For each configuration, 3D unsteady CFD simulations are performed by NEPTUNE_CFD code and the results compared with available experimental measurements (Dounit et al., Chem. Eng. J., 2008, Mayer et al., Applied Energy, 2015).

Dr. Ziad Hamidouche
???????IMFT, Toulouse, France

Liquid-solid simulations of fluidized beds with heat transfer at micro/meso scales

Fluidized beds are encountered in various domains such as oil and gas services and chemical engineering. The comprehension of flow properties and transfer in these systems is complex since spatial interaction occurs from the particle scale to the process unit scale. Particulate flows arising in fluidized beds are often coupled with heat and/or mass transfer through chemical reactions. The recent progress in high performance computing (HPC) and resources enables to simulate fluidized beds at micro scale (PRS) up to thousands of particles. The local information computed during the simulations provides a database to better understand momentum and heat transfer occurring in fluidized beds. Due to the wide range of scales in presence (micro to macro), a multiscale framework is used to study these processes. A mesoscale is also introduced corresponding to interactions between parcels of particles. In this work, microscale (DLM/FD) and the meso (Euler/Lagrange) scale simulations of liquid-solid fluidized beds with heat transfer are performed with our massively parallel code PeliGRIFF.

A comparison of system size at microscale is provided to select appropriate size allowing statistically averaged local and global momentum and heat transfer. Then, a direct comparison of the predictions obtained at both scales is performed and

suggest how the mesoscale modeling might be improved to provide more accurate solutions. Hydrodynamics improvements of the mesoscale model according to PRS results is realized by introducing a correction in the forces acting on the particles or by adding a fluctuating term in the eulerian variables. Correcting in a first time mesoscale hydrodynamics will give a hint on the need to add a correction term on heat transfer process into fluidized beds.

Florian Euzenat
???????IFP Energies nouvelles, Solaize, France

Heat transfer in a packed bed of particles for energy storage : an experimental and numerical study

Climate change concerns, the will to reduce dependence on fossil fuels and greenhouse gas emissions, are resulting in increased deployments of renewable energy technologies. But the intermittency of renewable power sources such as wind and photovoltaic presents a major obstacle to their extensive penetration into the grid. Electricity storage is a potential solution to address this intermittency problem by compensating for wind and sunshine’s variability. Among the many technologies available, Advanced Adiabatic Compressed Air Energy Storage (AA-CAES) is a promising technology since it is a zero-emission storage system with a potential round-trip efficiency close to 70%. AA-CAES stores not only the compressed air, but also the heat, which is released upon compression of the air, in a separate heat storage tank. In order to generate electricity, the heat is returned to the compressed air, which flows to the turbine. The Thermal Energy Storage (TES) system plays a prevailing role in the global efficiency of AA-CAES process. At IFP Energies nouvelles, we develop a technology for TES system, based on fixed bed reactors to store heat in particles.

In the present study, we investigate the heat transfer within a fixed bed using an experimental and a numerical approach. The objective of this study to better understand the heat transfer involved in such a system but also to validate the closure laws used in the numerical Euler-Euler approach.

Dr. Guillaume Vinay
???????IFP Energies nouvelles, Rueil-Malmaison, France

Particles and snowflakes falling through turbulence

The question of how turbulence affects the settling of small heavy particles is relevant to both industrial and natural settings. I will present laboratory and field measurements and numerical simulations, demonstrating how turbulence may lead to a multifold increase of particle fall speed. In the laboratory, we use a novel apparatus where microscopic particles fall through a large volume of homogeneous air turbulence. In the field, we image snowflakes settling in the atmospheric surface layer during snowfalls. Further insight is provided by direct numerical simulations of particle-laden turbulence, to which we apply a novel definition of cluster based on self-similarity.

Prof. Filippo Coletti
Aerospace Engineering and Mechanics
University of Minnesota
???????Minneapolis, USA

Settling of isotropic and anisotropic solid particles in homogeneous isotropic turbulence

In a first part, the behaviour of large and heavy particles settling in a decaying isotropic homogeneous turbulence has been investigated using experiments with glass beads in water turbulence. For a Stokes number, based on the Kolomogorov scale, close to unity, we measured a increase of the settling velocity compare to the one measured in a still fluid. In addition, an anisotropic response of the particles to the turbulence is measured. The turbulent agitation of the particles, which is of the same magnitude as turbulent kinetic energy of the fluid phase in the horizontal direction, is found to be much larger in the direction of the gravity. Those findings agree well with previous experimental and numerical results (e.g. Good, G. H. et al. J. Fluid Mech. 759, 2014). Using scaling arguments, we also show that enhancement of the settling velocity of heavy particles can only occur in specific turbulent flows. For heavy particles, with rp >> rf, criteria solely based on the properties of the turbulent flow are then proposed.

In a second part, we will present some preliminary results from a study of a jet of heavy inertial particles falling under gravity in a quiescent fluid and in an isotropic homogeneous turbulence. In absence of fluid flow, we found that the mean jet diameter remains constant at low volume fraction while a large dispersion of the jet particle is measured at higher volume fraction. A simple model in which the dense suspension is described as an effective liquid is proposed. The liquid-into-liquid jet description with as entrainment velocity depending on the particle volume fraction reproduces the observed trends. When the jet of particle falls in a turbulent flow we measured an increase of the dispersion as the volume fraction is reduced.

Asmaâ Aissaoui
???????IMFT, Toulouse, France

Preferential concentration of inertial particles in turbulent flows

Turbulent flows laden with inertial particles present multiple open questions and are a subject of great interest in current research. Due to their higher density compared to the carrier fluid, inertial particles tend to segregate in clusters, also leading to depleted regions (voids). This mechanism, called preferential concentration, results from the interaction of the particles with the multi-scale and random structure of turbulence. The exact mechanism at play and the full dynamical consequences still remain however to be unveiled. We will present an experimental investigation of the clustering phenomenon of heavy sub-Kolmogorov particles in homogeneous isotropic turbulence. We investigate the effects of Reynolds number (R?, quantifying the turbulence intensity), particles Stokes number (St, quantifying particles inertia) and seeding volume fraction on preferential concentration. We use Voronoï analysis to quantify clustering as well as the dimensions of cluster and void regions. An important result concerns the weak dependency on Stokes number observed, which lends support to the "sweep-stick" mechanism, where particles accumulate preferentially near zero-acceleration points of the carrie flow. To explore further this scenario, we investigate the clustering properties of specific topological points (suchs as zero-acceleration points and zero-vorticity points) of the velocity field of single phase homogeneous isotropic turbulence (obtained for instance from direct numerical simulations) which we compare to the clustering characteristics of particles in the experiments.

Dr. Mickael Bourgoin
???????Physics laboratory
ENS Lyon
Lyon, France

Large-Eddy Simulation of Coal Combustion

Coal boilers are a prime example for the advantages of LES: where experiments are hardly feasible, due to very poor optical access, RANS simulations would require very significant closure models, considering the strong turbulence-chemistry-radiation coupling between the Eulerian and Lagrangian phases. Given the uncertainties in these closures, LES can make a real difference with simple models already. The presentation introduces some of the relevant coal physics, it’s modelling, and recent, massively parallel examples of coal flame LES and DNS with common and detailed pyrolysis modelling.

Prof. Andreas Kempf
???????Fluid Dynamics
University of Duisburg-Essen
Duisburg, Germany

Use of gas/particles CFD codes in the IFPEN Chemical Engineering Department

The Chemical Engineering department of IFPEN is involved in the development of several processes with gas/particles flows such as oil conversion (Fluid Catalytic Cracking), Chemical Looping Combustion and biomass conversion. Within the last decade, gas/particles CFD tools have become more and more popular to help engineers in the development of reactor technologies and the troubleshooting of industrial units. In this presentation, we first compare the different approaches used for gas/particles CFD simulations (Euler-Euler, MP-PIC). Then, examples of the CFD tools usage going from simulation at cold flow model scale to simulation at industrial scales are presented. Finally, issues and limitations faced with the CFD tools currently used in the chemical engineering department are discussed.

Benjamin Amblard
???????IFP Energies nouvelles, Solaize, France

Development of a parallel CFD/DEM approach for the simulation of reactive fluidized bed reactors

This presentation focuses on the development of a CFD/DEM solver for Fluidized Bed Reactors (FBR) of complex shape. In the CFD/DEM formalism, the simulation of the fluid phase dynamics relies on the solving of the filtered Navier-Stokes equations at low-Mach number on unstructured meshes and the solid particles are tracked using the Discrete Element Method (DEM). This formalism is able to provide a local insight into i) multiple particle-particle and wall-particle contacts, and ii) gas/particles hydrodynamics and thermal coupling. A dynamically thickened flame approach, which is widely used for combustion Large-Eddy Simulation (LES), is retained allowing the spatial resolution of the flame front on a grid coarser than the flame thickness. The implemented approach is specifically tailored for massively parallel computing on unstructured meshes in complex geometries: it features a dynamic collision detection grid and packing/unpacking of the halo data for non-blocking MPI exchanges. The results of three-dimensional (3D) numerical simulations of a reactive semi-industrial FBR fed with a natural gas/air mixture are compared with available experimental measurements performed in the LGC laboratory.

Yann Dufresne
CORIA, Rouen, France

Three-dimensional numerical simulation of a lab-scale pressurized fluidized bed using a LES-DEM approach

In this work, three-dimensional (3D) numerical simulations of a lab-scale pressurized fluidized bed are performed using an Euler-Lagrange approach. The gas phase is modeled solving the low-Mach variable density Navier-Stokes equations in a LES framework, and the solid phase is tracked by the Discrete Element Method (DEM). The implemented approach allows detailed investigation of the effects of i) fluid-particle drag force and particle-particle soft sphere collision model, ii) particle-wall collisions, accounting for dynamic friction, and iii) multiple particle-particle contacts for collisions occurring in dense regime. The 3D unsteady numerical simulations are realized in the frame of the flat frictional wall assumption for the particle boundary conditions and for different particle-particle and particle-wall restitution coefficient values in order to analyze their influence on the dynamic behavior of the fluidized bed. Results from Euler-Lagrange numerical simulations are compared with the predictions obtained using a two-fluid continuum approach. Furthermore, time-averaged quantities are computed and numerical predictions compared with available experimental measurements, obtained from Positron Emission Particle Tracking for the same pressurized bed configuration.

Ainur Nigmetova
???????IMFT, Toulouse, France

Numerical modelling of deformable particles under flow: the example of red blood cells

In the context of suspension dynamics, blood occupies a very special place, due to the obvious interest in understanding its flow for medical applications, but also because of its staggering complexity. Indeed, blood is a dense suspension of highly deformable particles, the red blood cells, which control blood dynamics. Red blood cells consist of a drop of hemoglobin solution enclosed by a compound biological membrane. As other suspensions, blood rheology depends on the volume fraction occupied by the dispersed phase. However, blood behavior also depends on the dynamics of the cells themselves. Predicting blood flows by numerical simulation thus necessitates solving the intricate dynamics of its red blood cells.
In this talk, I will illustrate the complexity of blood flows and of isolated red blood cells dynamics under flow. I will also underline the numerical challenges associated with suspensions of deformable particles. Finally, I will present recent results showing that we are only at the early stages of understanding how blood flows.

Dr. Simon Mendez
???????IMAG laboratory
University of Montpellier
Montpellier, France

Program and Asbtract

Download the final program and abstract *(PDF - 317Ko)*

Workshop Particles & Fluids: from individual particle dynamics to collective effects and fluidized beds
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