



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

Roscoff biological station, France, April 24-27 2017

CODSPIT	MORE4LESS
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Program & Abstracts

Conference topics

Multi-scale modeling 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

MONDAY, APRIL 24, 2017

Mo 19:00 Aperitif Dinner in Roscoff (La Moule au Pot)

TUESDAY, April 25, 2017

Tu 08:45 Opening: Welcome addresses
Short presentation of the ANR projects CoDSPiT and More4Less

Chairman : P. Fede and M. Bourgoïn

Tu 09:00 Sticky and tricky: Cohesive-particle flows

C.M. Hrenya, *University of Colorado, Boulder, USA*

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.

Tu 09:50 Challenges of CFD modeling in the chemical industry: an example of multiscale modeling of dense liquid/solid suspensions

N. Perret, *Solvay R & I, Lyon, France*

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*, vol58, n°10). On the same device, a procedure using particle-unresolved simulation is validated and then applied to a higher scale in 1 liter reactor. At this scale, comparisons with experiments and Euler-Euler URANS models from a commercial software are done.

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

Many open questions remain such as the difficulty to acquire accurate measurements for opaque slurries, and mapping out the detailed impact of a great number of numerical parameters that one can find in Eulerian granular models.

Although the impact of non-ideal products (polydispersity, shape factors) still has to be investigated in depth, the results of comparisons showed that Eulerian granular models can be more confidently used to improve industrial scale reactors.

Tu 10:20 Coffee break

Tu 10:50 Rotation of non-spherical particles in shear

F. Lundell, *Linné FLOW Centre & Wallenberg Wood Science Center, KTH Mechanics, Stockholm, Sweden*

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 summarised in this talk.

Tu 11:30 Paths of Bodies Freely Rising or Falling in Fluids

J. Dušek, *ICube, Strasbourg, France*

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.

Tu 12:00 Flow past a yawed cylinder of finite length using a Finite Volume/Fictitious Domain Method

J. L. Pierson, A. Hammouti, *IFPEN, Solaize, France*

Fluidized beds are frequently encountered in various industrial processes such as catalyse 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 fluidised 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 analysed 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 are 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.

INOUE, O. and SAKURAGI, A., (2008), “Vortex shedding from a circular cylinder of finite length at low Reynolds numbers”, *Physics of Fluids*, 20, 033601.

SEARS, W. R., (1948) The boundary layer of yawed cylinders. *Journal of the aeronautical sciences*.

WACHS, A. HAMMOUTI, A., VINAY, G., et al., (2015) Accuracy of finite volume/staggered grid distributed lagrange multiplier/fictitious domain simulations of particulate flows. *Computers & Fluids*, 115, p. 154-172.

Tu 12:30 Lunch (Gulf Stream)

Chairman : O. Praud and F. Coletti

Tu 14:15 **Development of filtered particulate Eulerian modeling approach for the prediction of bi-disperse gas-solid fluidized bed**
S. Chevrier, P. Fede, E. Masi, O. Simonin, *IMFT, Toulouse, France*

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 leads 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. [2], 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 [3]. 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 [3, 4]. 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.

- [1] AGRAWAL, K., LOEZOS, P., SYAMLAL, M., SUNDARESAN, S., (2001), “The role of meso-scale structures in rapid gas–solid flows”, *J. Fluid Mech.* 445, 151–185.
- [2] IGCI, Y., ADREWS, AT., SUNDARESAN, S., PANNALA, S., O’BRIEN T., (2008), “Filtered two-fluid models for fluidized gas-particle suspensions”, *AIChE J.*, 54, 1431-1448
- [3] OZEL, A., FEDE, P., SIMONIN, O., (2013), “Development of Filtered Euler-Euler Two-phase Model for Circulating Fluidised Bed: High resolution Simulation, Formulation and a Priori Analyses”, *International Journal of Multiphase Flow*.
- [4] GERMANO, M., PIOMELLI, U., MOIN, P. and CABOT, W. H., (1991), “A dynamic subgrid-scale eddy viscosity model”, *Physics of Fluids A: Fluid Dynamics*, 3, 1760-1765.
- [5] PARMENTIER, J.F, SIMONIN, O., DELSART, O., (2012), “A functional subgrid drift velocity model for filtered drag prediction in dense fluidized bed.”, *AIChE Journal*, 58, 1084-1098. Chevrier, Fedde and Simonin

Tu 14:55 **Development of Numerical Approach for Gas-Solid Flows with Complex Particle-Particle Interactions**

A. Ozel, Y. Gu, J. T. Kolehmainen, Ch. M. Boyce, S. Sundaresan, *Dept. of Chemical and Biological Engineering, Princeton University, Princeton, USA*

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.

Tu 15:25 **Modulation of the onset of turbulence by finite size particles**

E. Climent, M. Abbas, G. Wang, V. Loisel, O. Masbernat, *IMFT, Toulouse, France*

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.

Tu 15:55 Coffee break

Tu 16:25 **Euler-Lagrange Modeling of Strongly Coupled Particle-Laden Flows**

O. Desjardins, *Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, USA*

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 macroscale.

Tu 19:30 Dinner in Roscoff (Chez Janie)

WEDNESDAY, April 26, 2017

Chairman : V. Moureau and O. Desjardins

We 09:00

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

J.A.M. Kuipers, *Multiphase Reactors Group, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, The Netherlands*

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 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 which need substantial further attention will be discussed.

We 09:50

Micro/meso numerical simulations of fluidized beds

A. Esteghamatian¹, A. Hammouti², Michel Lance³, A. Wachs¹, ¹*University of British Columbia, Vancouver, Canada* / ³*LMFA, ECL, Lyon, France*

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.

We 10:20 Coffee break

We 10:50 Theoretical modeling and three-dimensional unsteady numerical simulations of reactive fluidized beds

Z. Hamidouche, E. Masi, P. Fede, O. Simonin, *IMFT, Toulouse, France*

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).

We 11:20 Liquid-solid simulations of fluidized beds with heat transfer at micro/meso scales

F. Euzenat¹, A. Wachs², A. Hammouti¹, E. Climent³, P. Fede³

¹IFPEN, Solaize, France / ²University of British Columbia, Vancouver, Canada / ³IMFT, Toulouse, France

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. Experimental studies investigating hydrodynamic or heat transfer in these systems have been carried to provide a better comprehension of mean behavior of heat transfer into fluidized beds [1, 2, 3]. These studies provide reliable results for dilute regimes and recently converge in dense regimes [4, 5]. Only recent numerical works focused on local hydrodynamic/heat/mass transfer and fluctuations [5].

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 provide 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.

Preliminary to this study, heat transfer closure laws were derived from PRS for both dilute and dense regimes through fixed arrays of particles. Mesoscale momentum/heat transfer between the two phases are modeled using these closure laws. 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 [6].

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 [8]. 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 an hint on the need to add a correction term on heat transfer process into fluidized beds.

References

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- [2] W.E. Ranz and W.R. Marshall, Evaporation from drops, Part I and II. *Chemical Engineering Science*, vol. 48, pp.141-146; pp. 173-180, 1952.
- [3] Haid M. Heat transfer to liquid-solid fluidized beds, *Chemical Engineering and Processing*, vol. 33, pp. 211-225, 1994.

We 11:50

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

G. Després¹, E. Sanz², C. Plais², S. Poncet², D. Teixeira¹, G. Vinay¹

IFPEN ¹*Fluid Mechanics Department*, ²*Process Design and Modeling Department, France*

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.

We 12:20 Lunch (Gulf Stream)

- We 14:30 Excursion to the island of Batz. Crossing by boat from Roscoff (15 minutes).
- We 19:30 Tasting Breton beers followed by dinner at the restaurant “Le Gulf Stream”

THURSDAY, April 27, 2017

Chairman : J. Dusek and G. Vinay

Thu 09:00 Particles and snowflakes falling through turbulence

F. Coletti, *Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, USA*

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.

Thu 09:50 Settling of isotropic and anisotropic solid particles in homogeneous isotropic turbulence

O. Praud, R. Bazile, *IMFT, France*

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 $r_p \gg r_f$, 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.

Thu 10:20 Coffee break

Thu 10:40 Preferential concentration of inertial particles in turbulent flows

M. Bourgoïn, *Laboratoire de Physique, ENS de Lyon, France*

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 (Re_λ , 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 carrier flow. To explore further this scenario, we investigate the clustering properties of specific topological points (such 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.

Thu 11:20 Large-Eddy Simulation of Coal Combustion

A. Kempf, *Fluid Dynamics, University of Duisburg-Essen, Duisburg, Germany*

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, its modelling, and recent, massively parallel examples of coal flame LES and DNS with common and detailed pyrolysis modelling.

Thu 12:00 Use of gas/particles CFD codes in the IFPEN Chemical Engineering Department

B. Amblard, *IFPEN, Rueil-Malmaison, France*

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.

Thu 12:30 Lunch (Gulf Stream)

Chairman : E. Masi

Thu 14:15 Development of a parallel CFD/DEM approach for the simulation of reactive fluidized bed reactors

Y. Dufresne¹, V. Moureau¹, G. Lartigue¹, E. Masi², O. Simonin²

¹CORIA, Rouen, France / ²IMFT, Toulouse, France

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.

Thu 14:45 Three-dimensional numerical simulation of a lab-scale pressurized fluidized bed using a LES-DEM approach

A. Nigmatova¹, Y. Dufresne², E. Masi¹, V. Moureau², P. Fede¹, O. Simonin¹

¹IMFT, Toulouse, France, ²CORIA, Rouen, France

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.

Thu 15:15 Coffee break

Thu 15:45 Numerical modelling of deformable particles under flow: the example of red blood cells

S. Mendez, *IMAG, Université de Montpellier, France*

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.

Thu 16:25 Workshop ends

Thu 19:30 Dinner in Roscoff (Les Chardons Bleus)