New Frontiers in Multiphase CFD for the 21st Century Energy Mix (18w5139)

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1 Context

There is urgent need to reduce the environmental footprint of the process industry and to design new, sustainable processes, involving renewable energy and materials. The 21st century energy mix will comprise oil, gas, hydro, wind, sun, biomass and nuclear sources of energy. Major challenges are extracting and converting the largest amount of energy from these sources, and to prepare feedstocks from waste materials. The corresponding processes all involve multiphase flows that generally exhibit intricate mass, momentum and heat transfers. The overall efficiency of the processes is strongly dependent on the level of control over these transfers. Historically, most of the advances in this domain came from lab experiments, with costly up-scaling issues to solve and inherent limitations in what is accurately measurable in the core of flows. Although pilot plants are still tremendously helpful in the design of reliable and more efficient processes, the fast-evolving computer industry has been offering over the past 20 years unprecedented ways to perform large-scale computations and to gain insight in these flows. Combined to more realistic multiphase flow models, accurate numerical schemes and fast parallel solution algorithms, computational fluid dynamics (CFD) is progressively becoming a genuine game-shifter for technological breakthrough in the process industry.

However, the process industry is still far behind in terms of incorporating Computational Fluid Dynamics (CFD) practices in its design tool chain compared to other sectors in which engineering-based simulations have been recognized long ago as a provider of major knowledge for technological breakthrough and efficiency improvement. These other sectors include, e.g., reservoir modeling, weather forecast and automotive industry. The process industry still relies on design procedures and operational practices that date from the post-second world war era. It is quite obvious right now that experimental and theoretical work, although highly complementary to simulations & computations, will not be sufficient to address the 21st century technological challenges and its transition towards sustainability of the process industry. In other words, we need more advanced, more reliable and more insightful computational tools that are transferrable to and trusted by industrial partners.

The mathematical modeling of multiphase flows in the process industry (as well as in nature as, e.g., landslides, sediment transport in rivers, sea/atmosphere mass transfer) has not yet reached the expected level of maturity. Although significant progress has been made to provide scientists and engineers with more accurate models, new simulation methods combined to forefront parallel computations undoubtedly help to solve the well known issues in multiphase flows: coupled momentum-heat-mass transfer, multiplicity of scales, highly inertial or even fully turbulent flows, non-Newtonian behavior of fluids at play. For instance, micro-scale simulations, i.e., high-fidelity simulations at the level of individual particles/bubbles/droplets, became possible only through High Performance Computing (HPC) and have delivered precious data, that were not accessible by experiments and theory, to understand the complex behavior of the corresponding multiphase systems. One challenge is now to transfer that knowledge to higher scale models of industrial relevance.

HPC and CFD have been recognized as new powerful tools for innovation. The industry of supercomputers has been evolving very rapidly for the past 10 years and indeed faster than the software engineering of large scientific codes. The computing power that they offer is only going to grow. In the multiphase CFD community, very few codes have breached the 1 billion of unknowns barrier at a production level with a good overall computing performance. There is much to benefit from the computing/simulating capabilities of these numerical tools in terms of physical understanding. And the needs of the process industry to design new materials, improve the efficiency of existing processes and progressively move to a greener technology is an extremely strong incentive to extend the frontiers of advanced multiphase CFD tools. The societal expectations are high too. A lot is at stake in the 21st century energy transition.

Another challenge in this area is to foster team-work between academic research and industrial players. The fact that the problems we need to attack are extremely challenging (maybe more than in other aforementioned industries) and the somehow still existing visible gap between industrial expectations and what the leading academic researchers can deliver should not preclude extensive academia-industry team work. Although many productive academia-industry partnerships exist, an additional effort in that direction will represent a real catalyst for forefront advances and accelerated technological development.

2 Overview of the Field

Multiphase flows are widely encountered in various industrial applications, especially the energy industry. For the 21st century, the energy mix is progressively enriched with renewable energy such as solar, wind, and biomass. Hence, there is an urgent need to strengthen the computational fluid dynamics (CFD) modeling tools to provide fundamental knowledge and further translate the knowledge into tangible technological innovation for the process industry to secure clean and sustainable energy sources. This workshop brought experts from academia and industry to exchange the current state-of-art and discuss the challenges and possible path forward for the multiphase flow modeling community.

The topics communicated in this workshop covered different multiphase flow systems including gas-solid, gas-liquid, liquid-solid, and gas-liquid-solid. The majority of talks were focused on the particulate multiphase flow system and the scope ranged from fundamental rheology model and theory development to advanced numerical algorithm for high performance computing and large-scale simulations. Below are some key take-aways from the meeting:

1. It is well acknowledged that the complexity of multiphase flows encountered in many industrial applications is due to the wide span of spatial and temporal scales. There was consensus that a multi-scale modeling approach [1] should be used to address large-scale industrial problems.

2. Due to the advancement in computing hardware and numerical algorithm, in general the modeling work shifted toward high-fidelity and computationally intensive simulations. In this workshop, there were many talks on direct numerical simulation (DNS) and discrete particle modeling (DPM), front tracking methods for gas-liquid flows, etc. This approach generates significant data for mining and there were discussions about how these datasets could potentially be shared to accelerate knowledge and model creation.

3. In the current exercise of multi-scale modeling, usually only one way coupling is adopted, i.e., the knowledge propagates from small-scale to meso-scale further to large scale. For example, the development of drag model from DNS on particle-scale, then filtered drag model on meso-scale and finally those constitutive models are used for the large-scale modeling. However, it usually lacks of a mechanism to provide feedback from large scale to small scale as emphasized by Prof. Kuipers' talk.

4. The machine learning and data science are being utilized in the development of meso-scale constitutive closure and show promising outcomes by coupling with physical constraints - e.g., the work by Prof. Balachandar's group to couple theoretical approach with neural network to develop the next generation drag model for Euler-Lagrange modeling.
5. A guideline of best practices for multiphase flow modeling is needed for industry even just for several representative problems. This was highlighted by Dr. Khanna in his plenary talk.
6. The computational complexity increases as we start utilizing hi-fidelity simulations (e.g., DNS of particulate flows for drag laws revealed that it is not sufficient to have drag correlations as a function of point properties only). On the other hand, even with current models, it is not feasible to simulate industrial scale flows without significant assumptions and simplifications (and sometimes not fully supported). This opens up opportunities to multiscale methods that efficiently model global large-scale features while the local fine features are modeled and upscaled to refine the global solutions. One possible option is to develop models on two-point correlations or other ways to capture local and global interactions.
7. There is a need for renewed emphasis on traditional chemical engineering training at schools.

3 Recent Developments and Open Problems

Over the past 10-15 years, the field of CFD for multiphase flows has rapidly evolved, with more advanced physical models, more accurate numerical schemes and faster algorithms. Supported by the growing computing power of modern supercomputers, multiphase CFD is becoming more mature with predictive capabilities that the industry can use for a enhanced design and reliable control of processes. Among the recent developments, we would like to emphasize the following:

- most modern implementations of numerical methods are nowadays parallel by default to exploit the large computing power offered by supercomputers. It has become a standard to write scientific codes and develop new schemes and algorithms that can run in parallel,
- the lattice Boltzmann method (LBM) has been established as a trustworthy alternative for solving multiphase flow problems [2]. The attraction for LBM partly stems from its ease of programming and parallelizing,
- while numerical approaches for momentum transfer are progressively becoming more reliable, additional physical effects have been incorporated into the numerical models as, e.g., heat/mass transfer [3], cohesive [4] or electrostatic [5] interactions between particles, non-spherical shape of solid particles [6]. This has enabled the community to examine a wider range of problems with industrial relevance,
- as multiphase problems discussed in this workshop exhibit a wide range of scales, the benefit of adopting a multi-scale approach is now widely accepted in the community. In general, the multi-scale approach is based on a decomposition of scales with adapted models at each scale and a bottom-up strategy, i.e., what is learnt at small scales cascades upwards to the large scales,
- closure laws integrate more and more detailed physics based on reliable high fidelity simulations,
- data-driven/machine learning is entering the field as a tool to postulate the functional form of closure laws to better represent the flow complexity and to compute the coefficients entering the aforementioned functional forms,
- as numerical models for fluid/particle and fluid/fluid interactions improve, and the available computing power grows, there is sufficient incentive to attempt to examine 3-phase systems [7].

There are however many open problems that include:

- while developing codes and algorithms for parallel computing as a standard has been a big step forward, the new multi-core architecture introduced by the hardware industry has created new challenges that may require a change of programming paradigm,

- growing computing power does not mean infinite computing power and small scale high-fidelity computations are still limited to rather small systems with a maximum of $O(10^5)$ bubbles and/or particles. Additional efforts towards faster and more scalable algorithms are still required. The 1 billion of cells computing barrier in multiphase CFD has not yet been brought down. This also calls for extended code sharing,
- 3-phase flow problems are relevant of many industrial processes but have not yet received a lot of attention due to their inherent complexity, both at the physical modeling level and at the computational level,
- the problem of thin boundary layers prevent classical numerical schemes that use a constant grid size to examine certain ranges of parameters as, e.g., large Reynolds or Peclet numbers. A solution involves using adaptive mesh refinement (AMR) technique that are well established in the literature. However, the programming complexity associated to AMR has impeded its widespread use in the multiphase CFD community. There is however a huge benefit in porting all current numerical codes to AMR,
- there is a lot we still do not know in 2-phase flows about the functional form of some of the unclosed terms, especially if the flow is partly or fully turbulent. Designing more accurate coarse-grained models has been a sustained effort over the last decade that should be pursued.

4 Presentation Highlights

We give below a flavor of what was presented and discussed over the workshop. We summarize the contributions of the 4 plenary speakers and further illustrate the nature of the scientific exchanges through a selection of standard talks. Finally, the workshop held 2 round tables whose general outcome is shortly highlighted.

Plenary talks

1. Modeling polydisperse multiphase flows using quadrature-based moment methods, Rodney Fox, Iowa State University
Prof. Rodney Fox is Anson Marston distinguished professor in Engineering Center for Multiphase Flow Research and Education at Iowa State University. In this talk, he presented the theoretical derivation of quadrature-based moment methods (QBMM) to solve the generalized population balance equations (GPBE) for poly-disperse multiphase flows. Starting from a closed GPBE, the unclosed moment equations were formulated and closed using QBMM. The accuracy of the closure was controlled by the order of the moments used in QBMM. In practice, the choice of the moments used in the closure was crucial. Once the moment equations have been formulated, the numerical algorithms used to solve them must be consistent with the underlying GBPE. Several examples of the numerical issues arising with QBMM were discussed, along with some open issues related to the numerical algorithms.

2. Wet particle systems from fundamentals to applications, Raffaella Ocone, Heriot-Watt University
Prof. Ocone is Chair of Chemical Engineering in the School of Engineering and Physical Sciences at Heriot-Watt University (HWU) in the UK. She has 25-year experience in modeling complex systems, spanning from solid/gas suspensions, to complex reaction networks. In her talk, she presented their work on wet particles made cohesive through the existence of liquid bridges. She presented some rheological studies and numerical simulations all aimed at elucidating the role that liquid bridges play on the ”flowability” of particles with focus on the intermediate regime between the two limits of quasi-static and rapid flows. She discussed their past modeling efforts and how they could help bridge the gap between particle and equipment scales. The efforts included constitutive model development, experimental characterization, lab validation and a few examples of applications. She mentioned about a large project entitled ”a new multi-scale paradigm for particulate flows” to develop a user-inspired theory to help master the hydrodynamics of particulate media and improve the reliability of their industrial processing. She highlighted the need for genuine multi-scale approaches for modeling.

3. CFD Modeling in the Petrochemical and Chemical Industry, Ray Cocco, PSRI

Dr. Ray Cocco is president and CEO of Particulate Solid Research (PSRI) in Chicago. PSRI is an international consortium of companies focused on the advancement of technology in multiphase flows with granular and granular-fluid systems. In his talk, he provided a brief overview of history of fluidization and its applications in various industries. Then he showed some examples at PSRI utilizing CFD modeling tool, primarily CPFD with MP-PIC (multiphase particle-in-cell) method, in experimental design and testing to help understand and troubleshoot industrial problems. According to him, a successful model stems from how well the modeler and stakeholders understand the fundamentals and the constitutive equations used for closing those fundamentals. He summarized the requirements for higher order models in industry and pointed out some pitfalls and limitations with CFD in the petrochemical and chemical industry such as oversimplifying boundary conditions, ignoring transient versus steady-state behavior, and not realizing the benefits of a poor fit. At the end of his talk, he emphasized the need for further development of drag model for fluidization application and best practices for users.

4. CFD Applications and Challenges in BP, Samir Khanna, BP
Dr. Samir Khanna is modeling advisor at BP. He oversees the CFD modeling activities across BP for both upstream and downstream processes. In his talk, he first introduced his career as a CFD modeler in Corning and BP. He then provided a brief overview of various CFD modeling activities at BP including prediction of erosion, corrosion and flow-induced-vibration for upstream and crude blending in large tanks, thermal mixing points, fluid catalytic cracking, and bubble-column reactors in downstream processing. In all these examples, emphasis was on challenges faced in accurately predicting the phenomena of interest due to multi-phase/physics dynamics, moving/deforming boundaries or size of the industrial-scale equipment as well as turnaround time required by the industrial projects. At the end, he highlighted the importance of experimental validation, lack of good currently available data, and the need for industrial best practices.

Standard talks

Ali Ozel: Modeling of Gas-Solid Flows with Tribocharging
In this presentation, Prof. Ozel collaborated with Prof. Sundaresan to study the dynamics of tribo-electrically charged particles in gas-solid flows through a combination of computational modeling and experiments. On the modeling side, they developed a finite-volume based Poisson solver for electric field and a charge transfer model coupling with CFD-DEM to study how tribocharging affects hydrodynamics of gas-solid flows. The model was further validated against vibrated and fluidized bed experiments for measured average charge on polyethylene particles at different humidity conditions. They further formulated a kinetic-theory based Euler-Euler model for monodisperse particles with tribocharging by deriving the mean charge transport equation from the Boltzmann equation for conduction of mean charge through collisions in the presence of electric field, and boundary condition capturing tribocharging at the wall. These models were implemented in OpenFOAM and some verification and validation studies were presented. The modeling approach is capable of capturing the qualitative flow behavior of solid flow with tribocharging and it is of interest to adopt their model to understand the electro-static problems encountered in polymerization processes.

J.A.M. Kuipers: Multi-scale simulation of mass, momentum and heat transfer in dispersed multiphase flows with deformable interfaces
Prof. Kuipers talked about the multi-scale modeling approach being adopted by his group on modeling the complex industrial processes involving dispersed multiphase flows with deformable interfaces. The basic idea of multi-scale modeling is that detailed models are used to generate closures for the interphase transfer coefficients to feed coarse-grained (such as stochastic Euler-Lagrange) models that can be used to compute the system behavior on a much larger (industrial) scale. Some examples on modeling bubble column were shown including detailed validation of DNS for single bubble formation, breakup and coalescence, development of discrete bubble method as well as application to design optimization. At the end, some areas that need substantial further attention were discussed.

J. Capecelatro: Data-driven methods for multiphase turbulence modeling
Prof. Capecelatro discussed how to develop reliable closures for turbulent particle-laden flows. He explained that closures adapted from single-phase flows break down even in the most simplified two-phase

particle-laden flows with sufficient mass loading, i.e., in a two-way coupled flows. The functional form of the unclosed terms being known, machine learning can be used to determined the value of the coefficients in the closures. This can be done either with neural networks or sparse identification. Using sparse identification, two applications were examined. In the former application about single-phase turbulence, sparse identification allowed to identify a better model with off-diagonal Reynolds stresses than the standard LRR-IP model from the literature. In the latter application about turbulent particle-laden flows, sparse identification again showed promises to uncover complex dependencies on flow conditions that eventually let to improve the accuracy of the model.

Carl Wassgren: Continuum Modeling of Powder Flow, Blending, and Segregation
Prof. Wassgren presented the recent work of his group investigating the use of elasto-plastic continuum models for predicting the flow behavior of particulate materials. Several constitutive relations were implemented in a commercial finite element method (FEM) software package to predict flow and stress fields in hoppers and tumbling blenders. After matching with other widely accepted models and correlations for the stress, velocity fields and mass flow rates, the particle mixing and segregation were incorporated by coupling the FEM-predicted continuum flow field with an advection-diffusion-segregation equation. The correlations derived from simple experiments and DEM simulations were used to close the model. The model was shown to predict the blending and segregation results very well comparing to experimental results. These models hold the promise of modeling particulate flows at industrial scales.

Frederic Gibou: PDE solvers on Octree grids
Prof. Gibou presented the last advances in solving PDEs on an octree grid and showed the advantages of using a node-based storage of the data. The talk also addressed the problem of the ghost-fluid method in multi-dimensional systems that does not provide convergence of the gradient, i.e., the flux. This deficiency is fixed by introducing a local Voronoi partition on each side of the interface and then apply the ghost-fluid method in the normal direction. Doing this, the ghost-fluid method is shown to be order 1 convergent on the gradient.

Round Table Discussions

Two round table discussions were organized and the topics were ”current and coming challenges in computing multiphase flows”, and ”industrial challenges and needs in multiphase flow: combined efforts in experiments and computations”.

In the first discussion, several challenges were brought up including:

- the need of two-way coupling for multi-scale model instead of one-way coupling as currently employed,
- to identify a few key areas for study from large-scale systems,
- to establish and maintain a database for sharing experimental data or DNS results to help model validation and benchmark,
- to establish a mechanism to communicate the best practice guideline including what does not work such as a journal of failure.

In the second round-table discussion, some topics related to industrial challenges and needs were reiterated, including:

- interaction between industry and university,
- training for next generation of chemical engineer,
- role of government on promoting research in multiphase flow closely related to industrial applications.

5 Scientific Progress Made

The community has invested sustained efforts in developing high-fidelity DNS models to generate huge amounts of high quality and trustable data. To do this, assorted numerical models for fluid/particle and fluid/fluid interactions were developed, together with scalable codes and fast algorithms. For instance, surface tension in bubbly flows is now properly computed using height functions without spurious currents [8]. These DNS data represent invaluable knowledge in the core of the flow that is not accessible through experiments and are the foundations of the bottom-up multi-scale approach. A thorough post-processing of these data has led to new enhanced closure models. The community pursues its efforts in this direction.

Larger scale models as Euler/Lagrange [9] and Euler/Euler [10] are improved on the basis of DNS data. These models are very important at the industrial level as they are able to compute industrial scale flow configurations. Their predictive capabilities have improved significantly over the past 2 decades. As pointed out earlier, when theoretical arguments do not suffice anymore to mathematically formulate the functional form of the unclosed terms in momentum/heat/mass transfer, machine learning has shown to be able to support physical intuition.

Many research groups in multiphase CFD nowadays perform large parallel computations routinely. Most of the highly optimized codes use a constant cartesian grid while only a few codes can perform dynamic mesh adaption to the local features of the flow. Dynamic mesh adaption, whether body-conforming [11] or not body conforming [12] , will be a key feature of the next generation of multiphase CFD codes.

6 Outcome of the Meeting

The workshop was attended by world-leading experts in multiphase flow modeling from universities, research institutes, and industry which was a good mix of academia and industry. In total 37 lectures were given during the four and half day workshop including 4 one-hour plenary talks, 33 half-hour regular talks and 2 panel discussions. The topics mainly covered various multiphase flow systems including gas-solid, gas-liquid, liquid-solid, and gas-liquid-solid. Different aspects of multiphase flow modeling were discussed such as fundamental theory development, novel numerical algorithms for high performance computing, basic physical models, model validation and industrial applications. The challenges faced by the multiphase flow modeling for energy industrial applications were discussed during the panel sessions. The main take-away is that the computational complexity increases as we start utilizing hi-fidelity simulations (e.g., DNS of particulate flows for drag laws revealed that it is not sufficient to have drag correlations as a function of point properties only). Nonetheless, even with current models, it is not feasible to simulate industrial scale flows without significant assumptions and simplifications (and sometimes not fully supported). This opens up opportunities to multiscale methods that efficiently model global large-scale features while the local fine features are modeled and upscaled to refine the global solutions.

The workshop was a great success. The vast majority (if not all) of the attendees were extremely glad to attend the meeting and underscored the high quality of the scientific exchanges. There is certainly a consensus in the community about what are the primary research paths to follow to advance the field of multiphase CFD and mathematical modeling of multiphase flows. The workshop represented an additional opportunity to clarify what the research priorities are, both at the fundamental level and at the applied level. We hope that mixing academic reseachers with industry representatives also created opportunities for extended academia-industry collaborations and/or synergies. At the very least, the workshop enabled academic researchers to learn better (if needed) about industrial problems and conversely industry researchers where this field of research stands.

There was a strong support from all participants for meeting again in 2 years in a similar setting to follow up on the progress made in the field and to foster university-industry interactions.

References

[1] M.A. Van der Hoef, M. van Sint Annaland, N.G. Deen and J.A.M. Kuipers, Numerical simulation of dense gas-solid fluidized beds: A multiscale modeling strategy, *Annual Review of Fluid Mechanics*, (2008), 40, 47–70.

[2] L. Wang, B. Zhang, X. Wang, W. Ge, Wei and J. Li, Lattice Boltzmann based discrete simulation for gas–solid fluidization, *Chemical engineering science*, (2013), 101, 228–239.

[3] N.G. Deen, E.A.J.F Peters, J.T. Padding and J.A.M. Kuipers, Review of direct numerical simulation of fluid–particle mass, momentum and heat transfer in dense gas–solid flows, *Chemical Engineering Journal*, (2014), 116, 710–724.

[4] Y. Makkawi, P.C. Wright and R. Ocone, The effect of friction and inter-particle cohesive forces on the hydrodynamics of gas–solid flow: a comparative analysis of theoretical predictions and experiments, *Powder Technology*, (2006), 163, 69–79.

[5] J. Kolehmainen, A. Ozel, C.M. Boyce and S. Sundaresan, Triboelectric charging of monodisperse particles in fluidized beds, *AIChE Journal*, (2017) 63, 1872–1891.

[6] M. Rahmani and A. Wachs, Free falling and rising of spherical and angular particles, *Physics of Fluids*, (2014), 26, 083301.

[7] M.W. Baltussen, Q.I.E. Segers, J.A.M. Kuipers and N.G. Deen. Cutting bubbles with a single wire, *Chemical Engineering Science*, (2017), 157, 138–146.

[8] S. Popinet, An accurate adaptive solver for surface-tension-driven interfacial flows, *Journal of Computational Physics*, (2009), 228, 5838–5866.

[9] J. Capecelatro, O. Desjardins and R.O. Fox, Strongly coupled fluid-particle flows in vertical channels. I. Reynolds-averaged two-phase turbulence statistics, *Physics of Fluids*, (2016), 28, 033306.

[10] A. Ozel, P. Fede and O. Simonin, 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*, (2013), 55, 43–63.

[11] V. Moureau, P. Domingo and L. Vervisch, Design of a massively parallel CFD code for complex geometries, *Comptes Rendus Mécanique*, (2011), 339, 141–148.

[12] C. Min and F. Gibou, A second order accurate projection method for the incompressible Navier–Stokes equations on non-graded adaptive grids, *Journal of Computational Physics*, (2006), 219, 912–929.